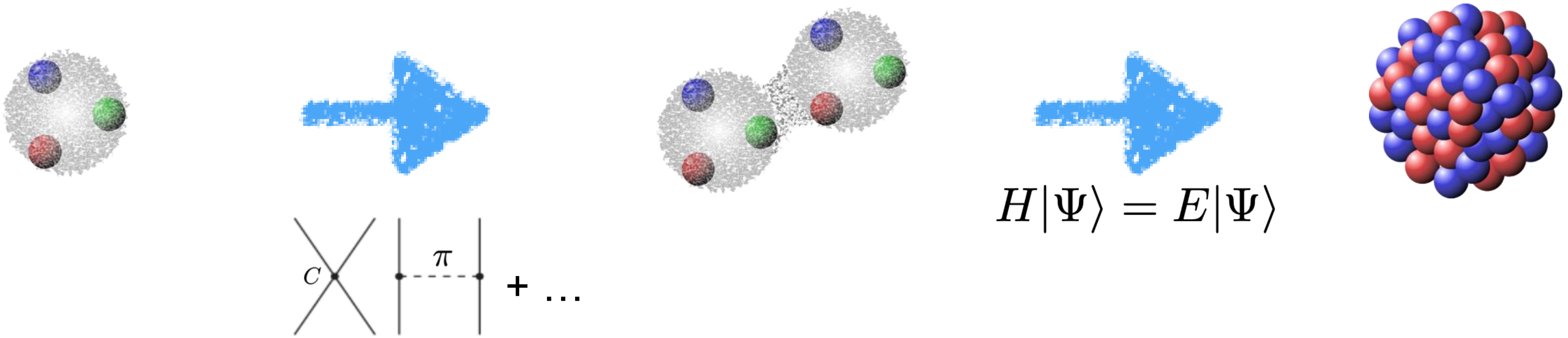
筑波大学
計算科学研究センター
Center for Computational Sciences

Valence-space in-medium similarity renormalization group description of calcium isotopes



Takayuki Miyagi (University of Tsukuba, Japan)

Ab initio many-body calculations: where has the nuclear pairing gone?

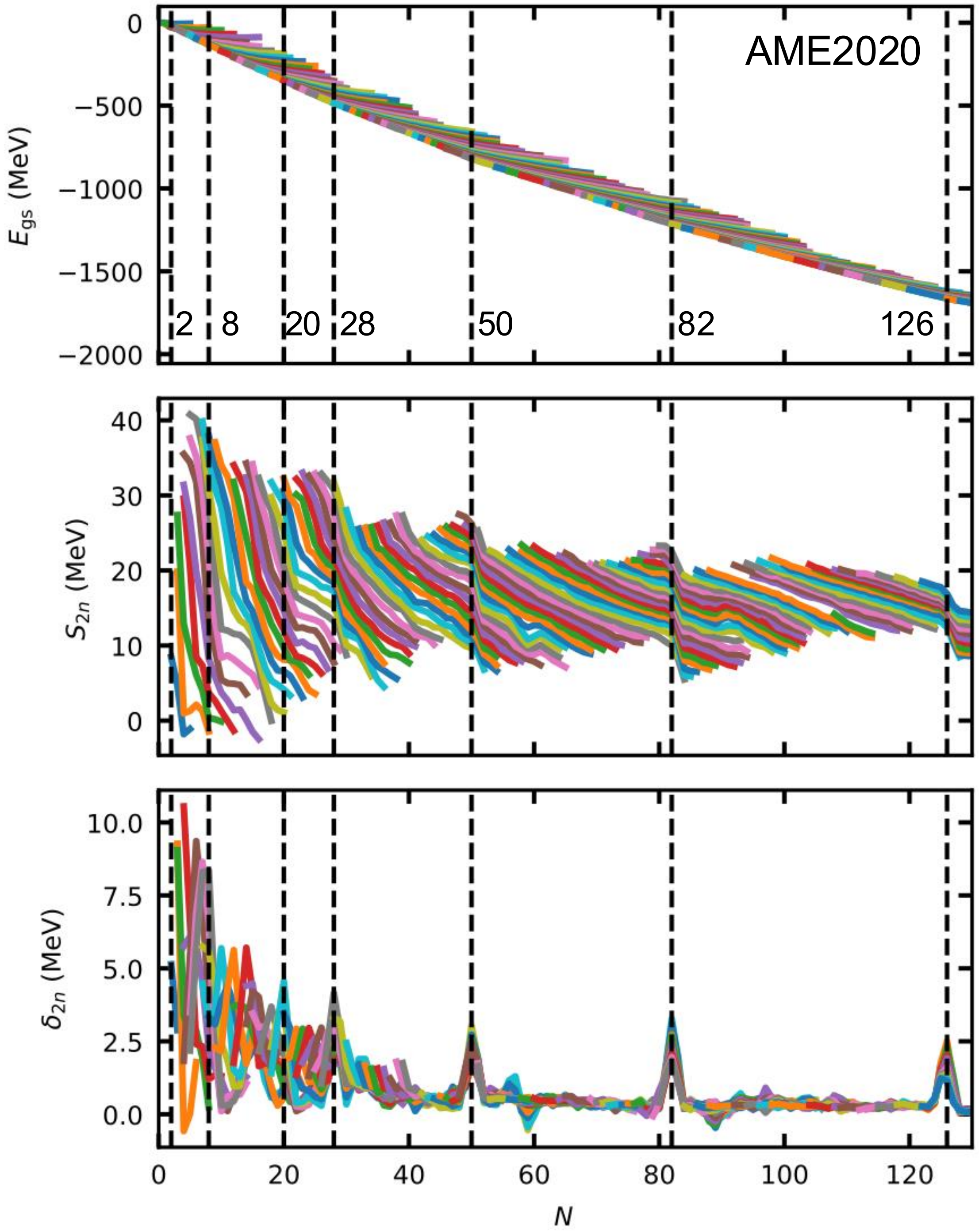
@ CEA, Saclay, France, May 14, 2025

Energies and radii

- Ground-state energies are fundamental properties of nuclei

$$S_{2n}(Z,N) = E_{\mathrm{g.s.}}(Z,N) - E_{\mathrm{g.s.}}(Z,N-2)$$
$$\delta_{2n}(Z,N) = \frac{1}{2}\left[S_{2n}(Z,N) - S_{2n}(Z,N+2)\right]$$

- The magic signature can be found!



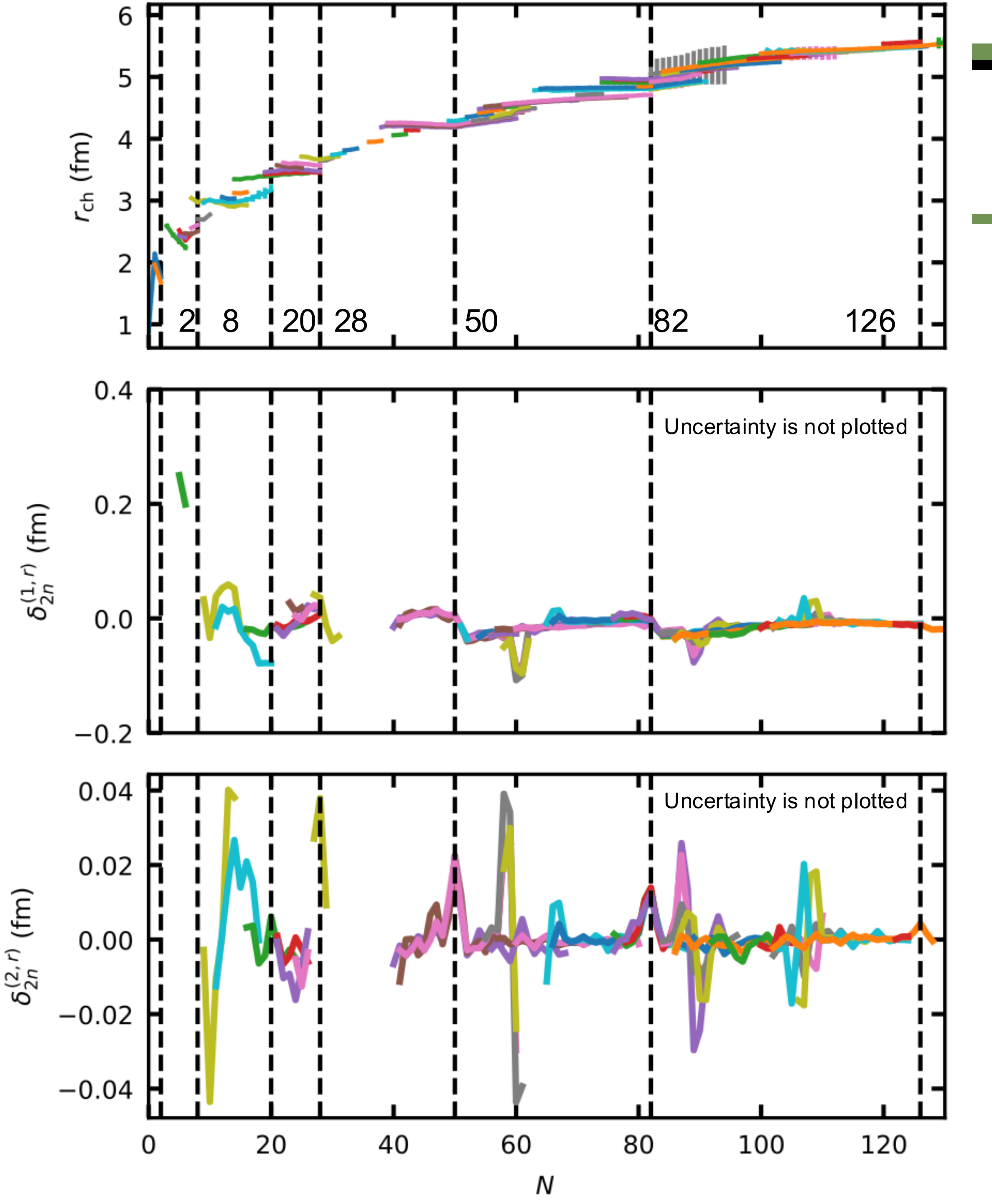
Energies and radii

- Radii are also fundamental properties of nuclei

$$\delta_{2n}^{(1,r)}(Z,N) = r_{\mathrm{ch}}(Z,N) - r_{ch}(Z,N-2)$$
$$\delta_{2n}^{(2,r)}(Z,N) = \frac{1}{2}\left[\delta_{2n}^{(1,r)}(Z,N) - \delta_{2n}^{(1,r)}(Z,N+2)\right]$$

- Some shell closures, such as near ^{132}Sn and ^{208}Pb, can be detected.

- Computing Egs' and radii would be a good test of a theoretical model.



I. Angeli and K. P. Marinova 2013

Ca radii puzzle

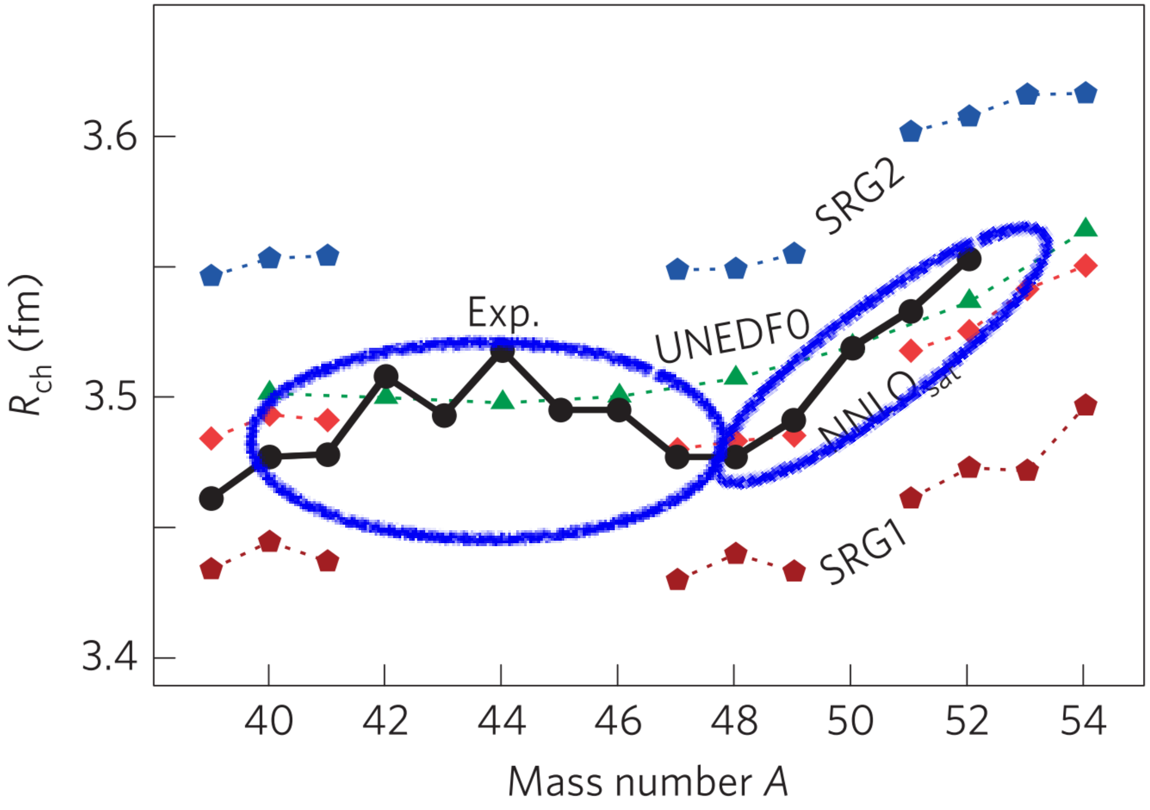
筑波大学
計算科学研究センター
Center for Computational Sciences

- Charge radii of Ca isotopes
  - 48 to 52
  - 40 to 48

ARTICLES
PUBLISHED ONLINE: 8 FEBRUARY 2016 | DOI: 10.1038/NPHYS3645
nature physics

Unexpectedly large charge radii of neutron-rich calcium isotopes

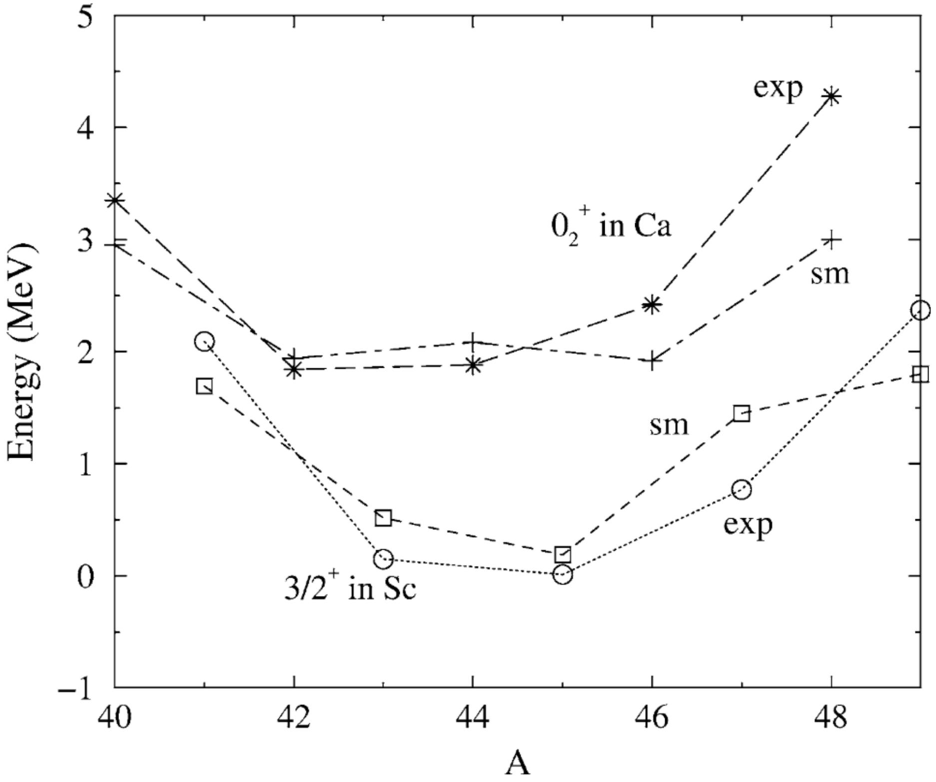
R. F. Garcia Ruiz[1*], M. L. Bissell[1,2], K. Blaum[3], A. Ekström[4,5], N. Frömmgen[6], G. Hagen[4], M. Hammen[6], K. Hebeler[7,8], J. D. Holt[9], G. R. Jansen[4,5], M. Kowalska[10], K. Kreim[3], W. Nazarewicz[4,11,12], R. Neugart[3,6], G. Neyens[1], W. Nörtershäuser[6,7], T. Papenbrock[4,5], J. Papuga[1], A. Schwenk[3,7,8], J. Simonis[7,8], K. A. Wendt[4,5] and D. T. Yordanov[3,13]



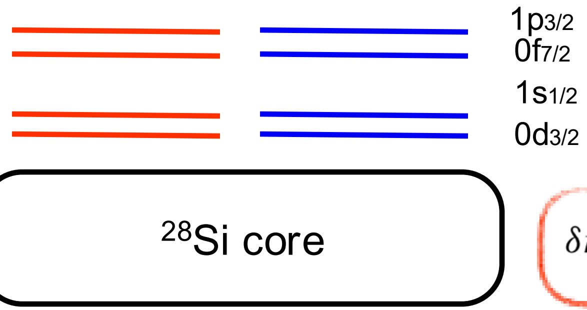
Ca radii puzzle

- Shell-model calculation

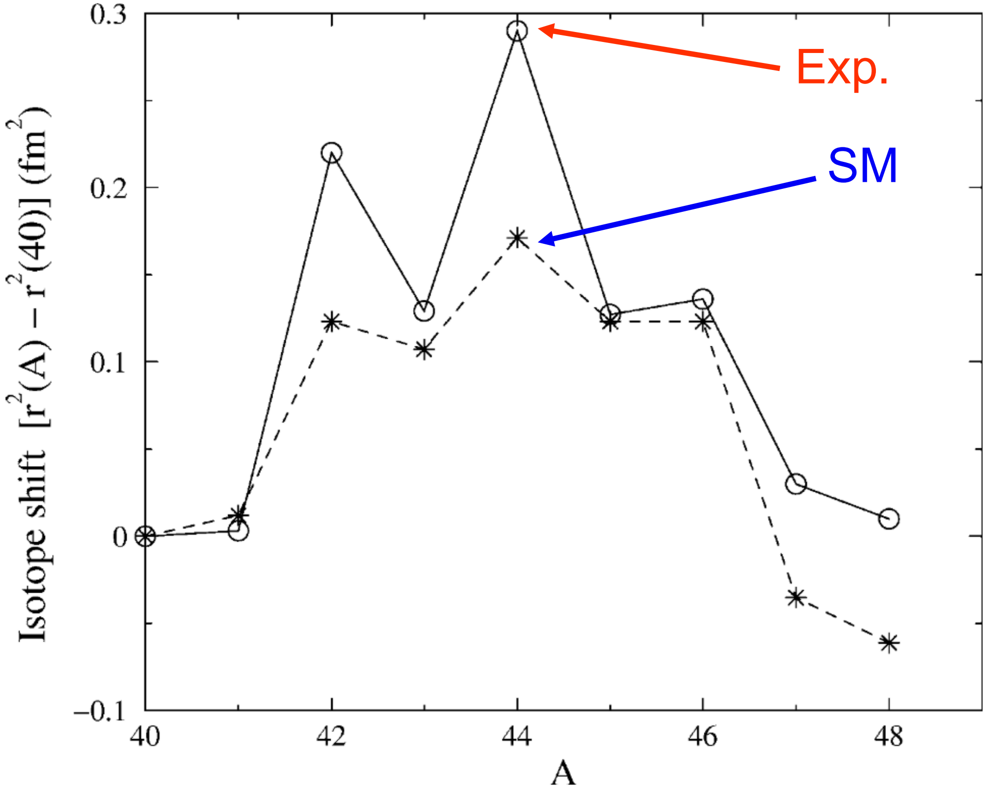
  Explicit inclusion of excitations across the N=Z=20 gap seems essential.



E. Caurier et al., Phys. Lett. B 522, 240 (2001).



$$\delta r_c^2(A) = \frac{1}{Z} n_{fp}^{\pi}(A) b^2,$$

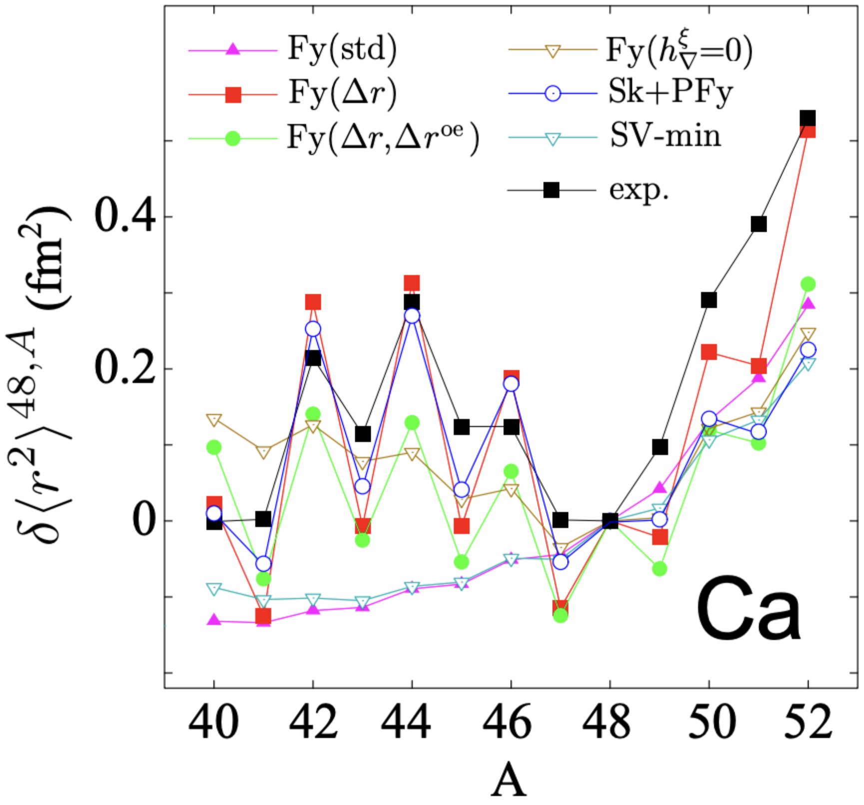


Ca radii puzzle

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

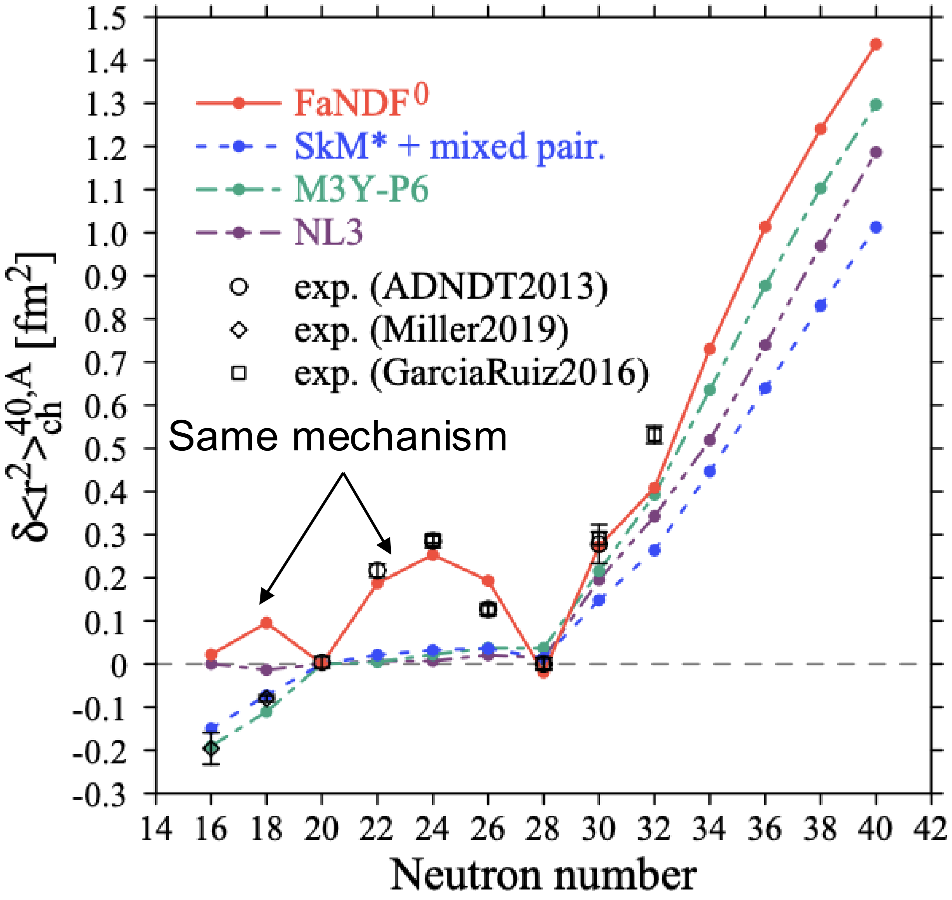
- DFT results

Fayans functional



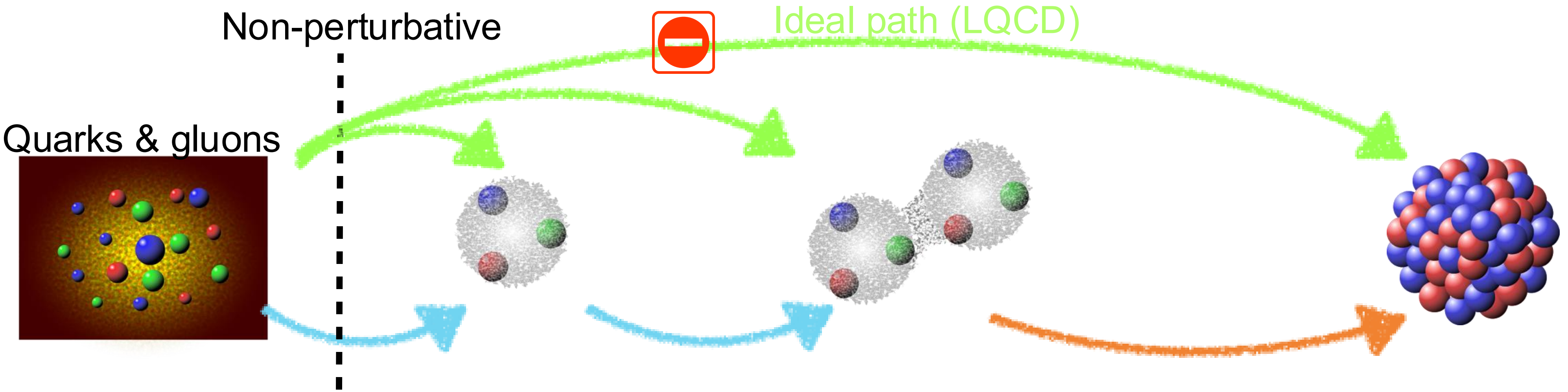
P.-G. Reinhard and W. Nazarewicz, Phys. Rev. C 95, 064328 (2017).

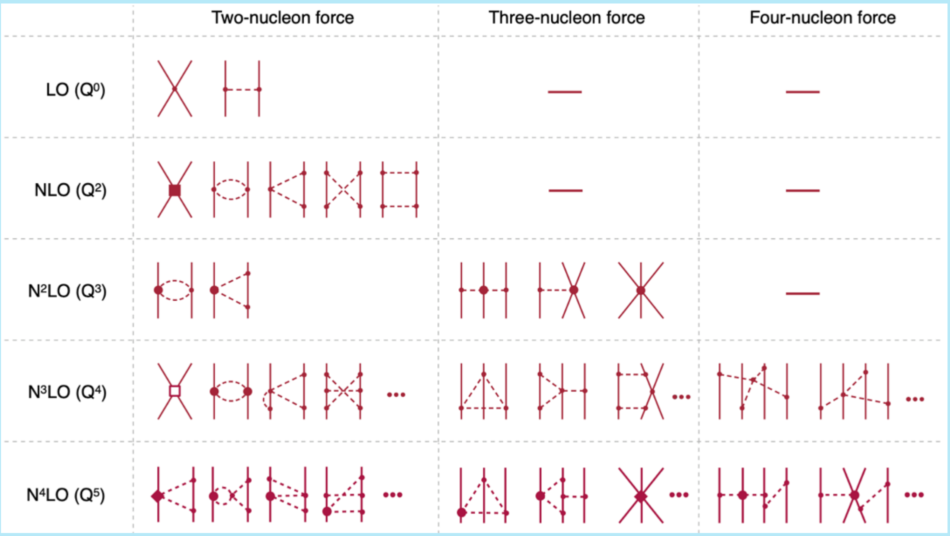
20<=N<=48 and N<20 cannot be explained simultaneoulsly.



T. Inakura, N. Hinohara, and H. Nakada, Phys. Rev. C 110, 054315 (2024).

Nuclear ab initio calculations





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

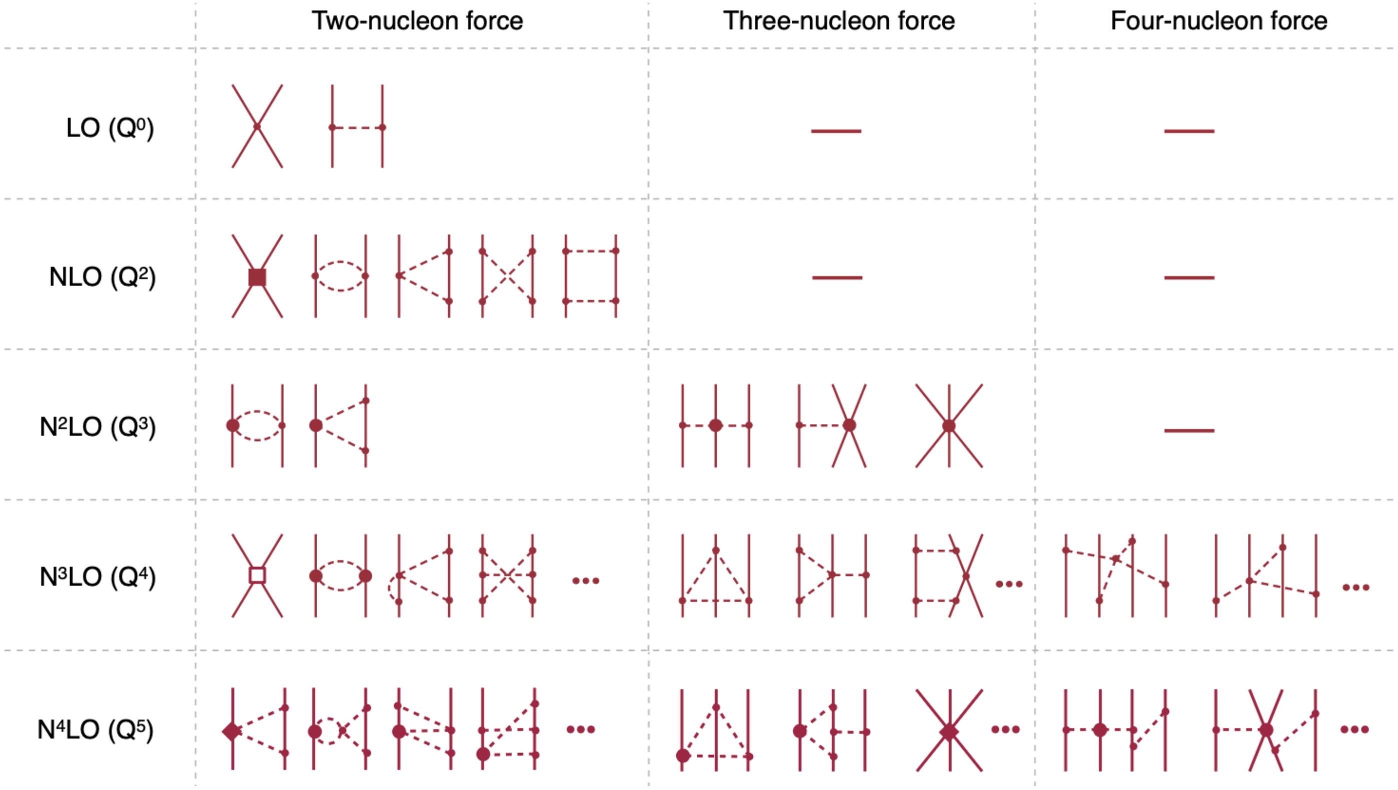
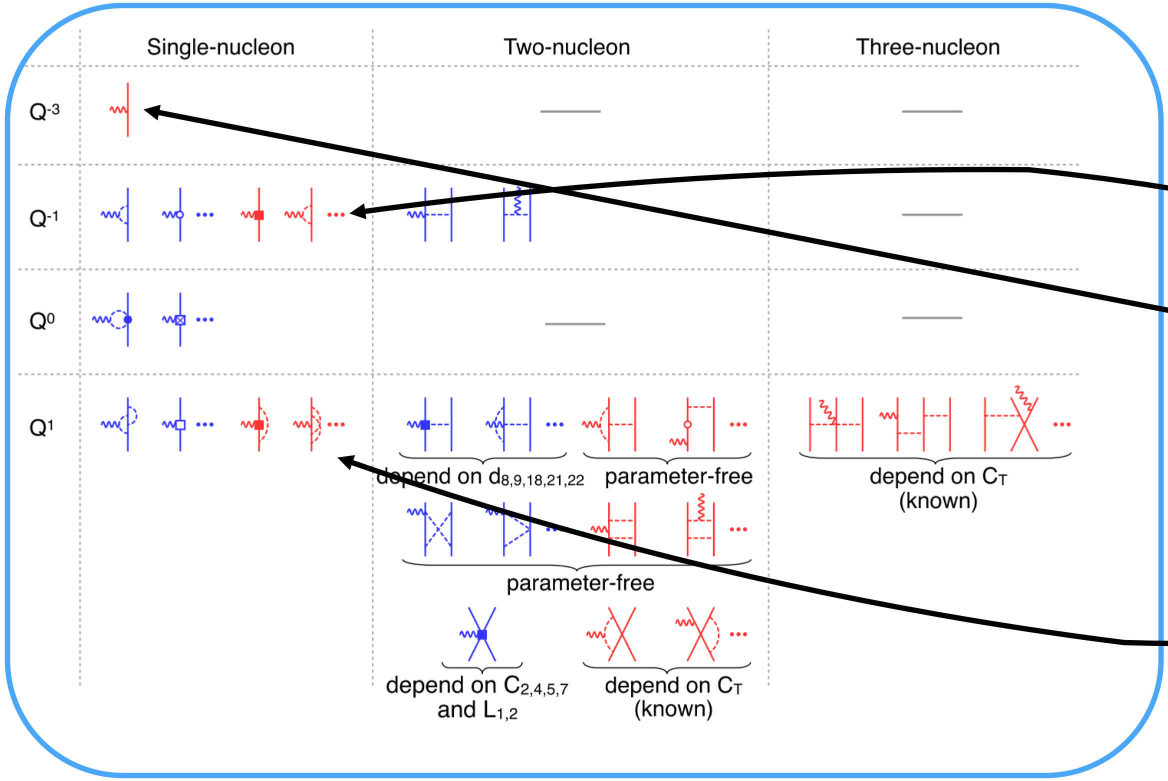


Figure is from E. Epelbaum, arXiv: 1510.07036

The 1.8/2.0 (EM) interaction will be used

Nuclear currents from chiral EFT

- The charge radius is measure through EM probes.
- Chiral EFT allows us a systematic expansion for charge and current operators.

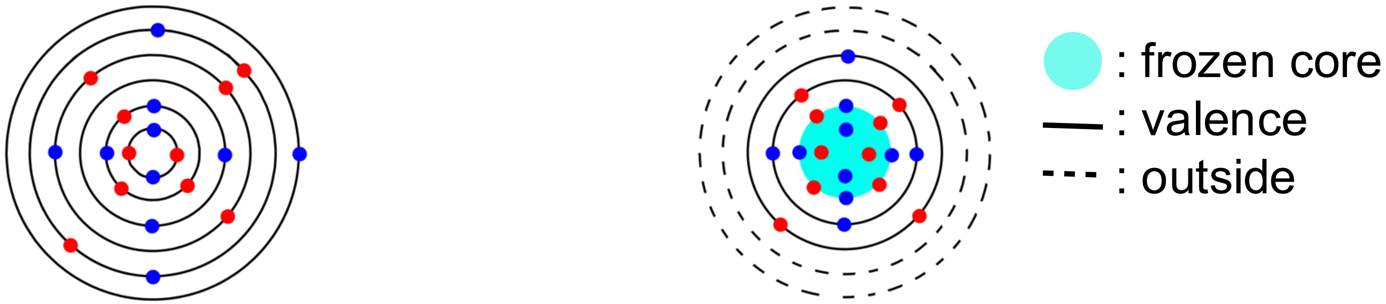


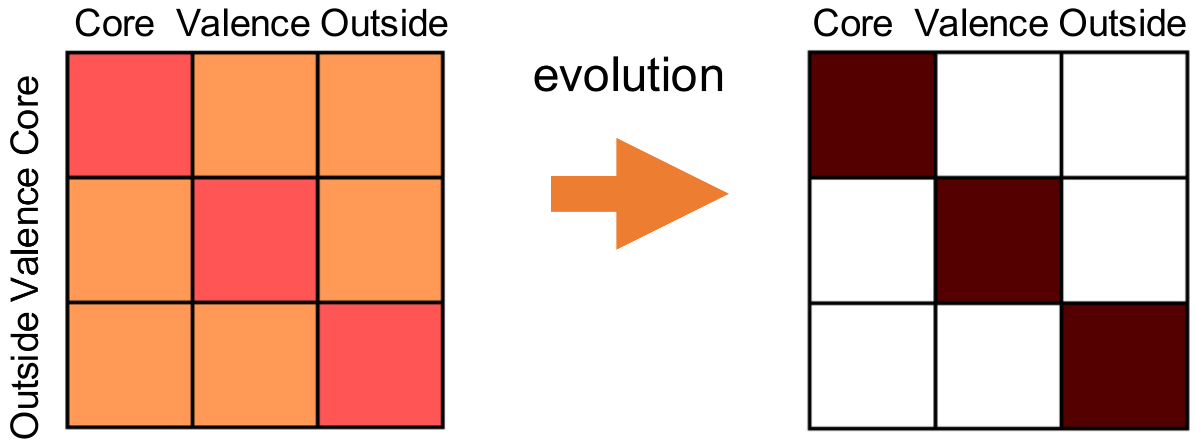
$$r_{\rm ch}^2 = -\frac{6}{Z}\lim_{Q\to 0}\frac{dF_{\rm ch}(Q^2)}{dQ^2},\quad F_{\rm ch}(Q) = \frac{1}{4\pi}\int d\hat{\mathbf{Q}}\tilde{\rho}(\mathbf{Q})$$

$$r_{\rm ch}^2 = r_{pp}^2 + r_p^2 + \frac{N}{Z}r_n^2 + r_{\rm DF}^2 + r_{\rm SO}^2$$

E. Epelbaum, arXiv:1908.09349.

Valence-Space In-Medium Similarity Renormalization Group





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

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

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

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

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

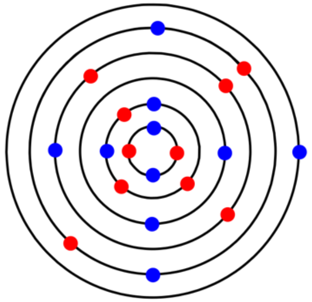
$$A_{1234} = \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}$$

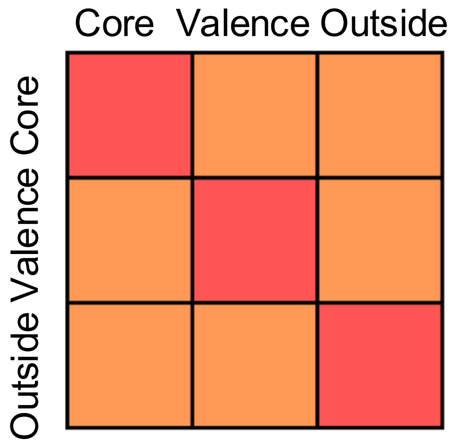
f_{12}, Γ_{1234} : matrix elements to be suppressed

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

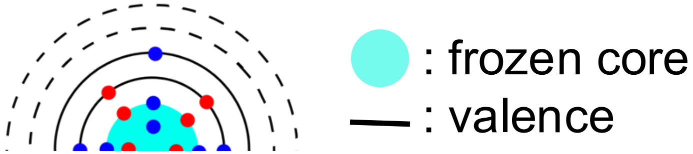
H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rep. **621**, 165 (2016).

Valence-Space In-Medium Similarity Renormalization Group

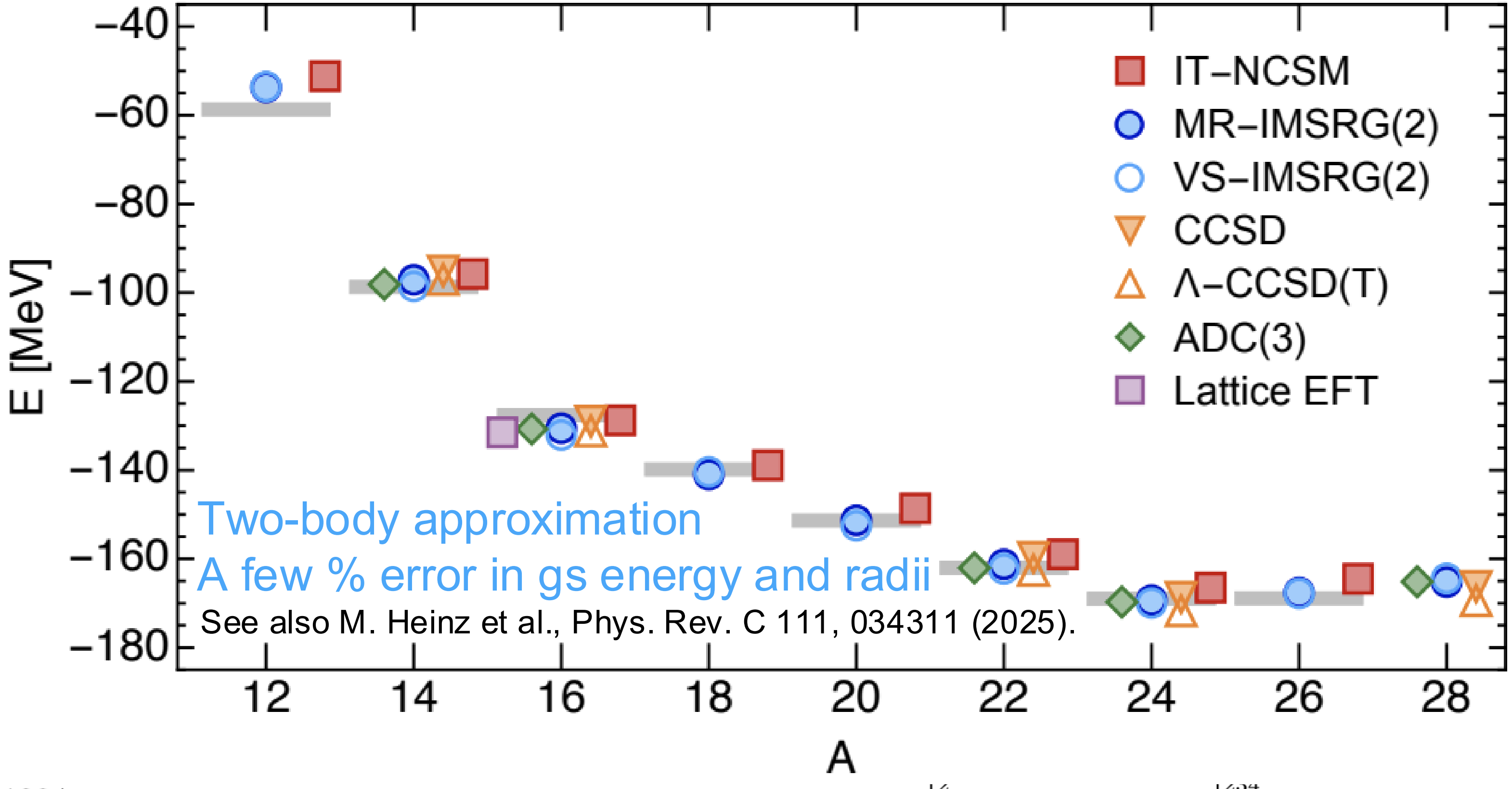




evolution



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

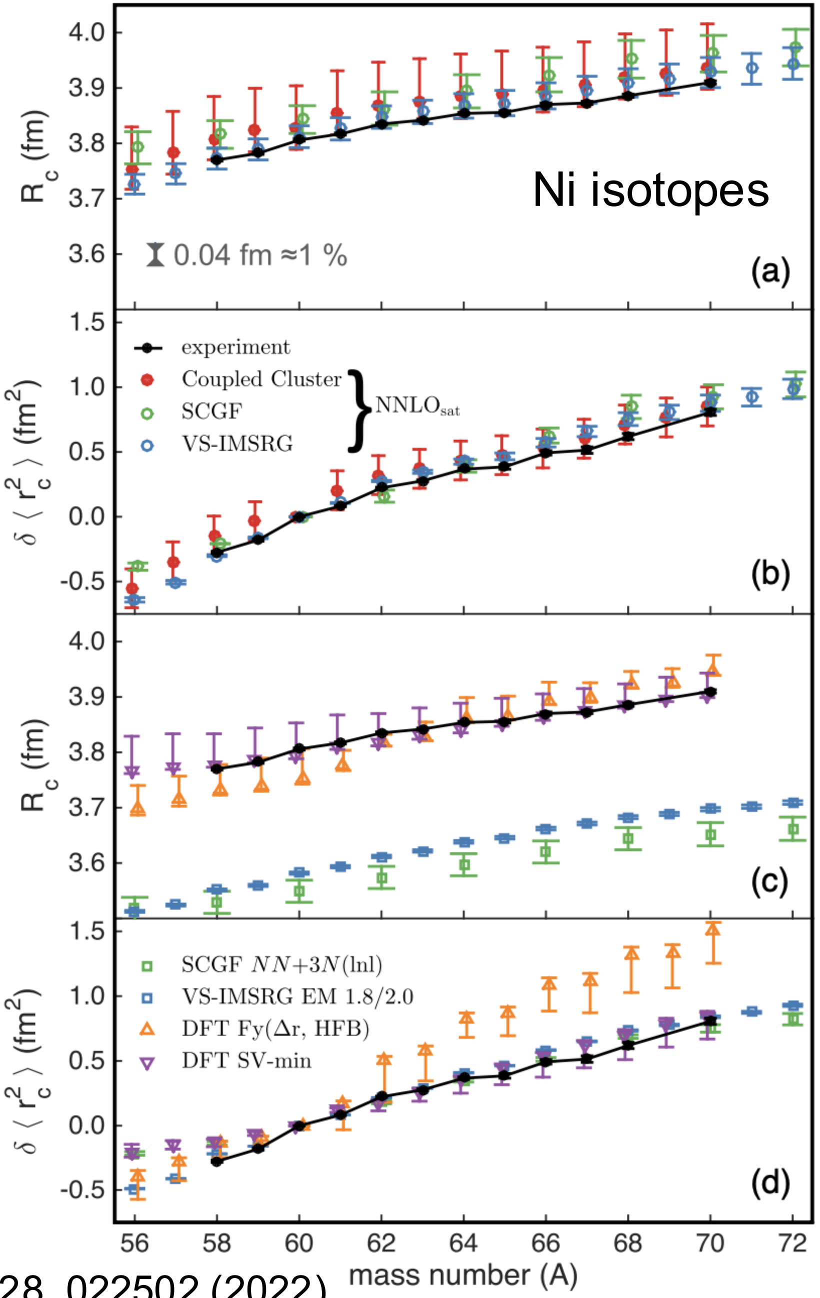
$$H(s) \approx E(s) + \sum_{12} f_{12}(s)\{a_1^\dagger a_2\} + \frac{1}{4} \sum_{1234}$$

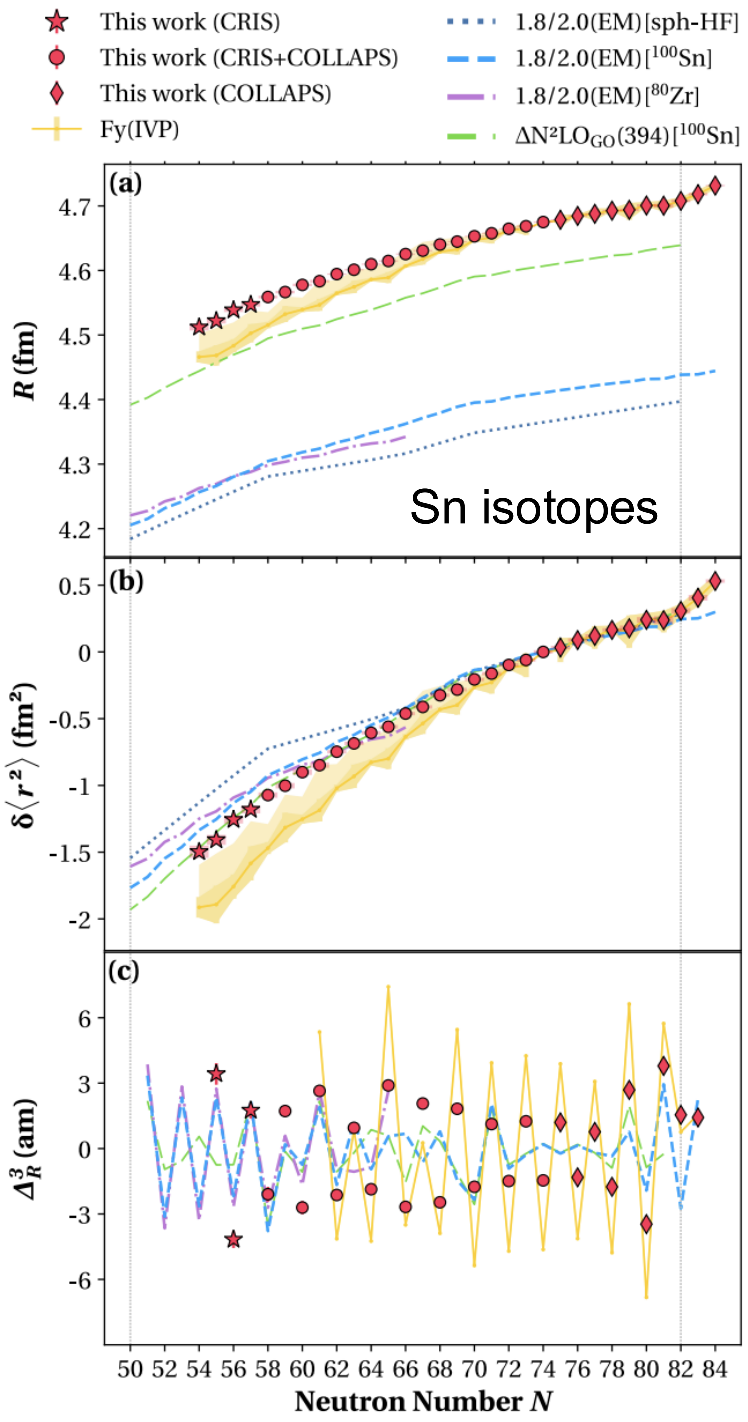
s: flow parameter

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

Some radii results

- Ni and Sn isotopes
- Isotope shifts are well reproduced with the 1.8/2.0 (EM) interaction





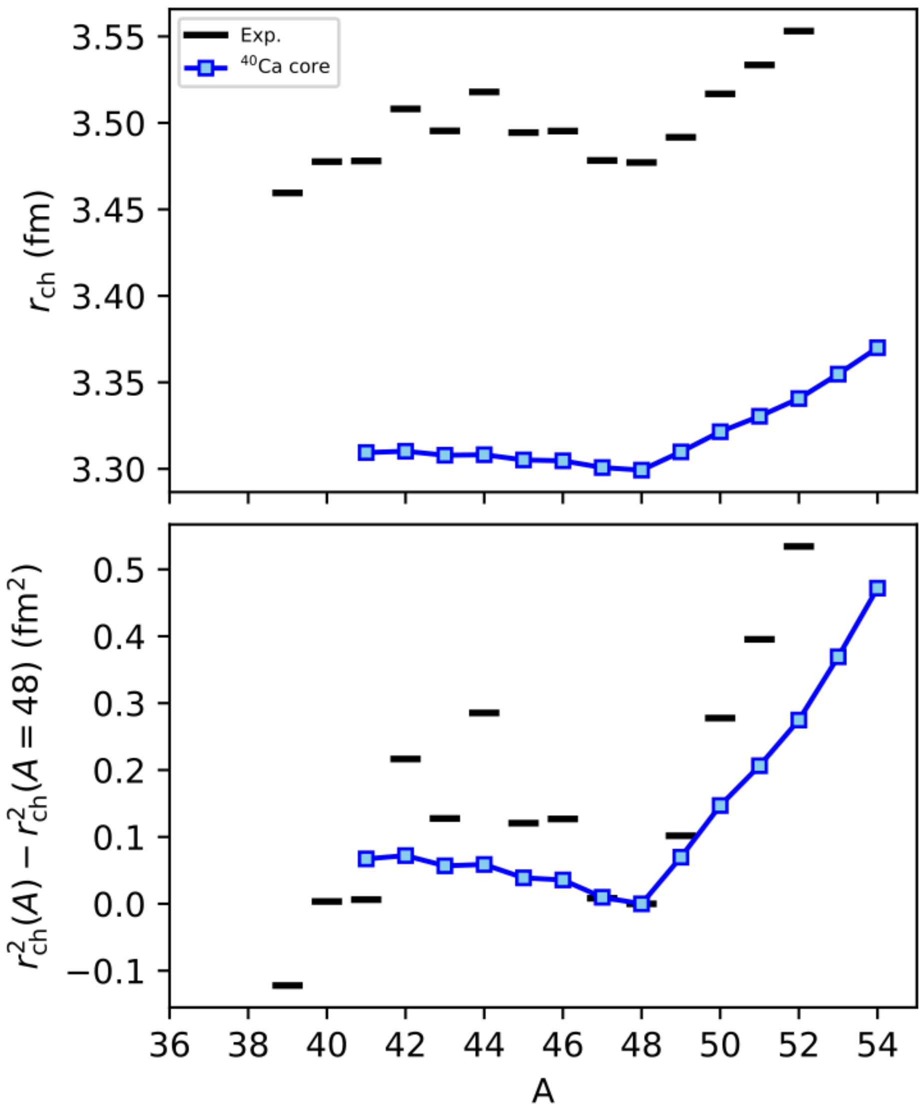
S. Malbrunot-Ettenauer et al., Phys. Rev. Lett. 128, 022502 (2022).

F. P. Gustafsson et al., arXiv: 2504.17060 (2025).

Ca radii with one major-shell valence space

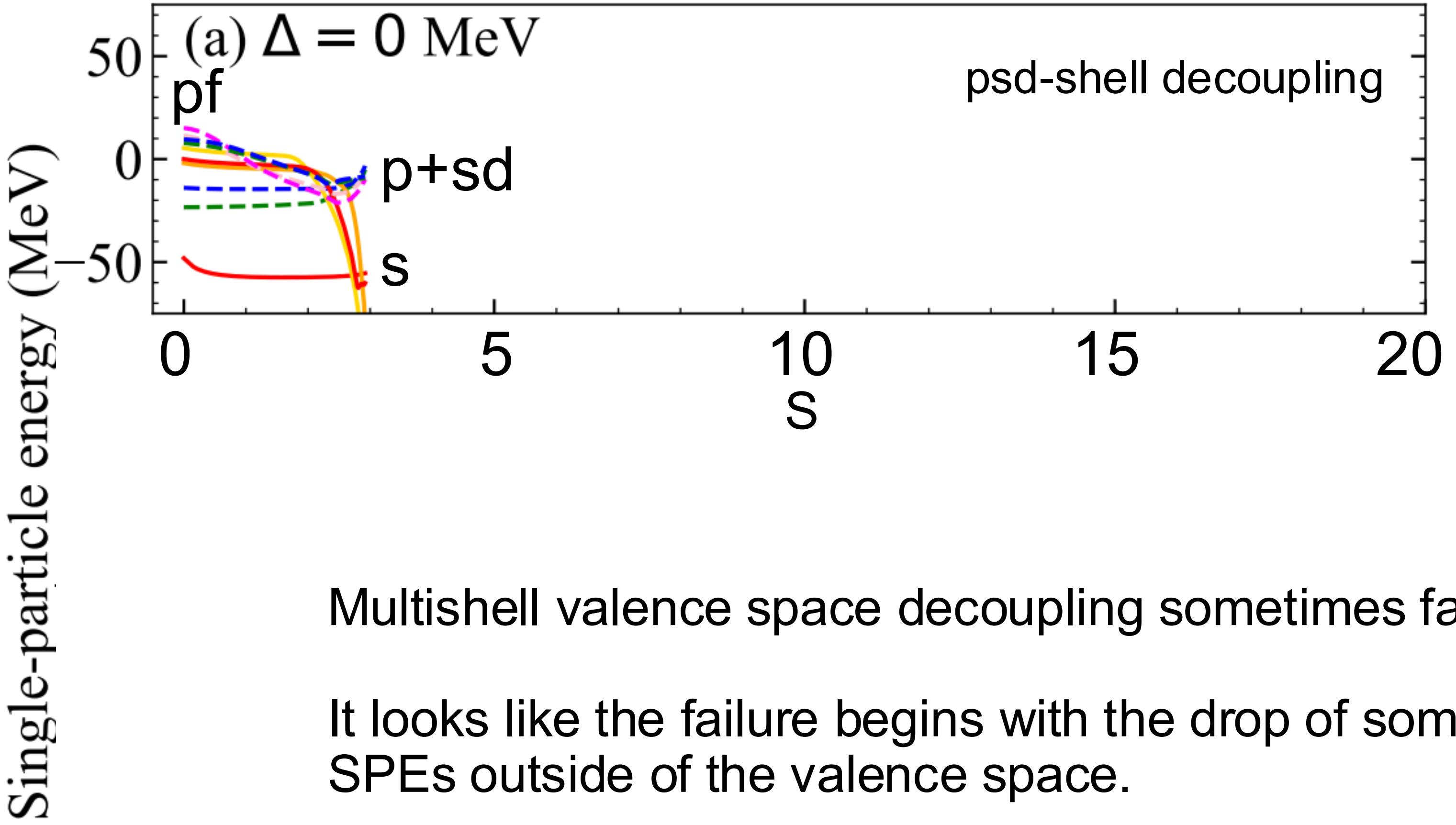
- The computed radii are significantly smaller than the experiments due to the 1.8/2.0 (EM) interaction.
- 40 < A <= 48 behavior is totally off from the data.
- The enhancements in A>48 can be observed, but not enough.
- Explicit excitations across Z=N=20 gap?

E. Caurier et al., Phys. Lett. B 522, 240 (2001).



Multishell valence-space decoupling

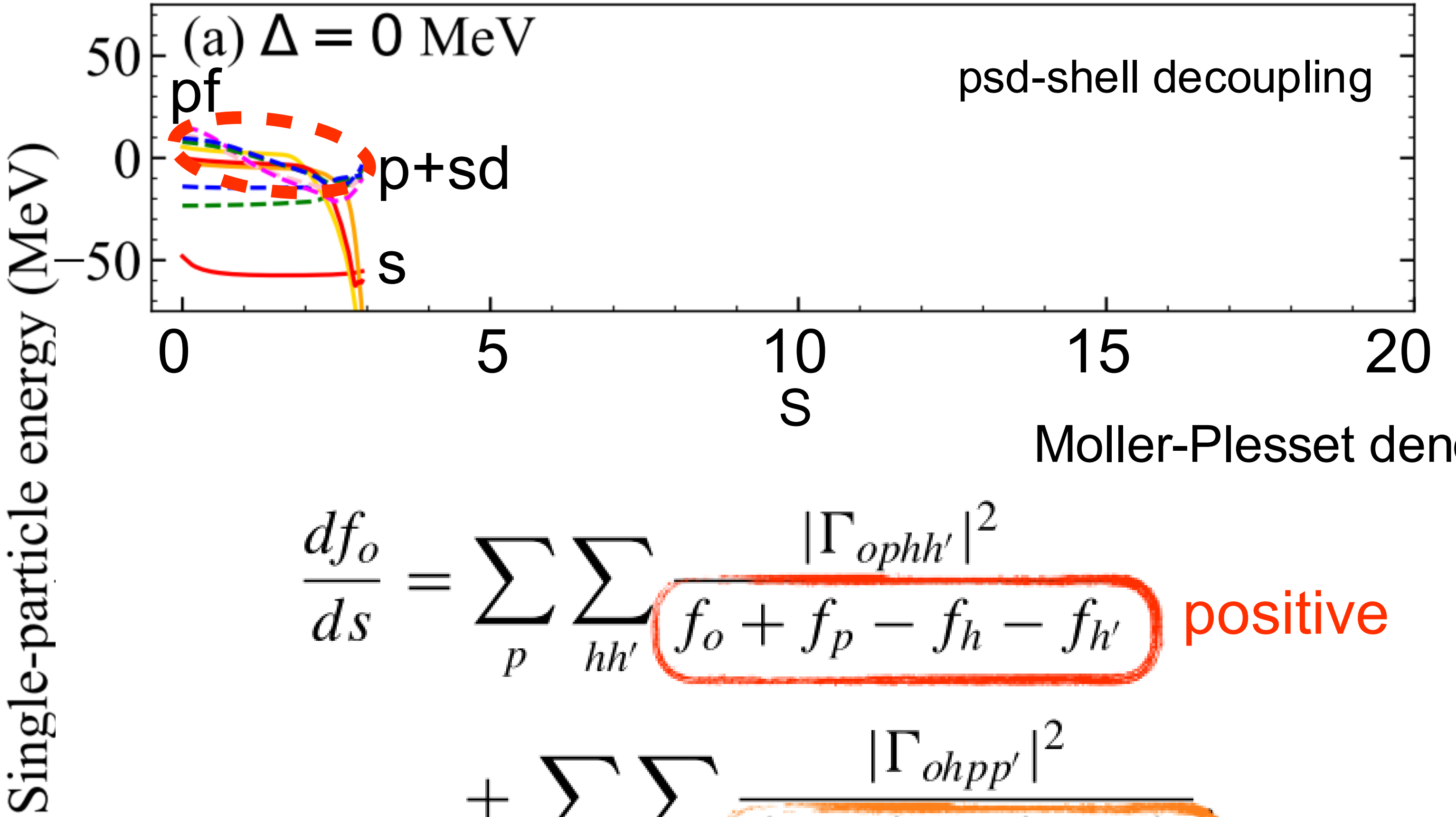
筑波大学 計算科学研究センター Center for Computational Sciences



Multishell valence space decoupling sometimes fails…

It looks like the failure begins with the drop of some SPEs outside of the valence space.

Multishell valence-space decoupling



Moller-Plesset denominator

$$\frac{df_o}{ds} = \sum_{p}\sum_{hh'} \frac{|\Gamma_{ophh'}|^2}{f_o + f_p - f_h - f_{h'}}$$ positive

$$+ \sum_{pp'}\sum_{h} \frac{|\Gamma_{ohpp'}|^2}{f_o + f_h - f_p - f_{p'}}$$ can be negative

Multishell valence-space decoupling

Moller-Plesset denominator

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

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

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

$$\frac{df_o}{ds} = \sum_p \sum_{hh'} \frac{|\Gamma_{ophh'}|^2}{f_o + f_p - f_h - f_{h'}} + \sum_{pp'} \sum_h \frac{|\Gamma_{ohpp'}|^2}{f_o + f_h - f_p - f_{p'}}$$

↓

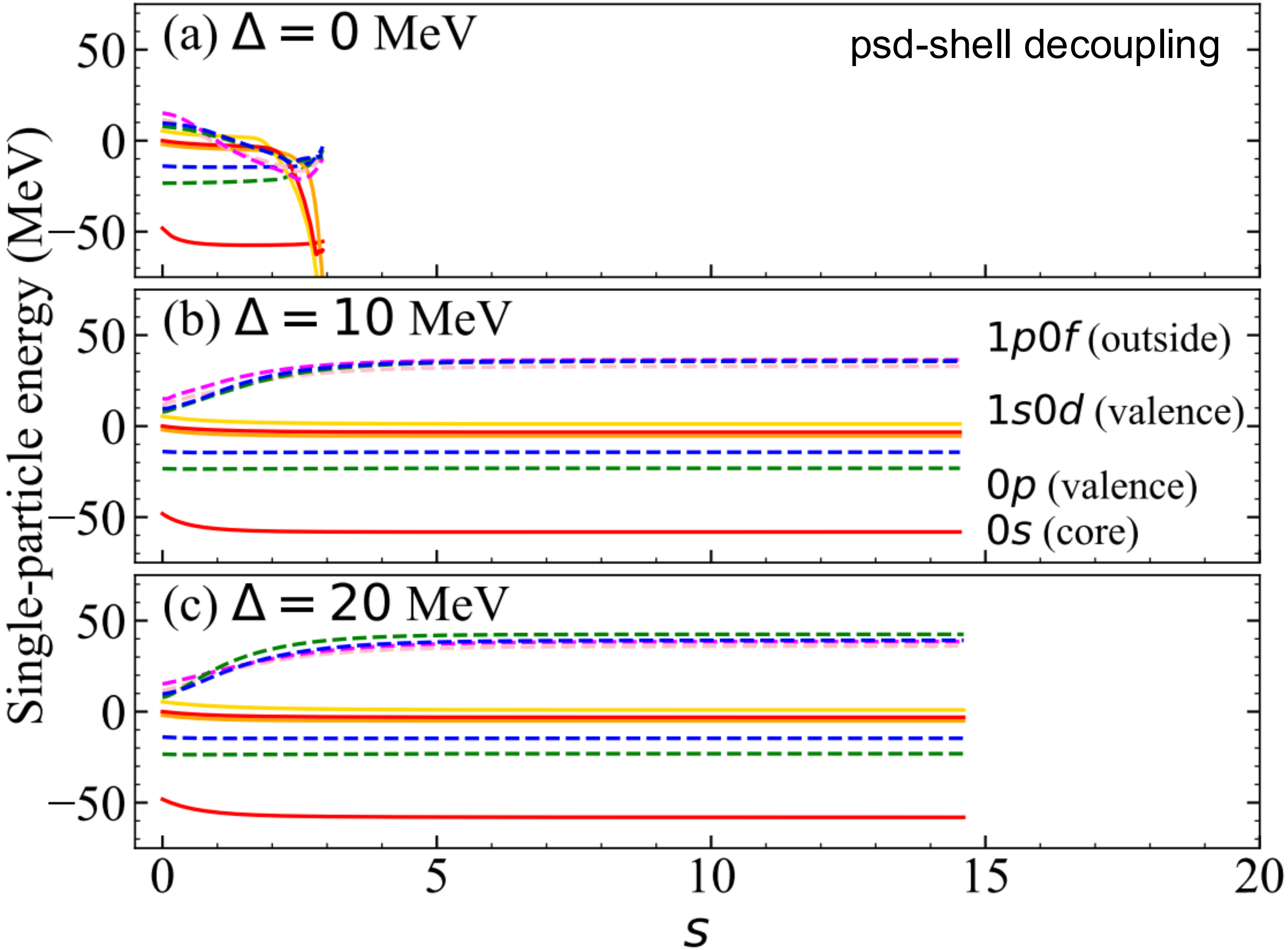
$$\eta_{12} = \frac{1}{2}\arctan\left(\frac{2f_{12}}{f_{11} - f_{22} + \Gamma_{1212} + \Delta}\right)$$

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

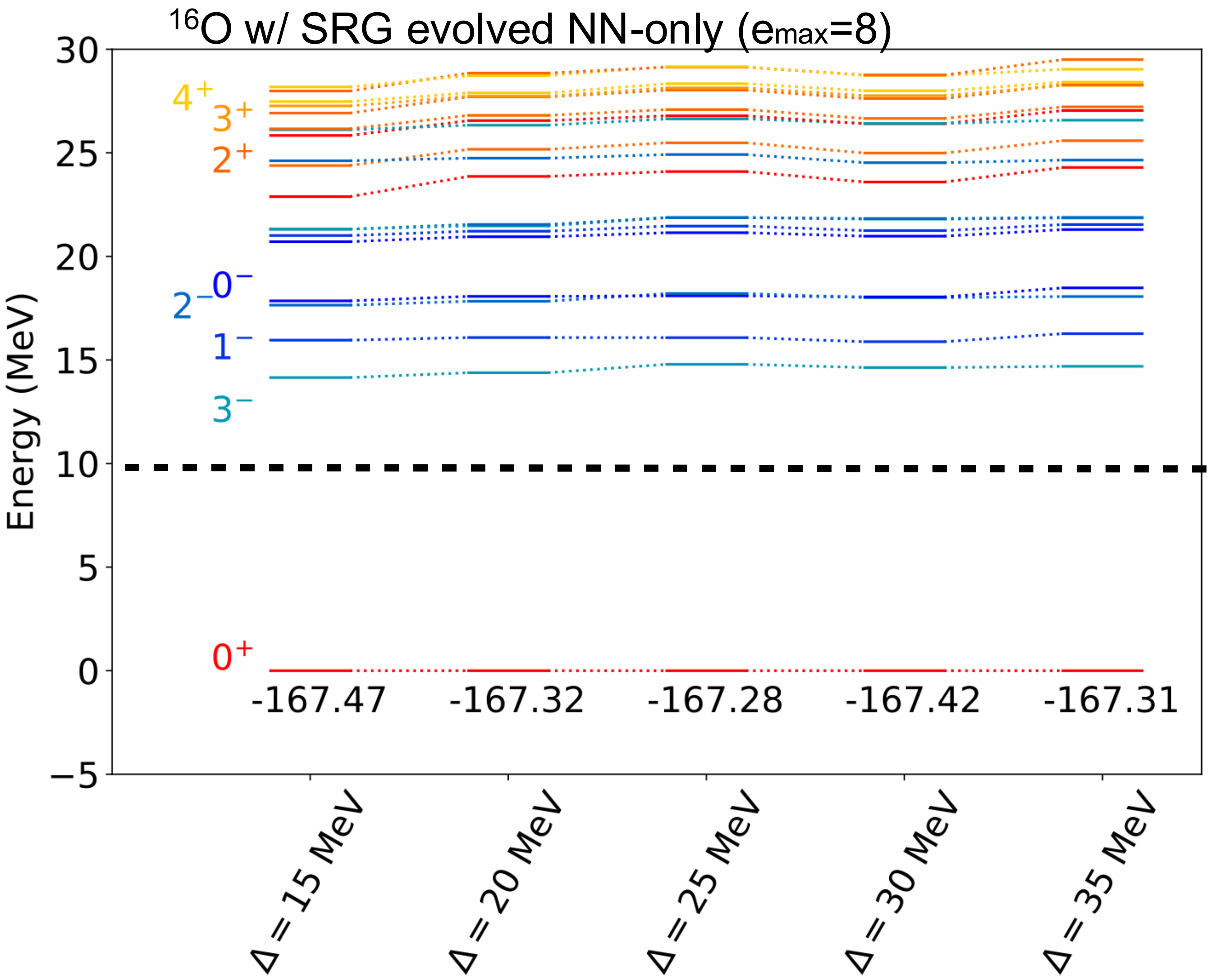
$$A_{1234} = \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}$$

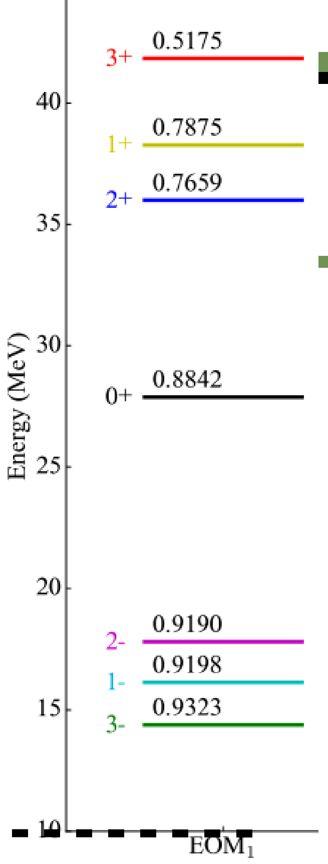
$$\frac{df_o}{ds} = \sum_p \sum_{hh'} \frac{|\Gamma_{ophh'}|^2}{f_o + f_p - f_h - f_{h'} + \Delta} + \sum_{pp'} \sum_h \frac{|\Gamma_{ohpp'}|^2}{f_o + f_h - f_p - f_{p'} + \Delta}$$

Multishell valence-space decoupling



Multishell valence-space decoupling





1p1h dominant lowest 3^-, 1^-, 2^- agree well with the EOM-IMSRG results.

EOM-IMSRG results are take from N. M. Parzuchowski, T. D. Morris, and S. K. Bogner, Phys. Rev. C **95**, 044304 (2017).

Multishell valence-space decoupling

Center-of-mass issue

A prescription in usual shell-model diagonalization method:

$$H_{\text{valence}} \rightarrow H_{\text{valence}} + \beta H^{\text{HO}}_{\text{c.m.}}$$

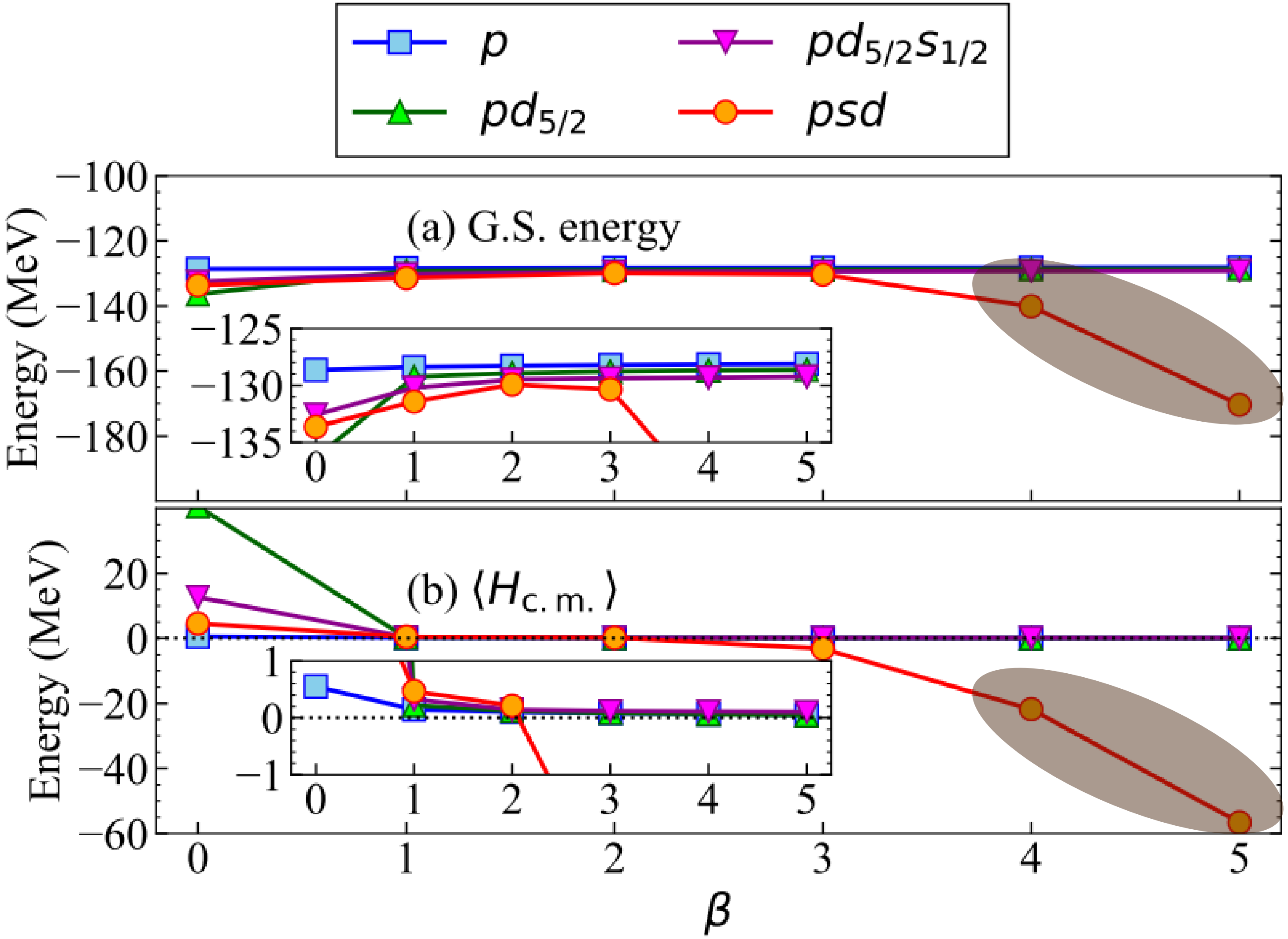
Our basis is no longer HO

$$H_{\text{intr}} \rightarrow H_{\text{intr}} + \beta H^{HO}_{\text{c.m.}} \xrightarrow[\text{IMSRG}]{} H_{\text{valence}}$$

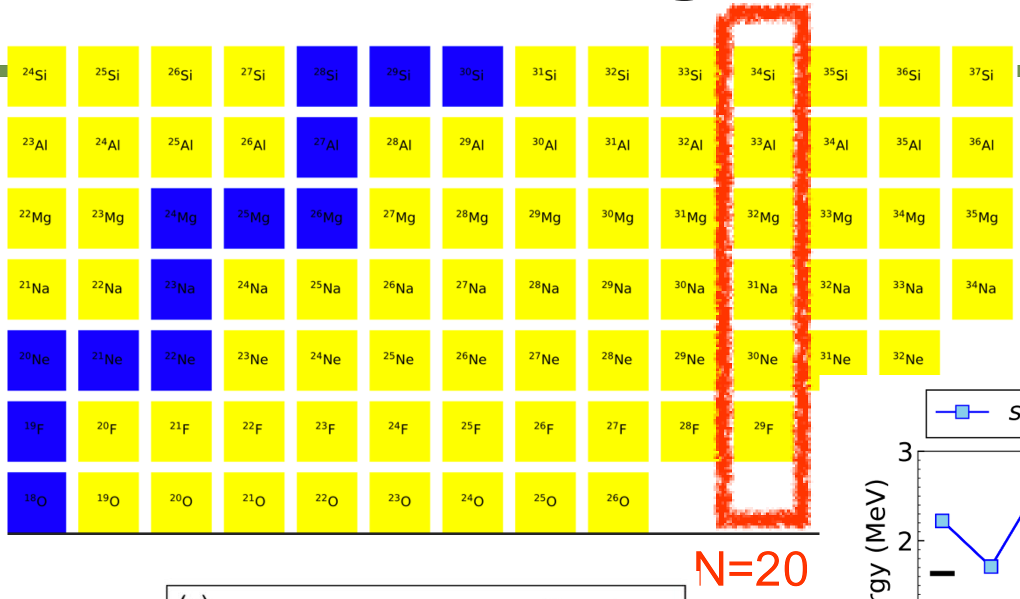
IMSRG(2) breaks down

Valence-space choice is crucial

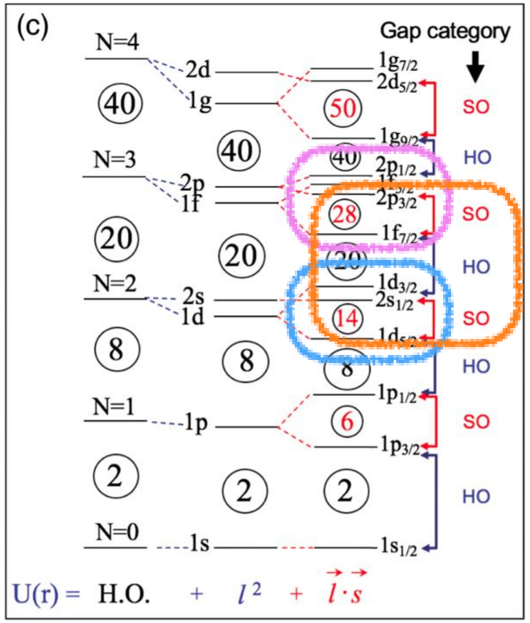
^{16}O @ e_{max}=8

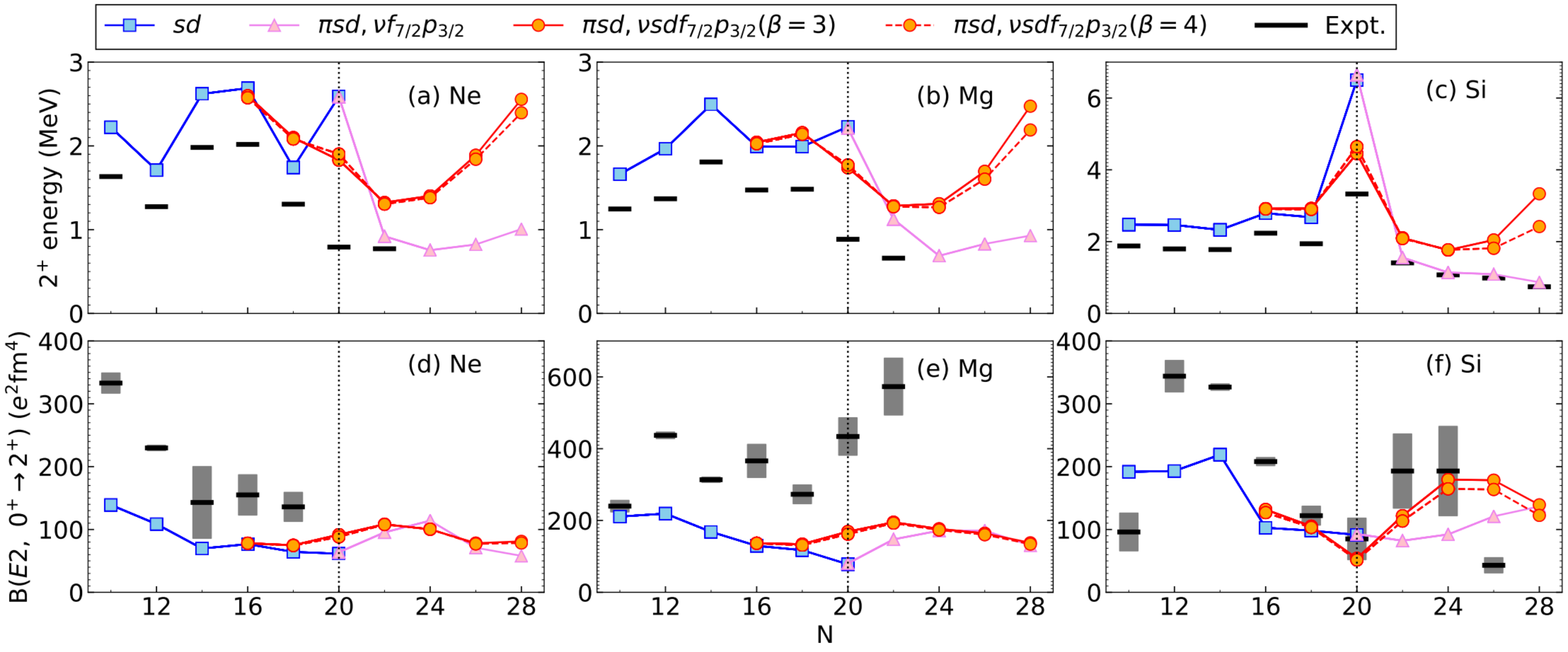


Island of inversion @ N=20

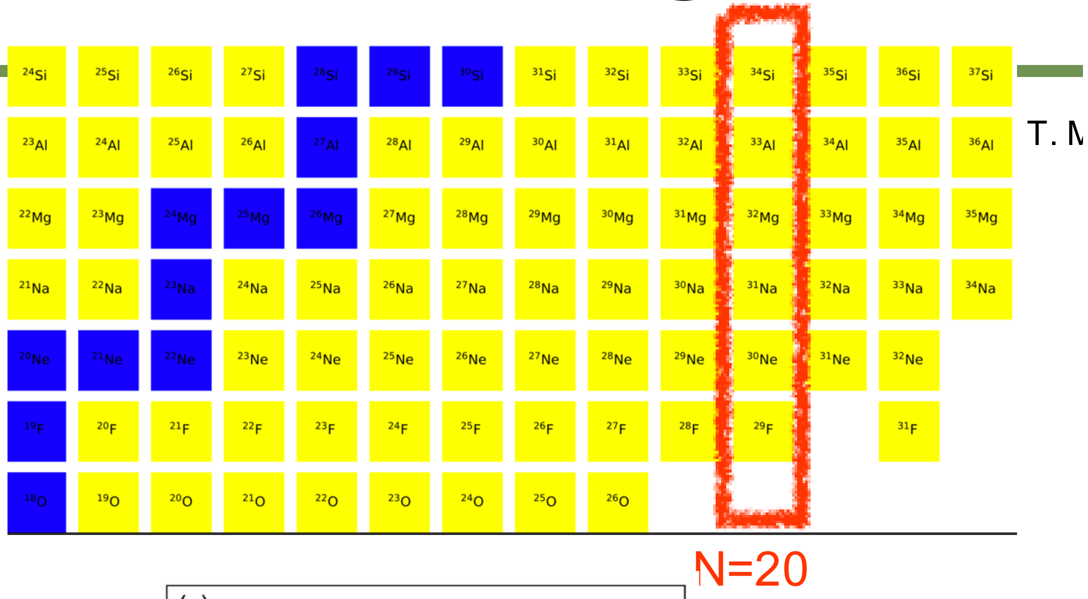


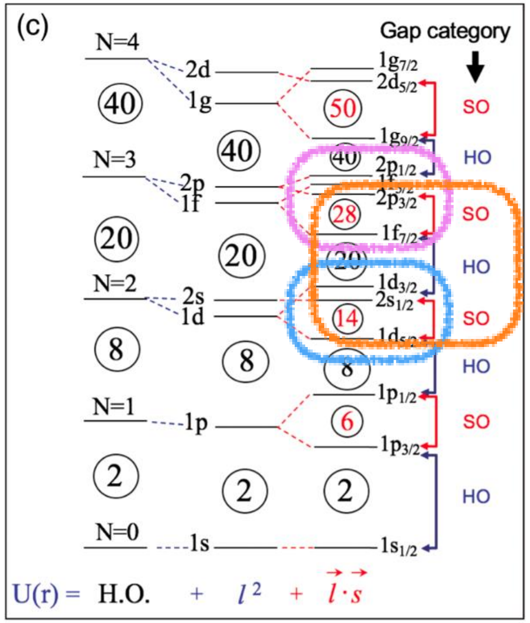
T. Miyagi, S. R. Stroberg, J. D. Holt, and N. Shimizu, Phys. Rev. C 102, 034320 (2020).

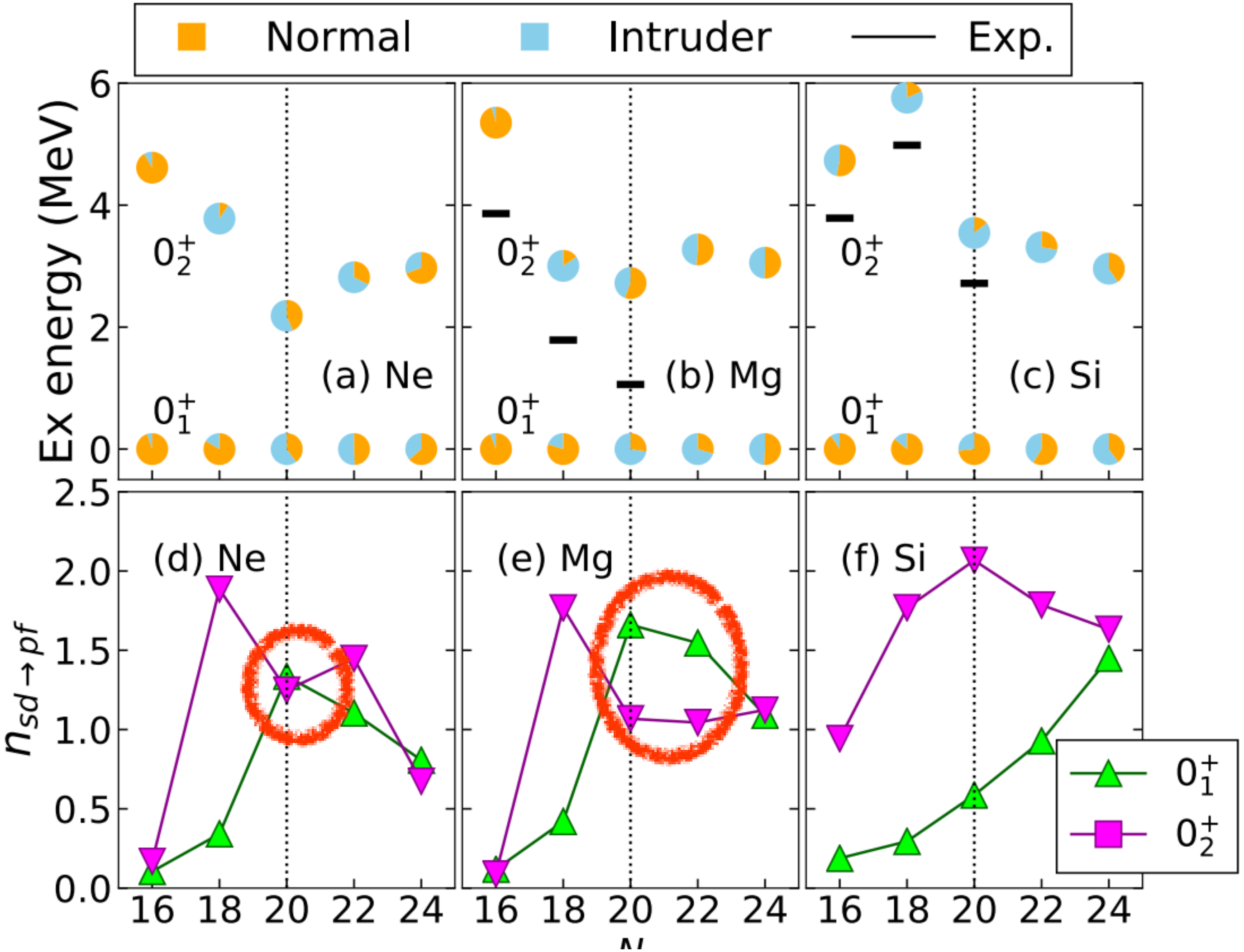




Island of inversion @ N=20



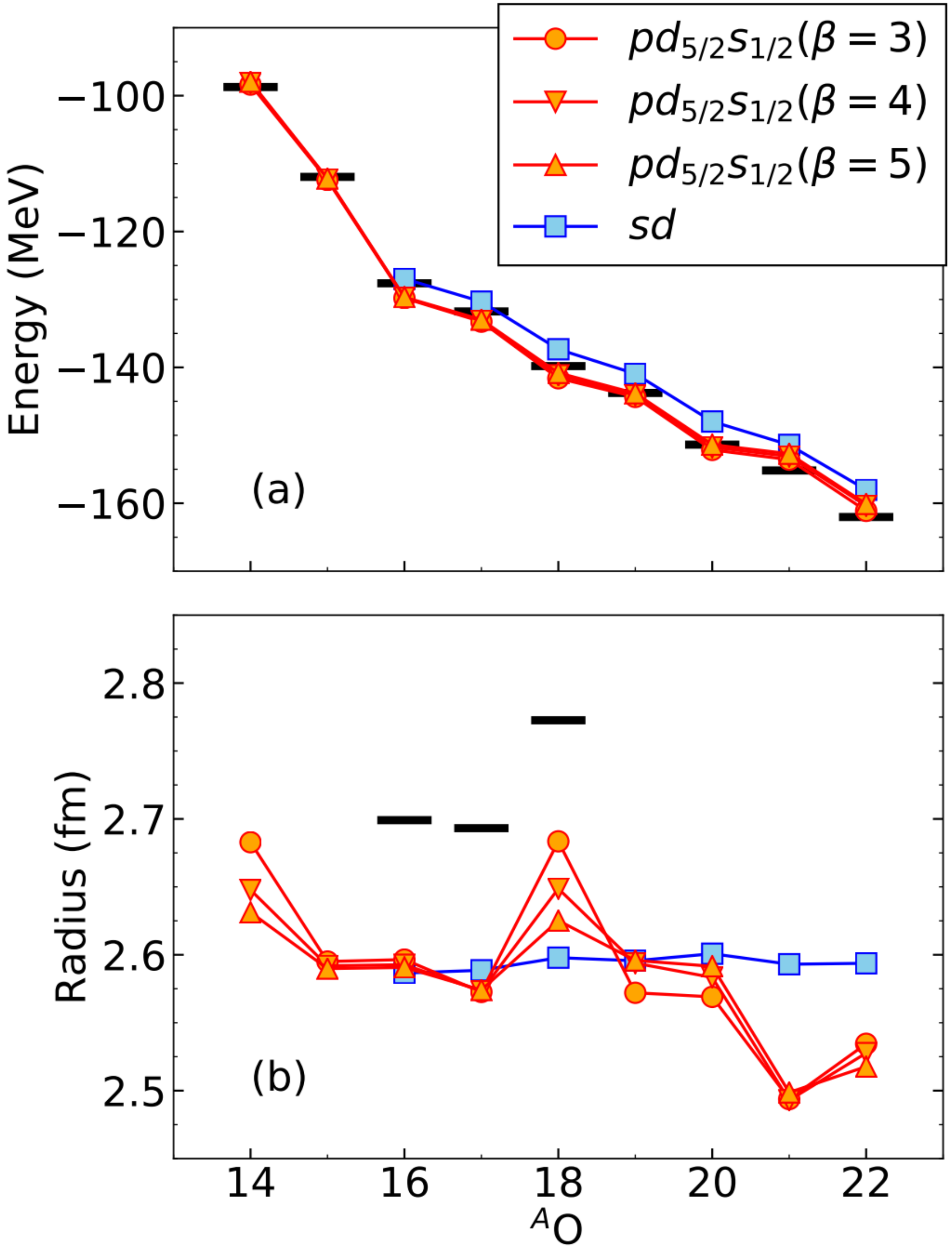




Island of inversion from underlying nuclear forces.

Oxygen radii

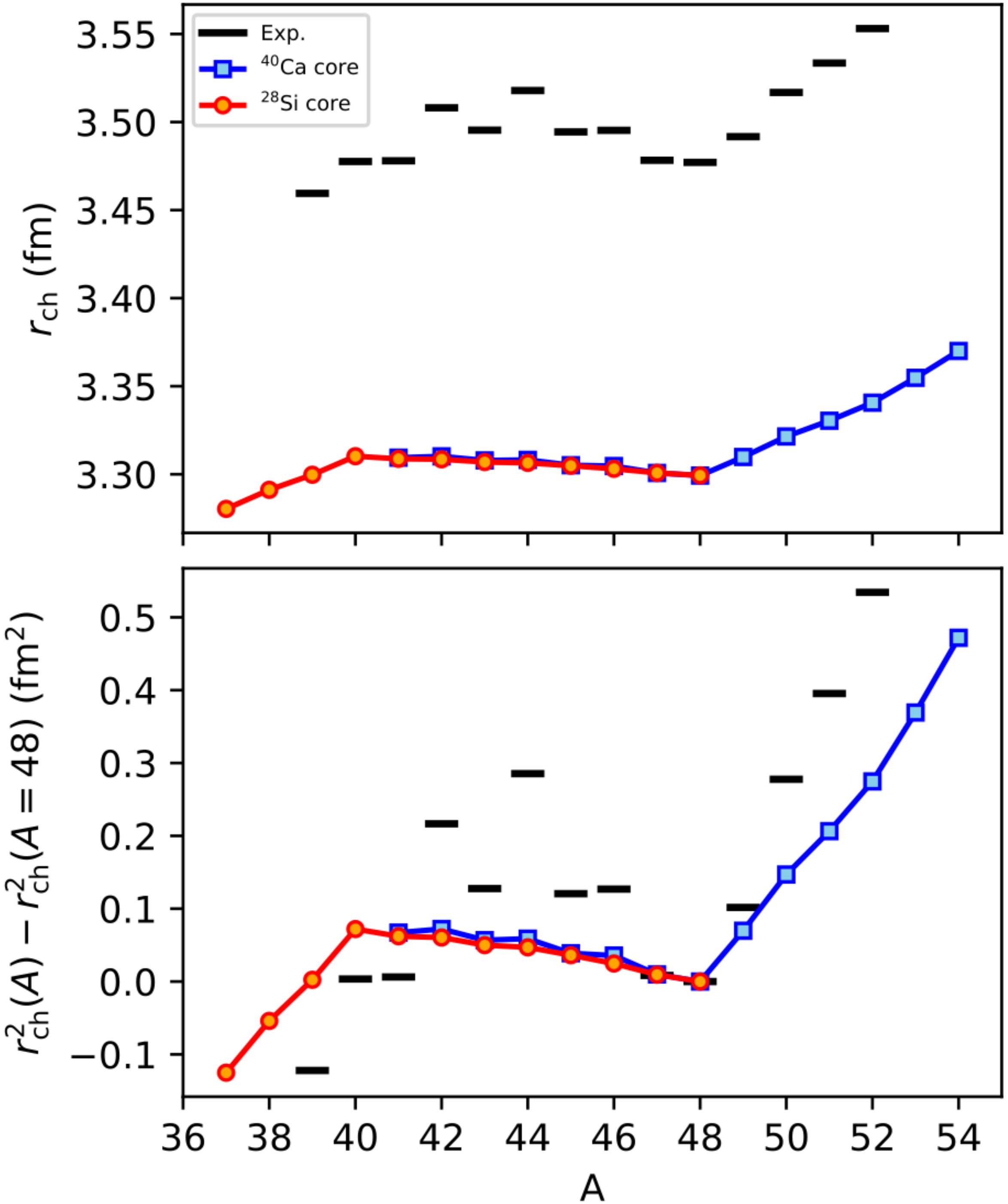
- The oxygen radii trend is also non-trivial.
- The computed radii are not fully β-independent
- $R_{ch}(A=17) < R_{ch}(A=16) < R_{ch}(A=18)$ trend can be seen in the multishell valence-space results.
- 0hw components (beta=3):
  - ^{16}O: 0.71
  - ^{17}O: 0.71
  - ^{18}O: 0.42



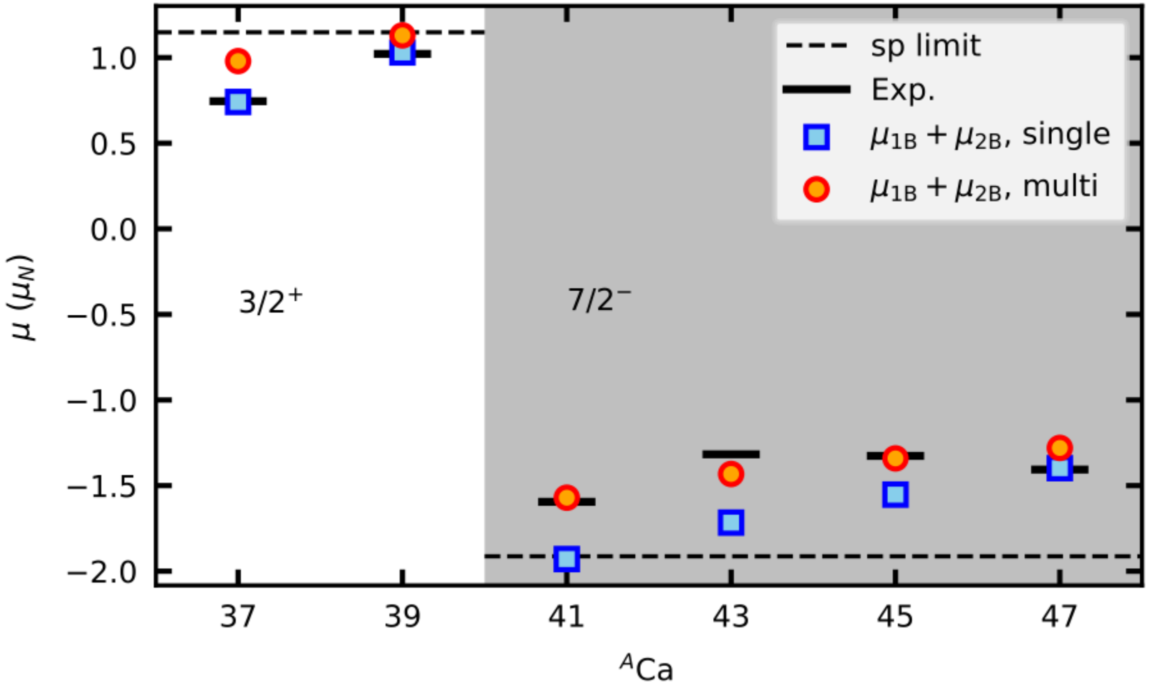
Ca radii

- The ^{40}Ca and ^{28}Si core results are almost the same.
- The beta dependence is weak.

- 0hw components:
  - ^{40}Ca: 0.49
  - ^{42}Ca: 0.50
  - ^{44}Ca: 0.54
  - ^{46}Ca: 0.65
  - ^{48}Ca: 0.81

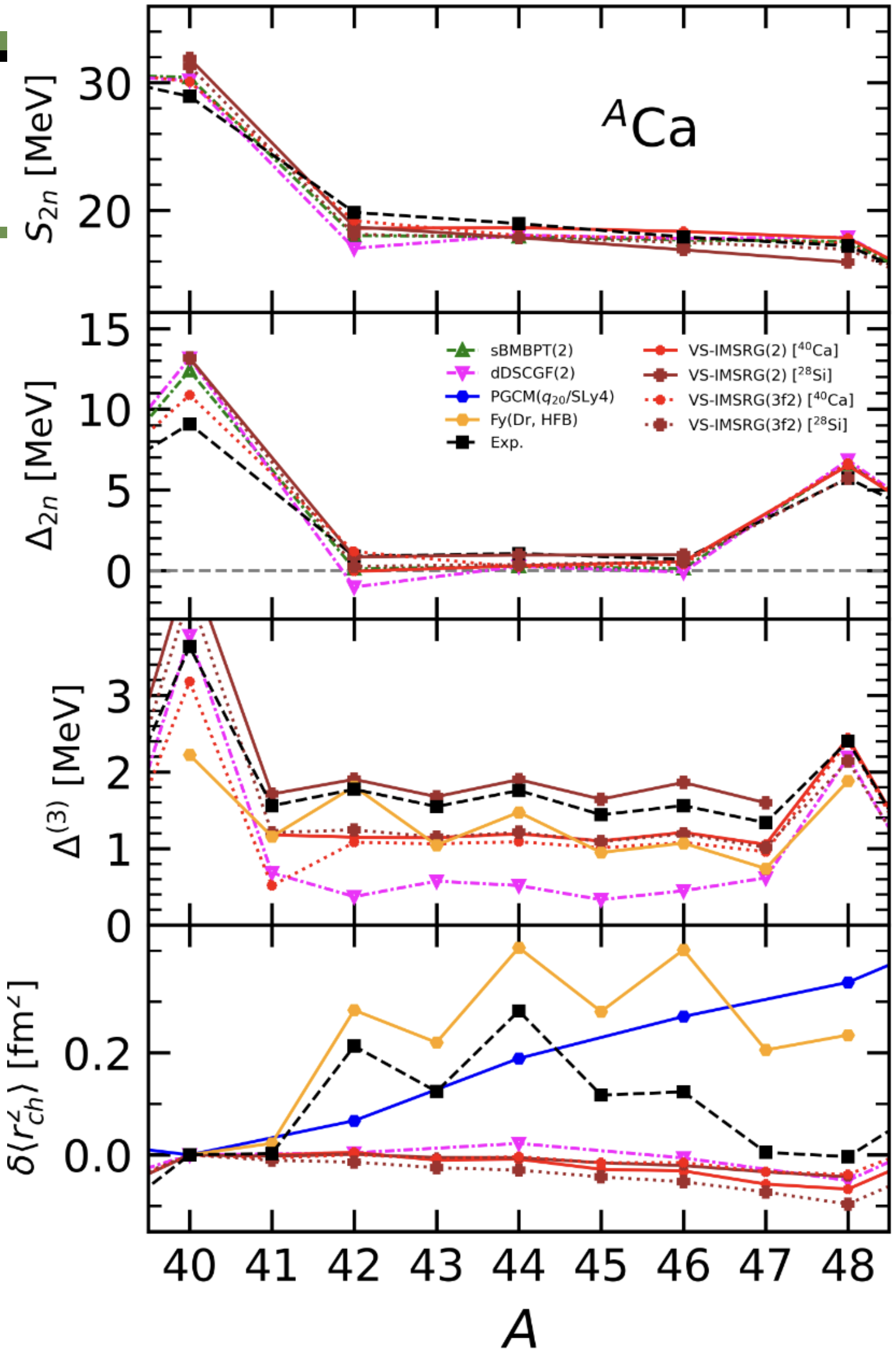


Other observables



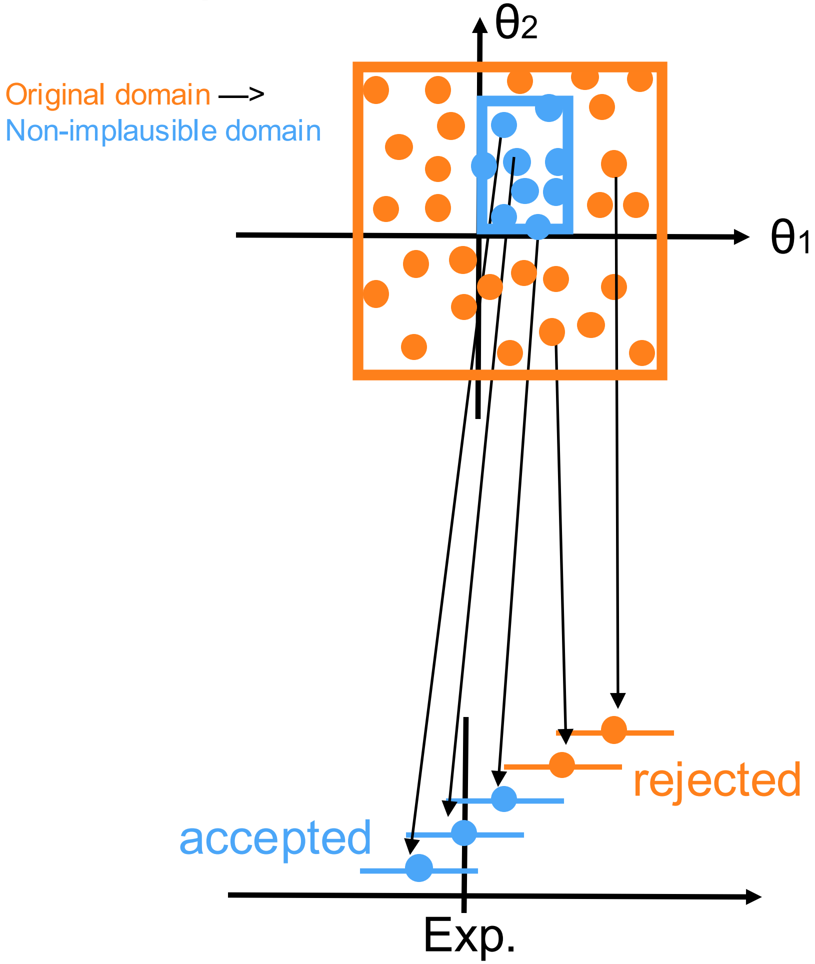
VS-IMSRG(2), 1.8/2.0 (EM)

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

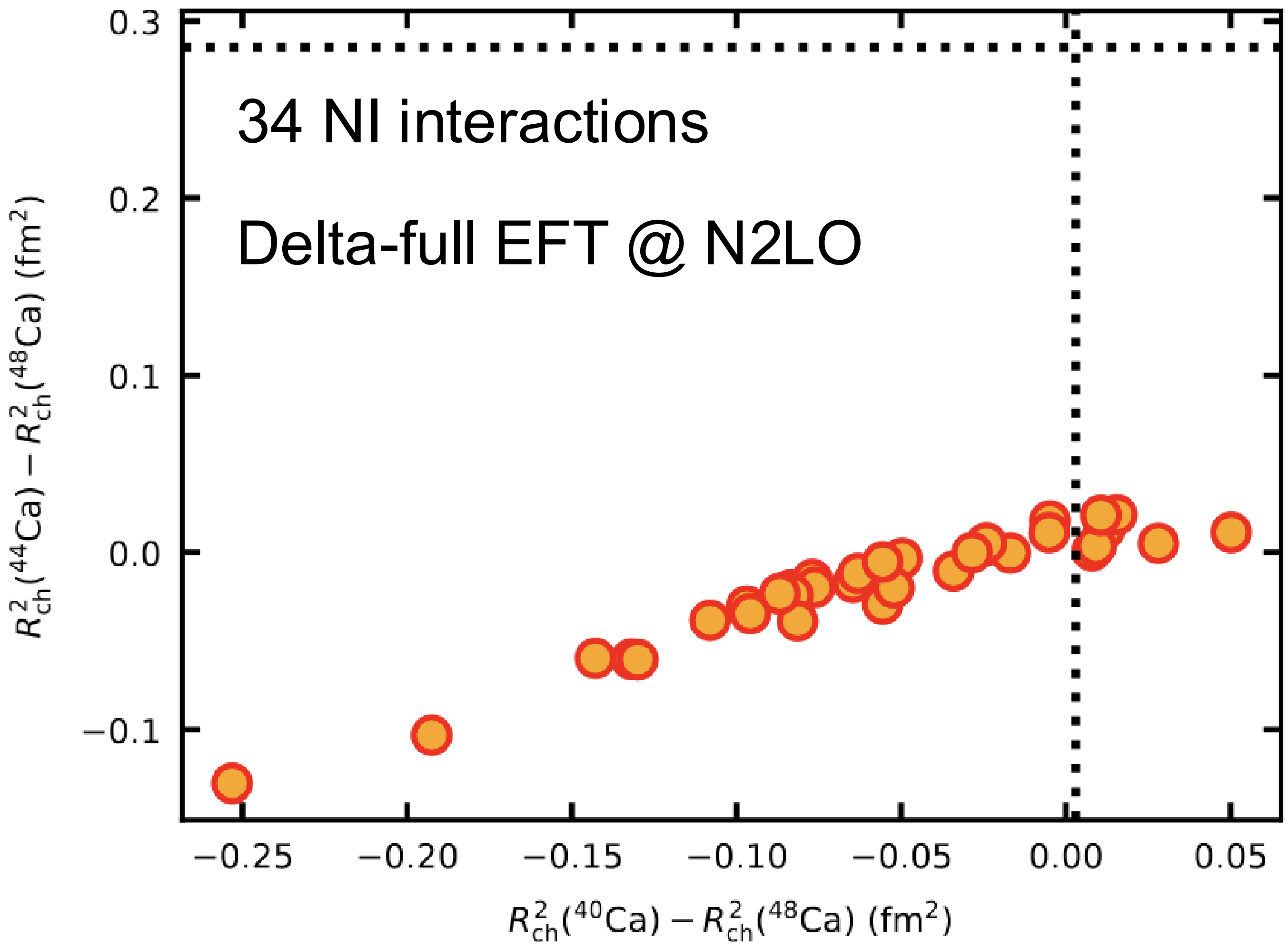


Hamiltonian issue?

Non-implausible interactions

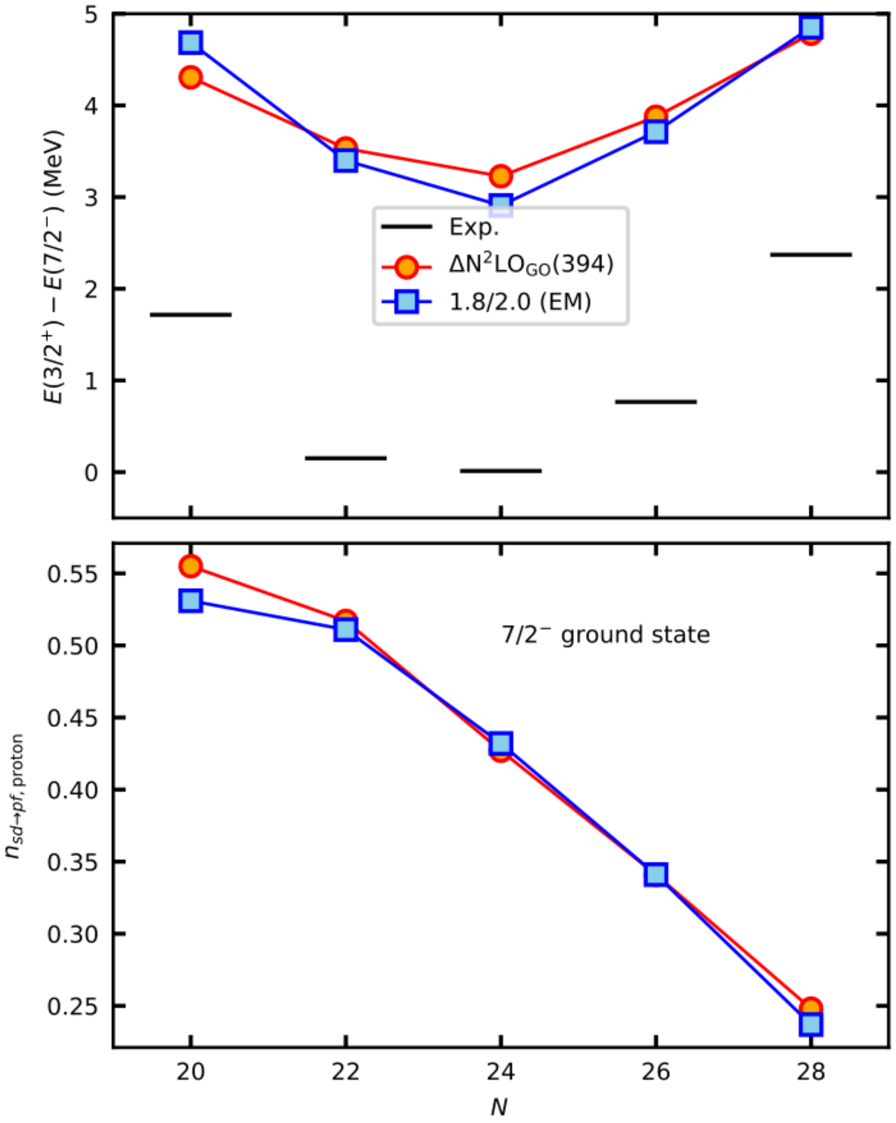


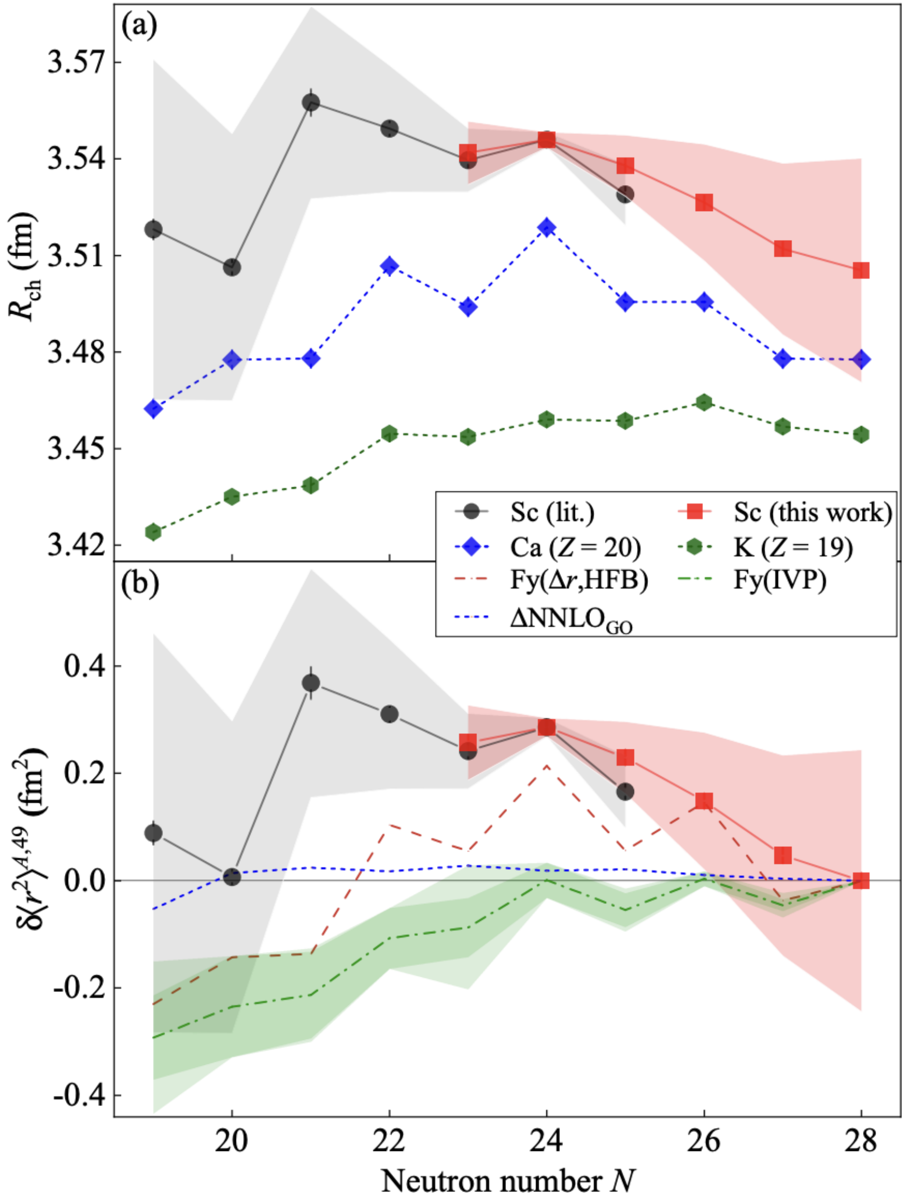
Target observable (few-body systems & ^{16}O)



VS-IMSRG(2), 34 Non-implausible interactions

Pontentially related issues





S. W. Bai et al., Phys. Rev. Lett. 134, 182501 (2025).

Maybe Isomer shifts as well

Summary

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

- Nuclear charge radius is a fundamental observable and provides us with an insight into the nuclear structure.

- The Ca radii behavior in 40 <= A <= 48 is a long standing issue.

- With VS-IMSRG, we have included explicit excitations across Z=N=20 gap.
  - The results are almost the same as the pf-shell calculation results

- Other many-body calculaitons with deformation also fail to reproduce the trend.
- Hamiltonian dependence not seems to explain it.

- What is the missing physics?