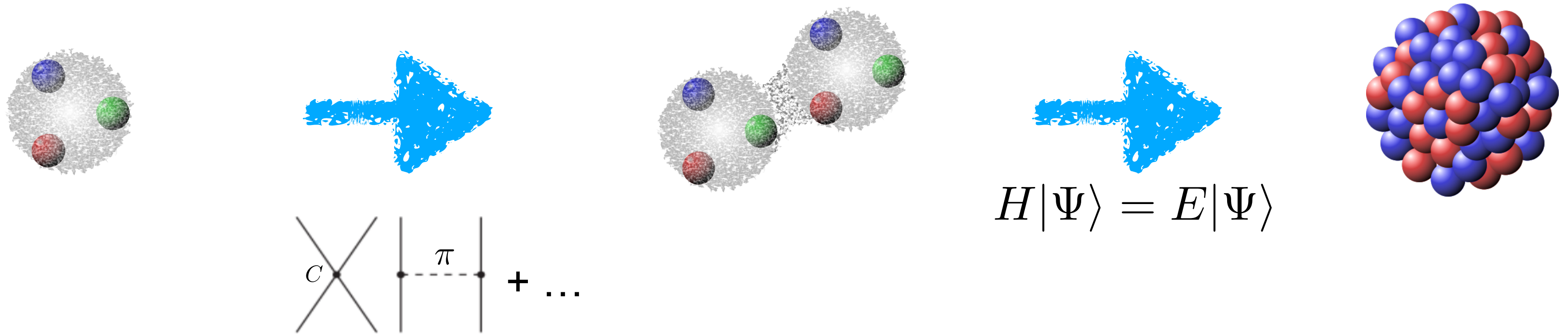
Nuclear ab initio calculations with in-medium similarity renormalization group

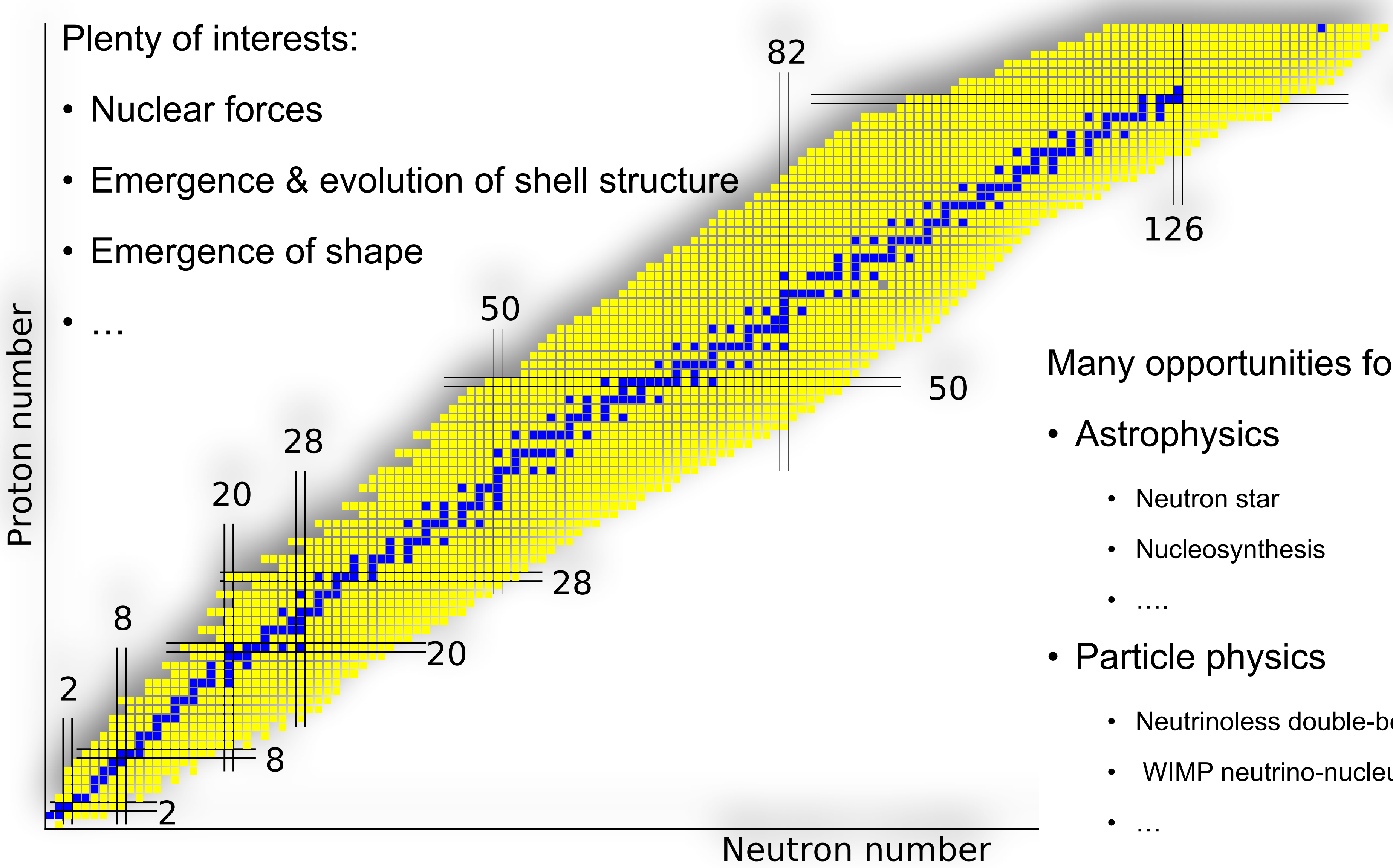


$$H|\Psi\rangle = E|\Psi\rangle$$

Takayuki Miyagi (University of Tsukuba, Japan)

Intersection of nuclear structure and high-energy nuclear collisions 2026 @ YITP, Kyoto, April 13-24, 2026

Motivations



Plenty of interests:

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

Many opportunities for interdisciplinary studies!

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

K. Murano et al., Prog. Theor. Phys. 125, 1225 (2011).
S. Aoki and T. Doi, Front. Phys. 8, (2020).
T. Otsuka et al., Rev. Mod. Phys. 92, 015002 (2020).
A. N. Andreyev et al., Nature 405, 430 (2000).

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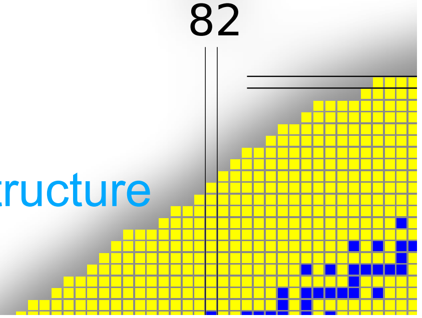

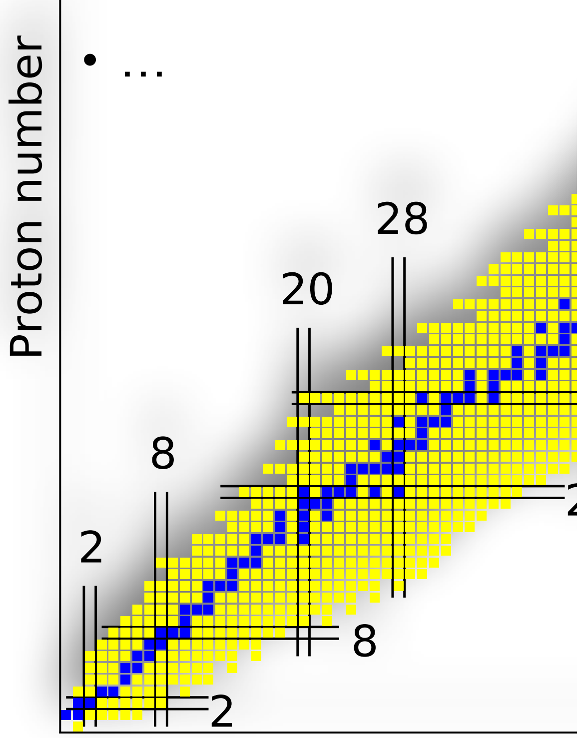

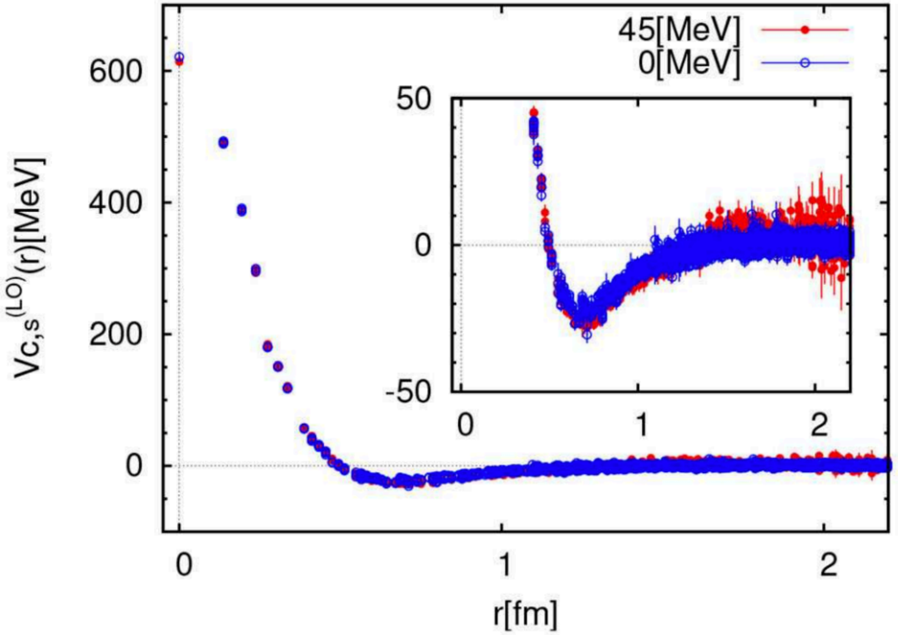

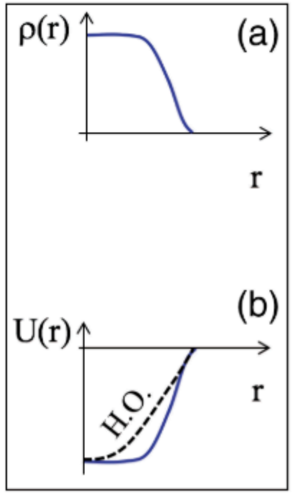

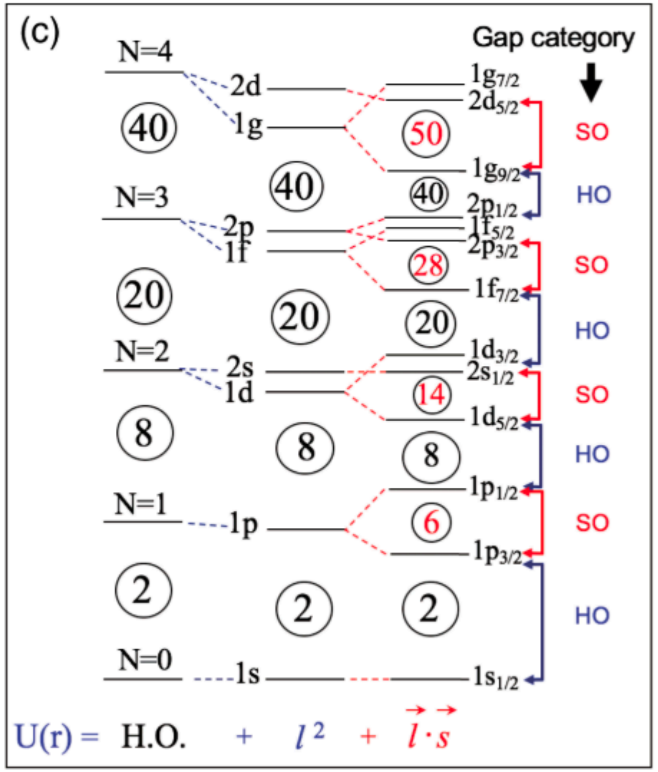

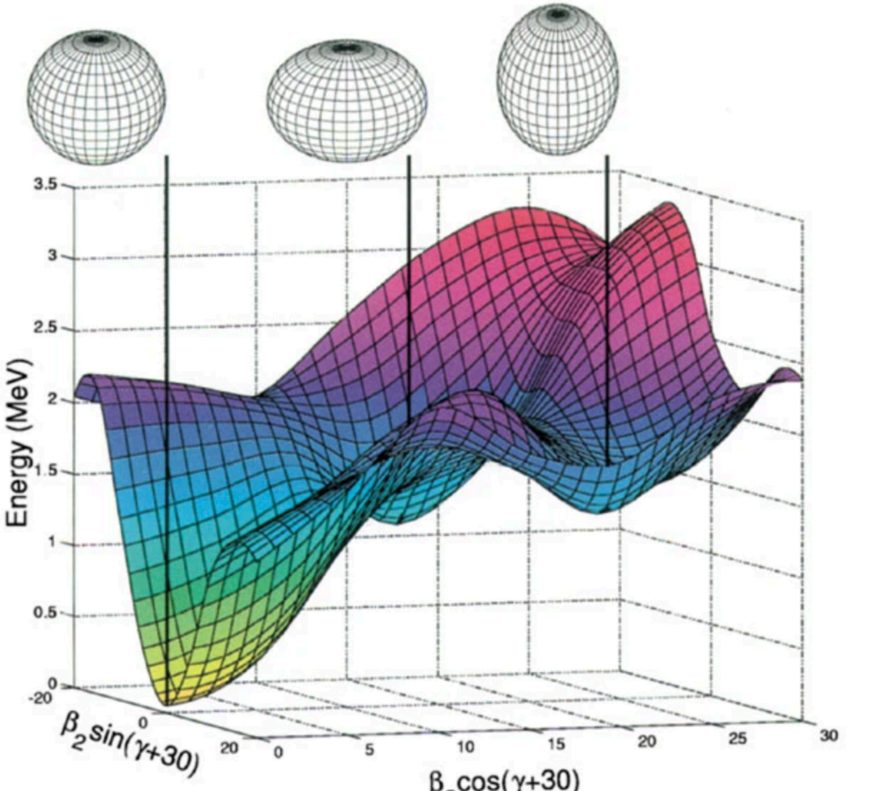

Motivations

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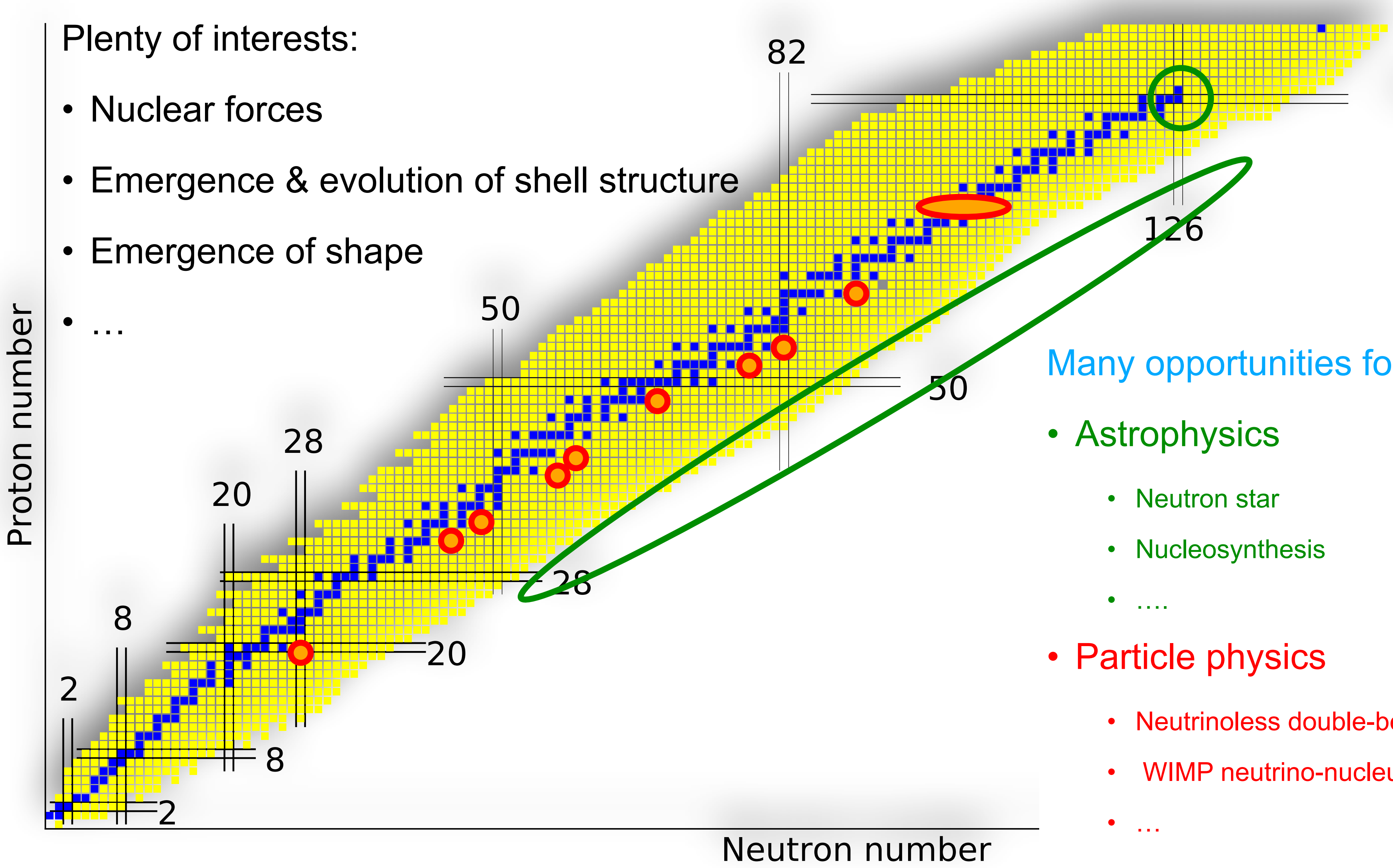

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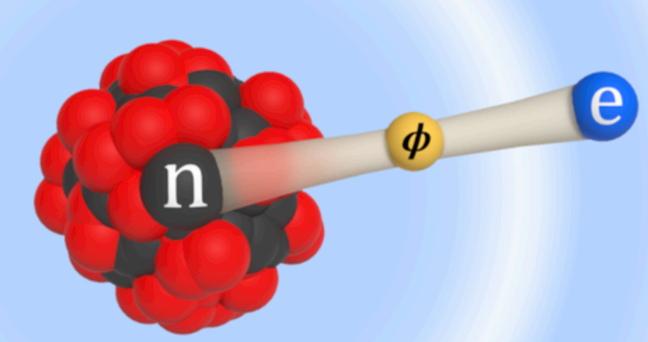
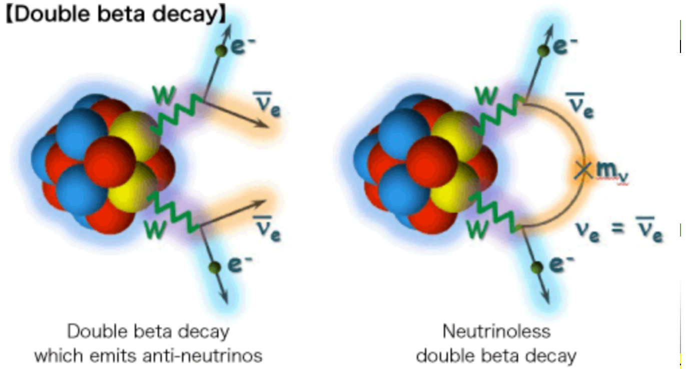
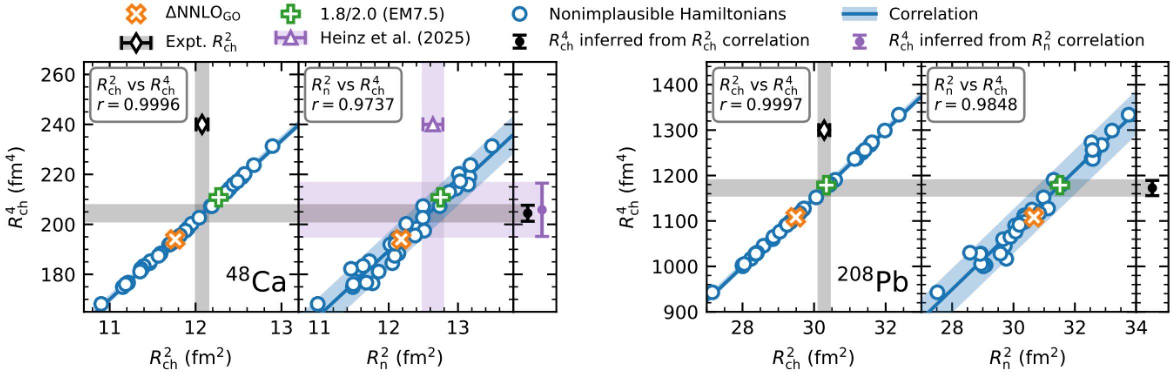


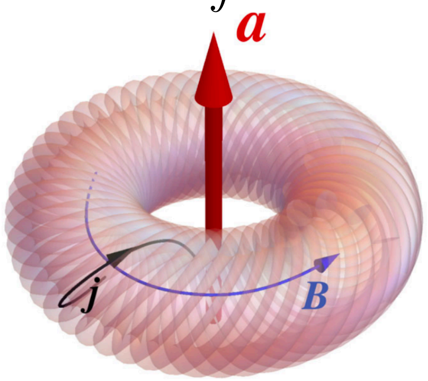
I. Counts et al., Phys. Rev. Lett. 125, 123002 (2020).

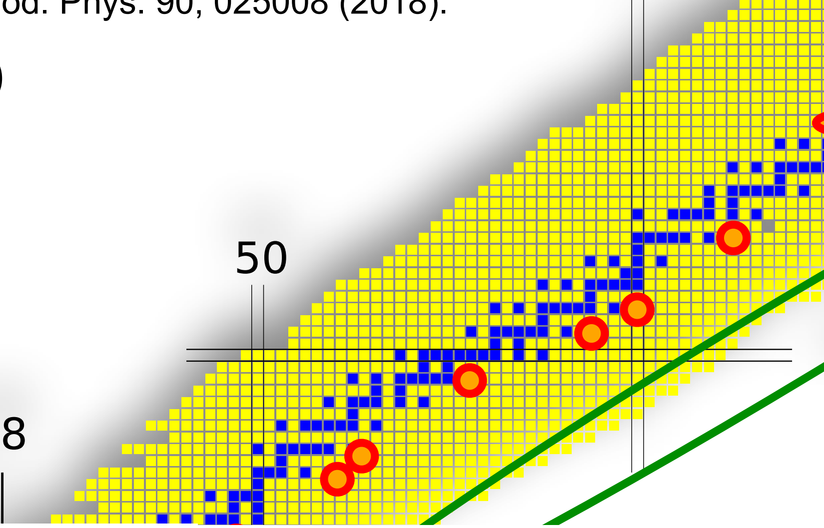
M. S. Safronova et al., Rev. Mod. Phys. 90, 025008 (2018).



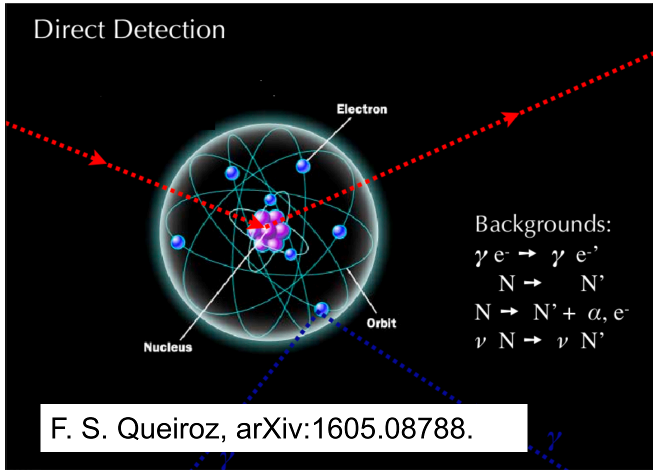


$$a = -\pi \int dx x^2 j(x)$$

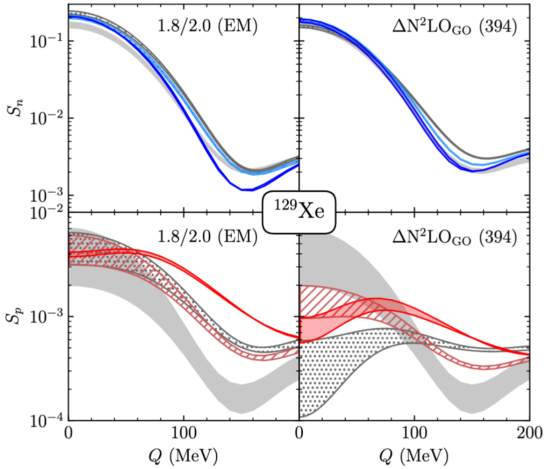




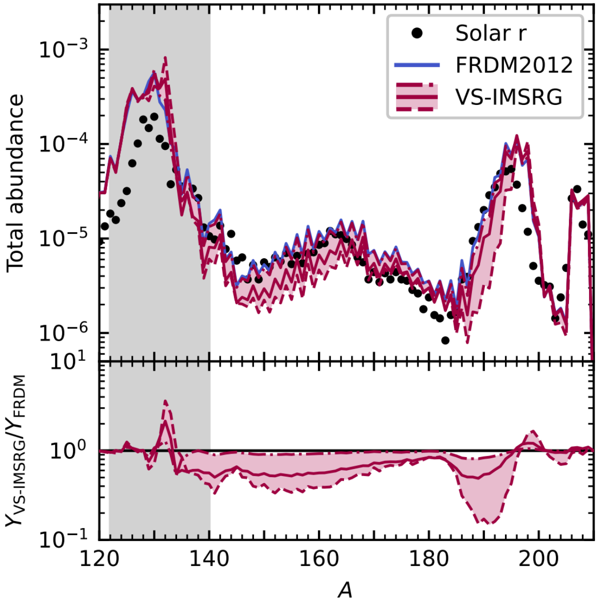
Many opportunities for interdisciplinary studies!

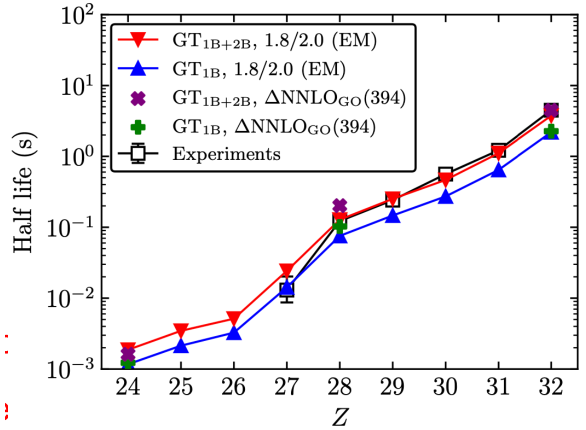


F. S. Queiroz, arXiv:1605.08788.



n nu





Making a prediction

*If the importance of models is known, combining models should also be possible.

- How can we make a prediction?
  - ✦ A probability distribution of target unknown data $\tilde{D}$ conditioned on known data D, based on a model I: $P(\tilde{D}\,|\,D, I)$
  - ✦ It can be realized with the help of model predictions:

$$P(\tilde{D}|D,I) = \int d\boldsymbol{\theta} \boxed{P(\tilde{D}|\boldsymbol{\theta},I)} \boxed{P(\boldsymbol{\theta}|D,I)}$$

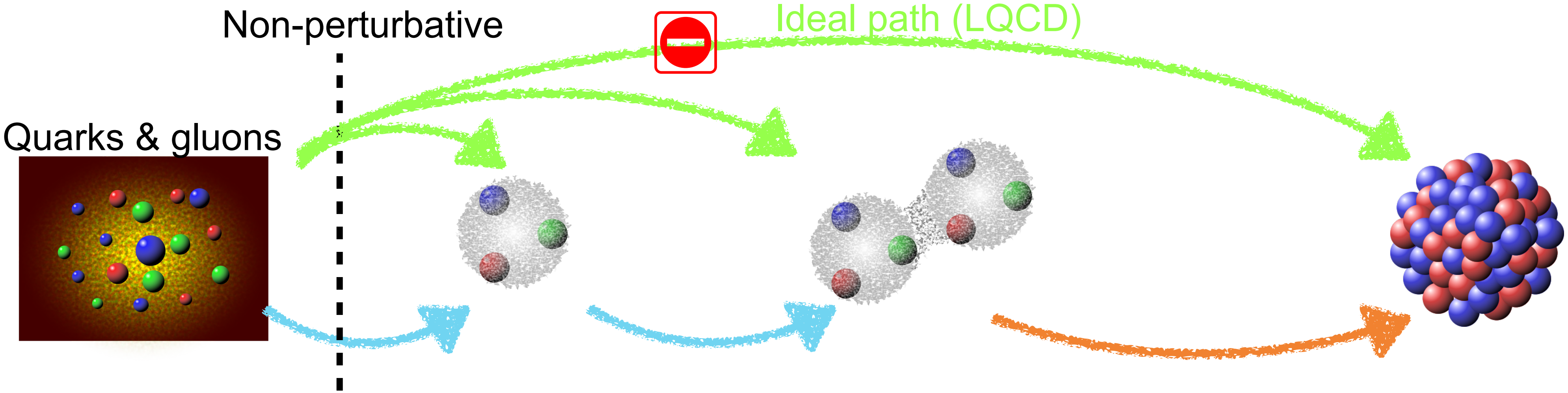
Model parameters Model prediction Posterior parameter dist.

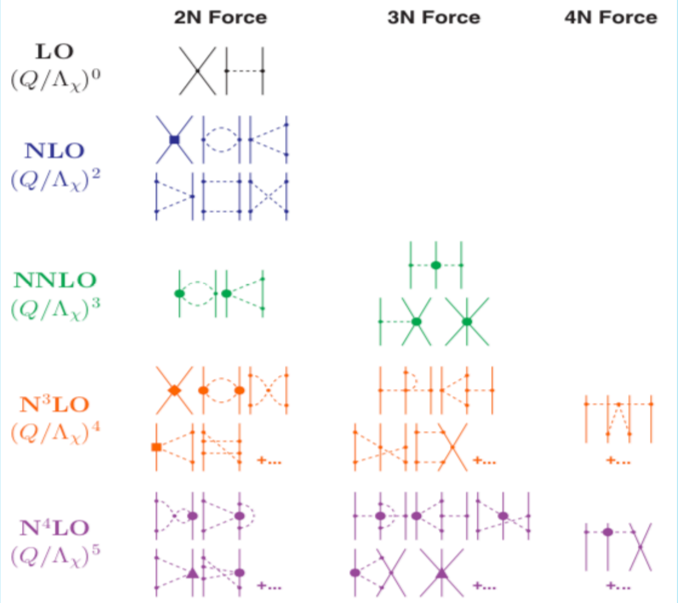
- Posterior parameter distribution

Likelihood Prior parameter dist.

  - One can use Bayes' theorem: $\boxed{P(\boldsymbol{\theta}|D,I)} \propto \boxed{P(D|\boldsymbol{\theta},I)} P(\boldsymbol{\theta})$
  - In practice, a sampling method is needed, for example Markov-chain Monte Carlo (MCMC) method.
- **Uncertainty quantification** is necessary in steps **model predictions** and **Likelihood evaluations!**
  - Systematically improvable theory is required.

Theoretical framework





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

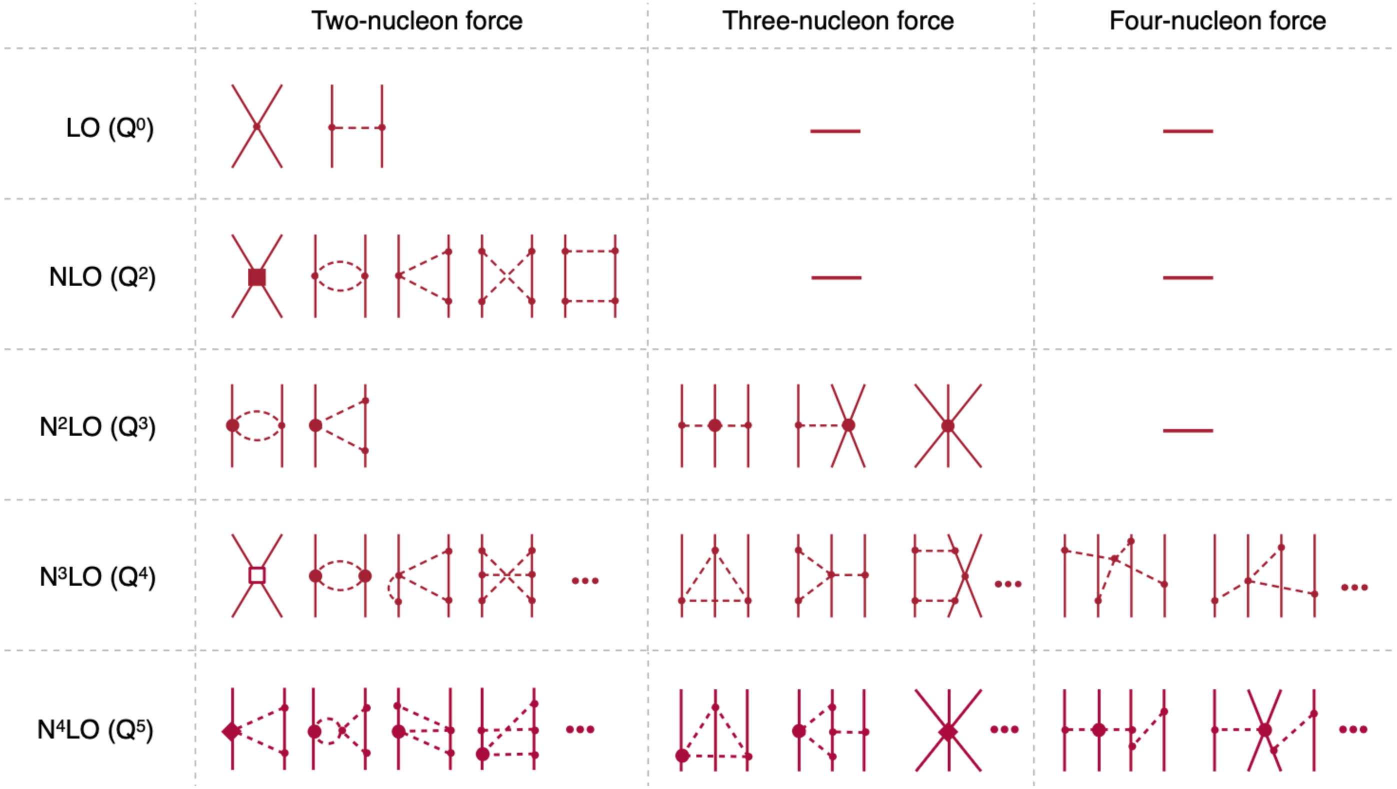


Figure is from E. Epelbaum, H. Krebs, and P. Reinert, Front. Phys. 8, 1 (2020).

Uncertainty quantification

- EFT convergence model for observable y

$$y = y_{\text{ref}} \left(\sum_{i=0}^{k} c_i Q^i + \underbrace{\boxed{\sum_{i=k+1}^{\infty} c_i Q^i}}_{\text{Error}} \right)$$

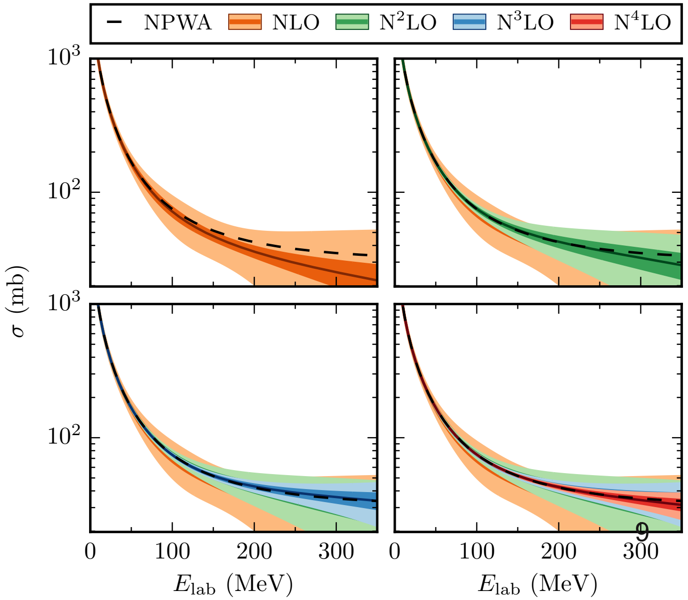
y_{ref} : absolute scale of the observable
k : expansion order considered
c_i : expansion coefficient $\mathcal{O}(1)$
Q : expansion parameter $\sim \max(m_\pi, p)/\Lambda_b$

- Assume that all c_i are independently taken from a single Gaussian.

$$\frac{1}{\bar{c}\sqrt{2\pi}} e^{-1/2\bar{c}^2}$$

- Using an actual order-by-order calculation results, one can obtain the distribution for $\bar{c}$.

- Once $\bar{c}$ is obtained, the EFT truncation uncertainty can be estimated.



R. J. Furnstahl, N. Klco, D. R. Phillips, and S. Wesolowski, Phys. Rev. C 92, 024005 (2015).
J. A. Melendez, R. J. Furnstahl, D. R. Phillips, M. T. Pratola, and S. Wesolowski, Phys. Rev. C 100, 044001 (2019).

Nuclear many-body problem

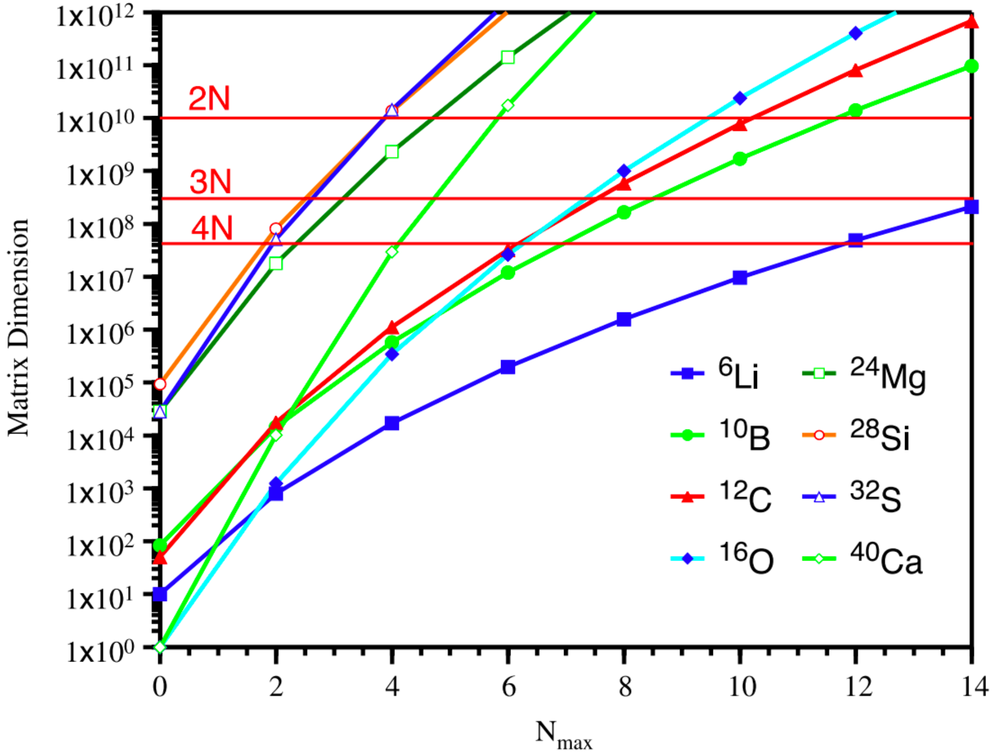
- Non-relativistic many-body Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$
- A straightforward way is to diagonalize the Hamiltonian matrix

$$\begin{pmatrix} \langle 1|H|1\rangle & \langle 1|H|2\rangle & \cdots & \langle 1|H|N\rangle \\ \langle 2|H|1\rangle & \langle 2|H|2\rangle & \cdots & \langle 2|H|N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle N|H|1\rangle & \langle N|H|2\rangle & \cdots & \langle N|H|N\rangle \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$$

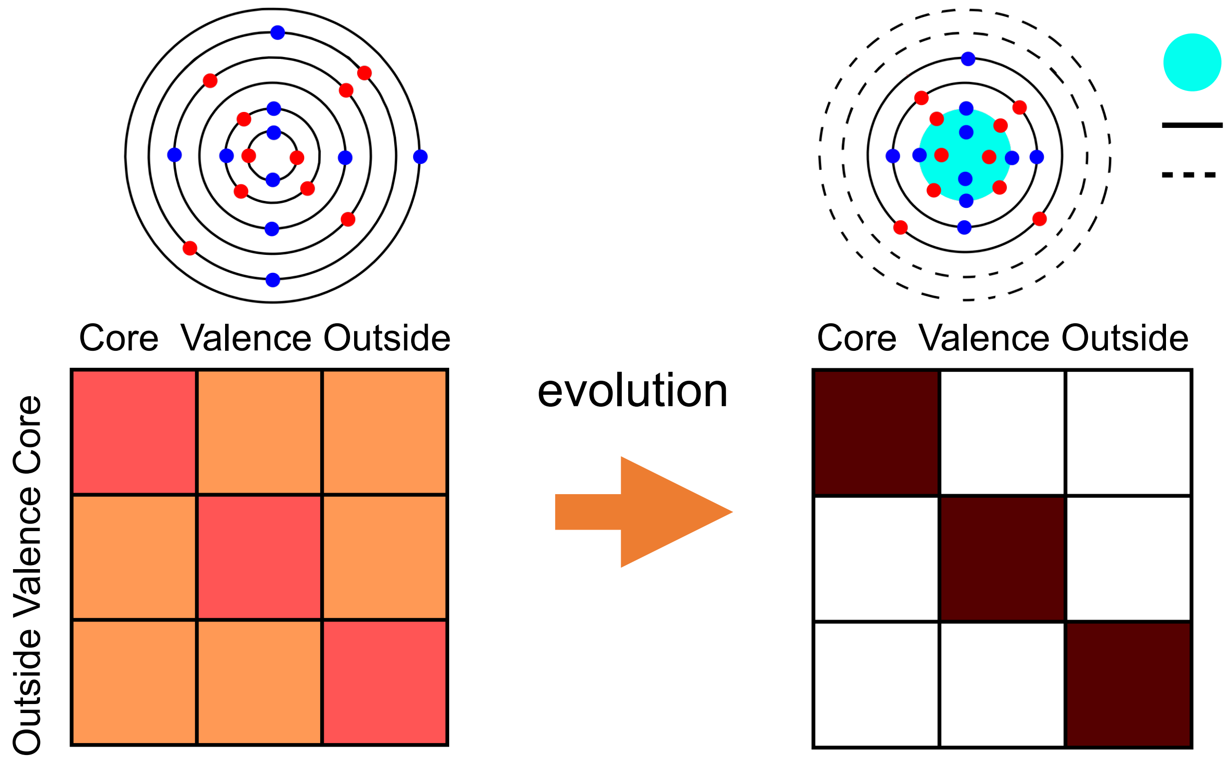
$|1\rangle, |2\rangle, \ldots |N\rangle$ are Slater determinants

- N exponentially scales with system size
- Brute force diagonalizations for heavy systems are impossible.
- The limit of brute force calculation method is A ~ 20.
  - ✦ No-core shell model
  - ✦ Quantum Monte Carlo

B. R. Barrett, P. Navrátil, and J. P. Vary, Prog. Part. Nucl. Phys. 69, 131 (2013).



Valence-Space In-Medium Similarity Renormalization Group



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

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

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

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

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

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

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

Similarity transformation

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

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

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

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).

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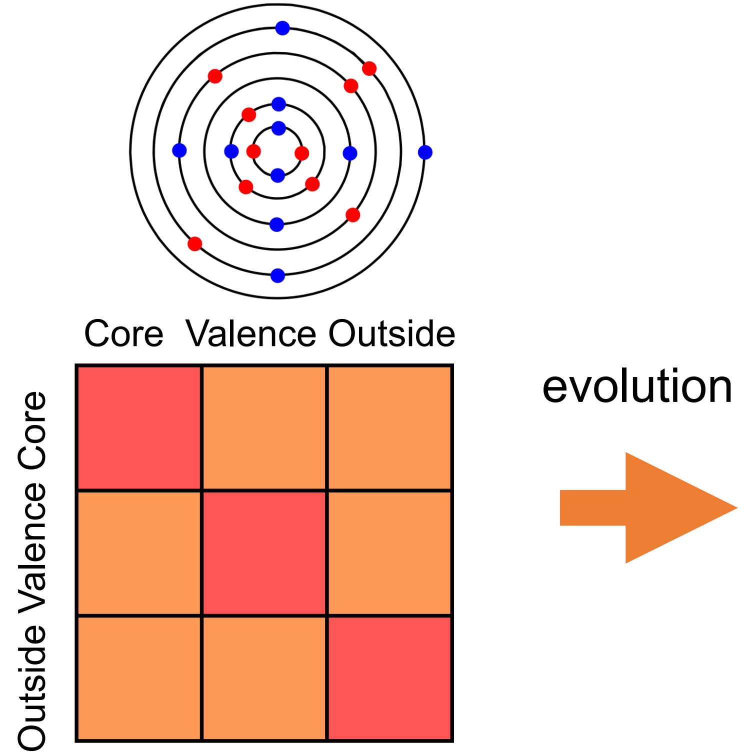
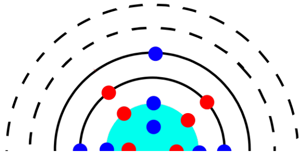
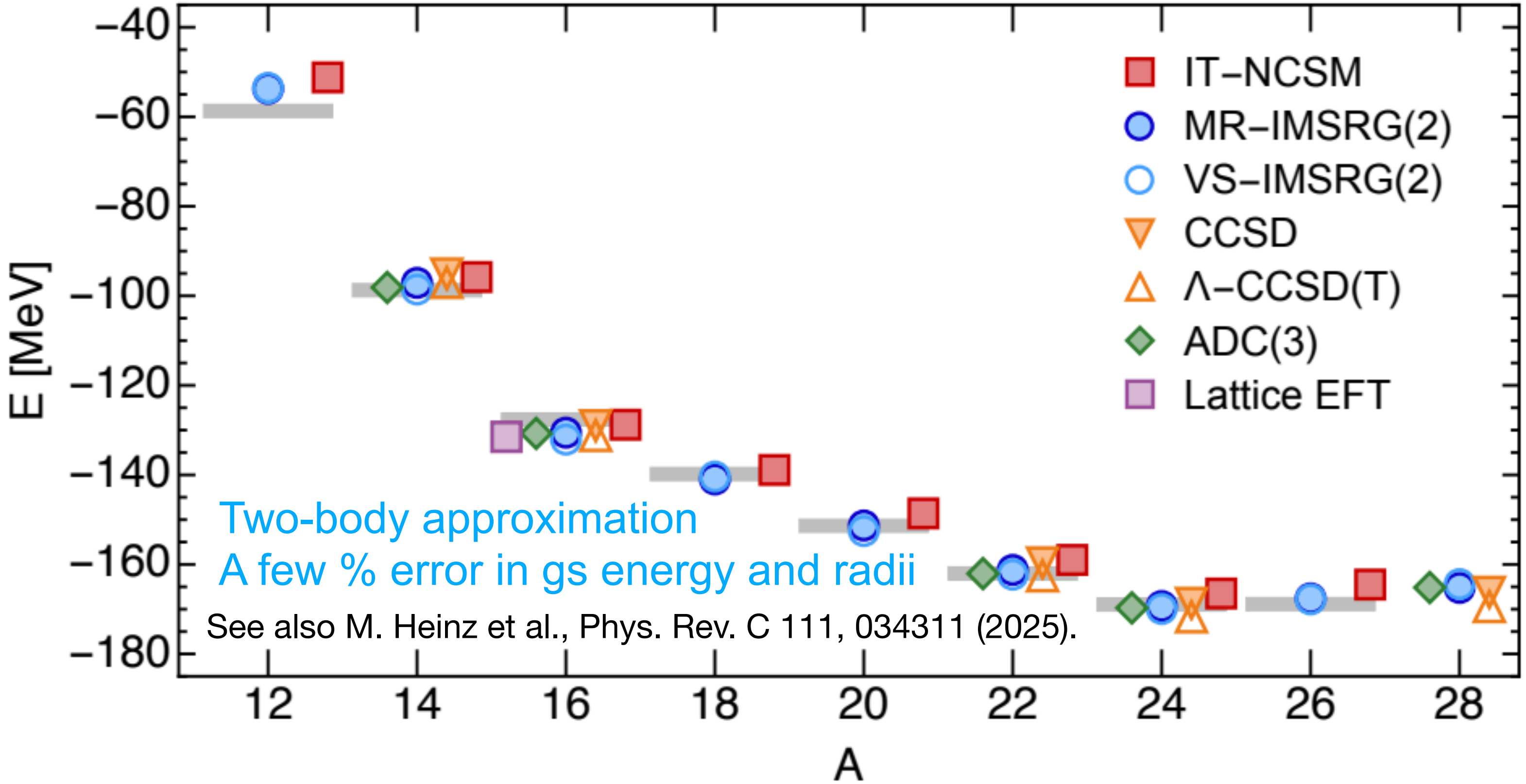




H. Hergert, Front. Phys. 8, 1 (2020).



Two-body approximation
A few % error in gs energy and radii

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

Similarity transformat

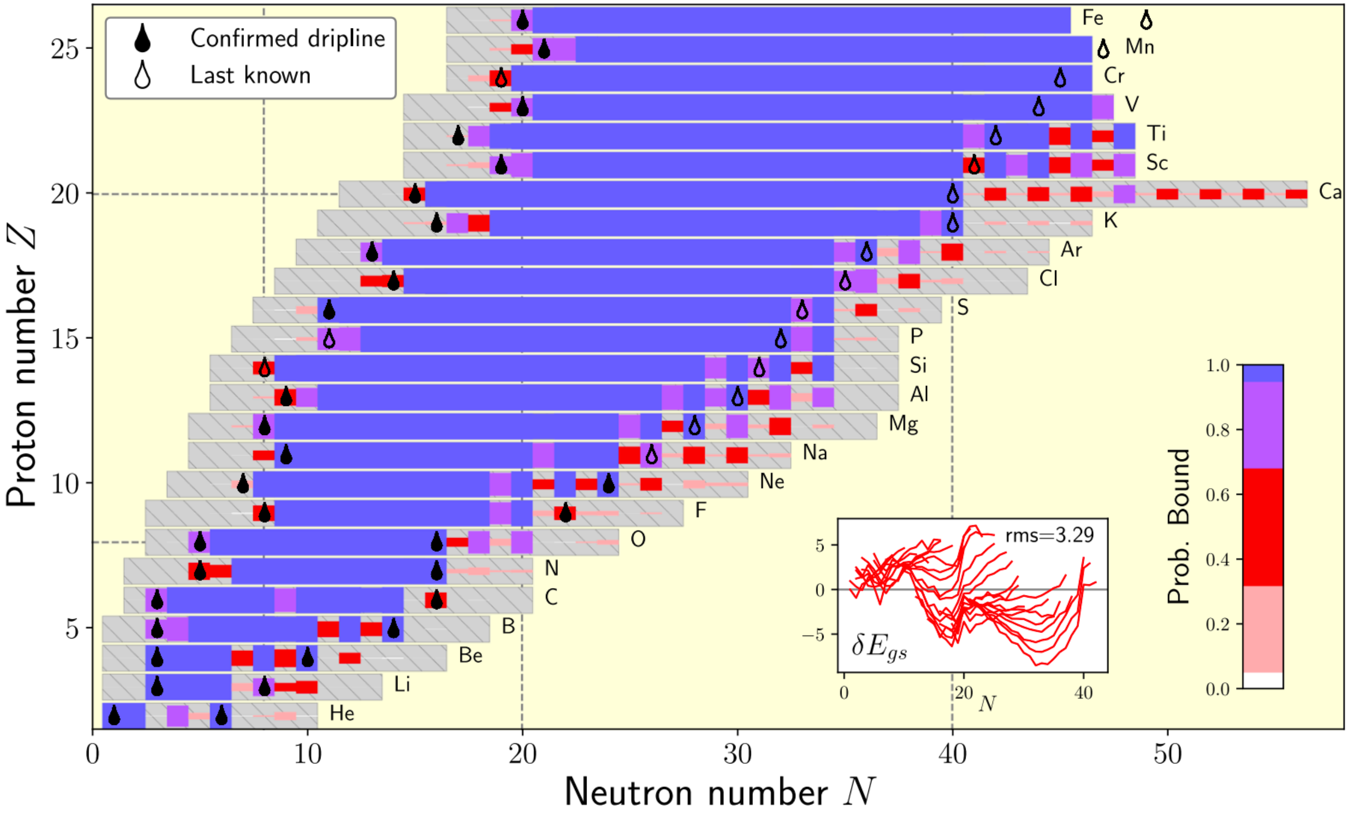
H

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

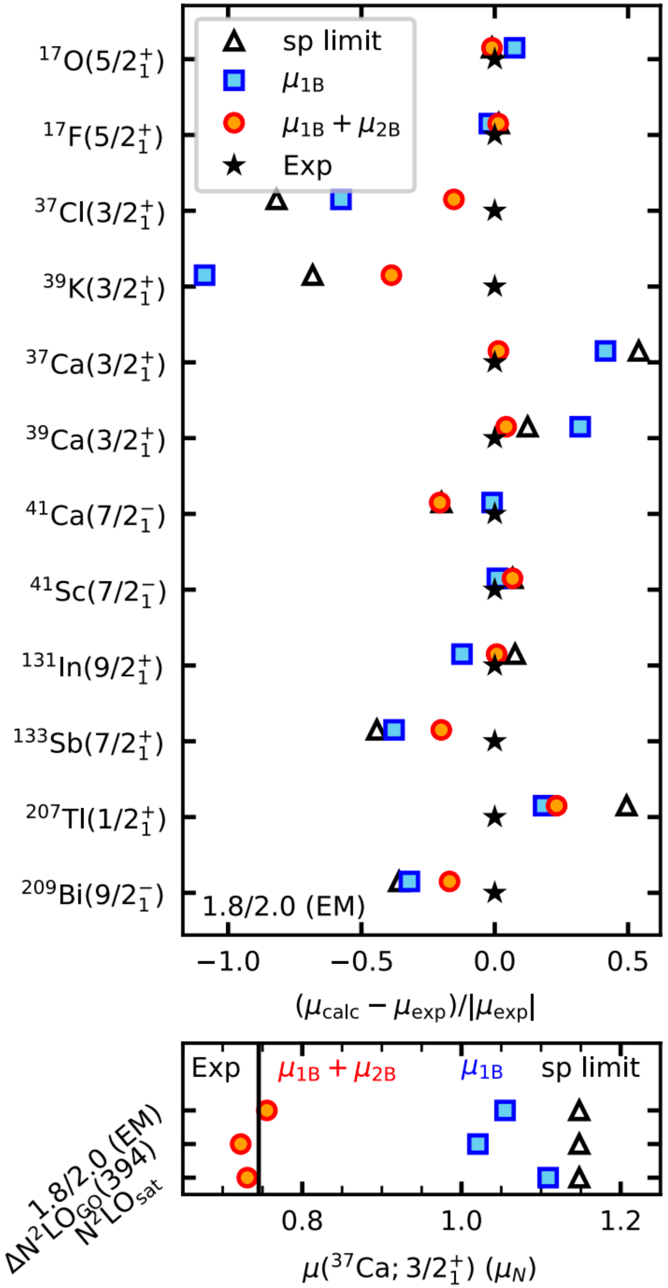
s: flow parameter

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).

Some results



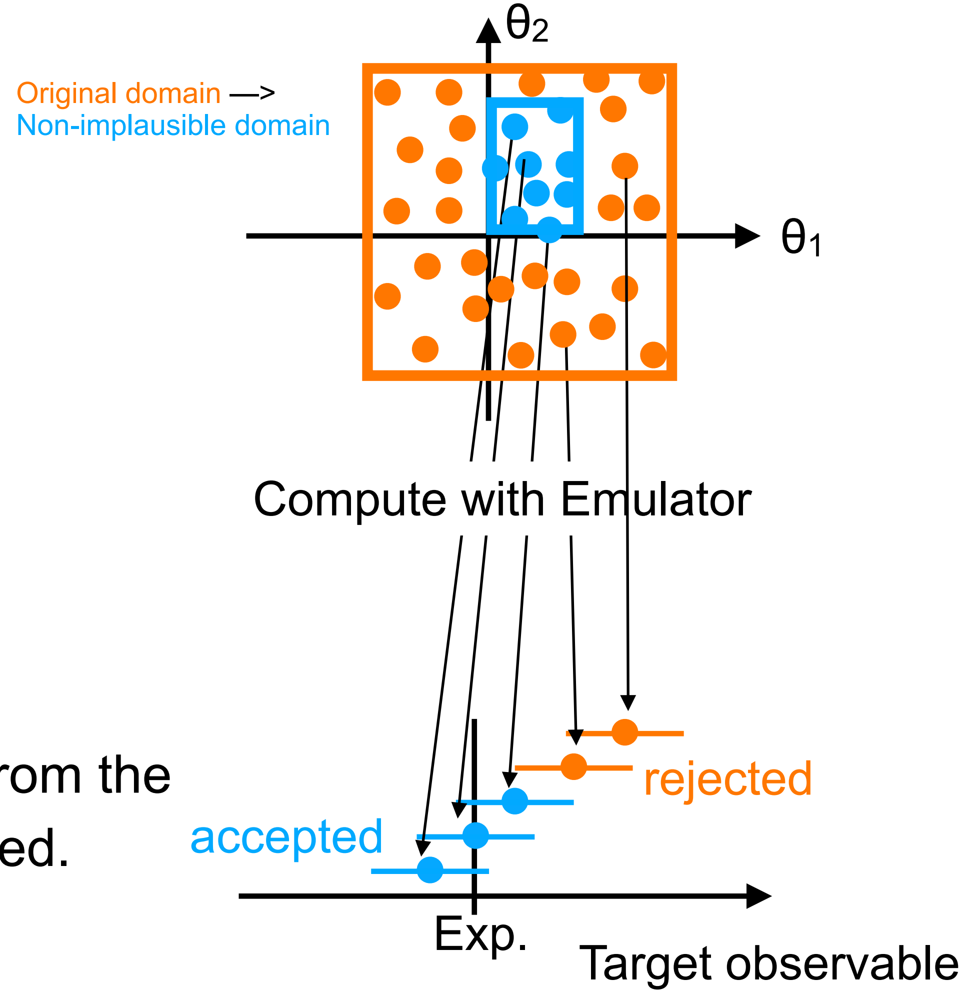
S. R. Stroberg et al., Phys. Rev. Lett. 126, 022501 (2021).



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

Sampling parameters

- Non-implausible samples
  - 17 Unknown LECs @ Delta-full N2LO
    - Constraints:
      - Naturalness: LECs should be O(1)
  - Steps:
    - (1) Generate a random 17 dimensional vector θ
    - (2) Evaluate the selected observables
    - (3) Measure how the calculated observables are far from the experiments. If it is too far, θ is implausible and rejected.
- Out of ~ 10^9 parameter sets, 34 NI interactions were found.

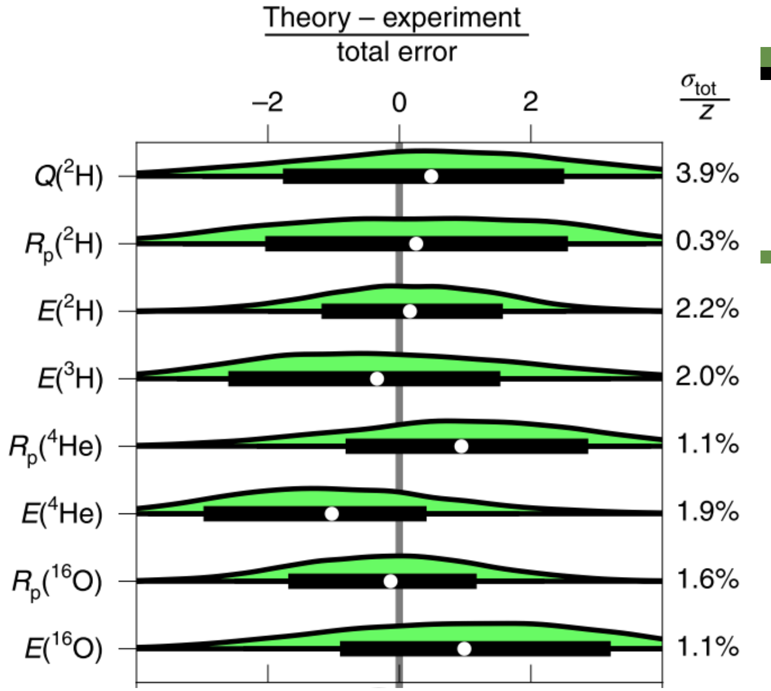


B. Hu et al., Nat. Phys. 18, 1196 (2022).

Neutron skin thickness of ^{208}Pb

- History matching:
  - Sampling 17 parameters in (delta-full) chiral EFT such that the parameter set is consistent with some selected data.
  - Proton-neutron scattering phase shifts, E(^{2}H), R$_p$(^{2}H), Q(^{2}H), E(^{3}H), E(^{4}He), R$_p$(^{4}He), E(^{16}O), and R$_p$(^{16}O).

History matching



~ 10^9 parameter sets → 34 NI parameter sets

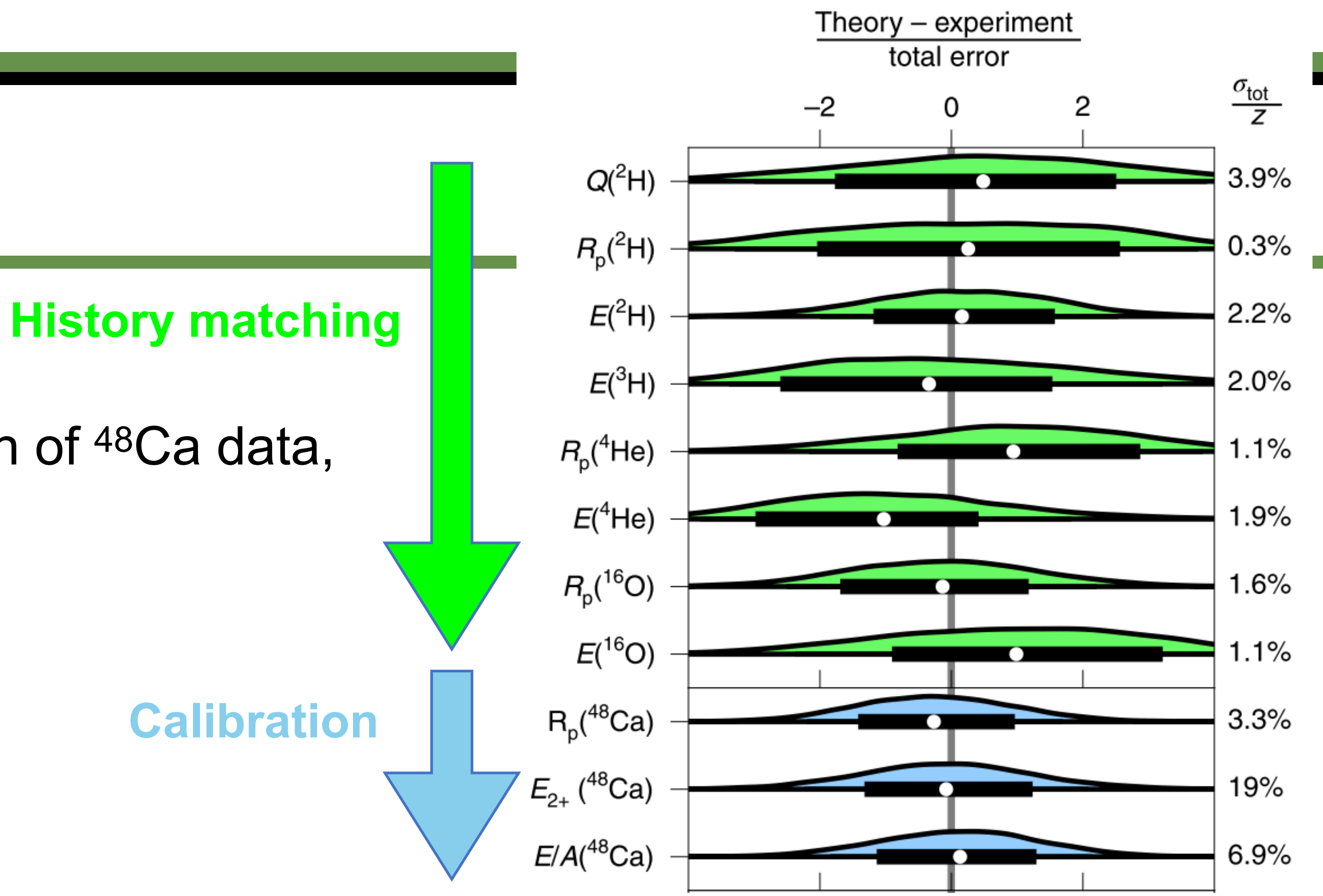
B. Hu, W. Jiang, T. Miyagi, et al., Nat. Phys. 18, 1196 (2022).

Neutron skin thickness of ^{208}Pb

- Calibration:
  - ✦ Assign weights according to the reproduction of ^{48}Ca data, known as importance resampling method.

$$w_i = \frac{\mathcal{L}(D|\boldsymbol{\theta}_i)}{\sum_{j=1}^{34} \mathcal{L}(D|\boldsymbol{\theta}_j)},$$

$$\mathcal{L}(D|\boldsymbol{\theta}_i) = \mathcal{N}(D, \sigma^2_{\mathrm{exp}} + \sigma^2_{\chi\mathrm{EFT}} + \sigma^2_{\mathrm{MB}})$$



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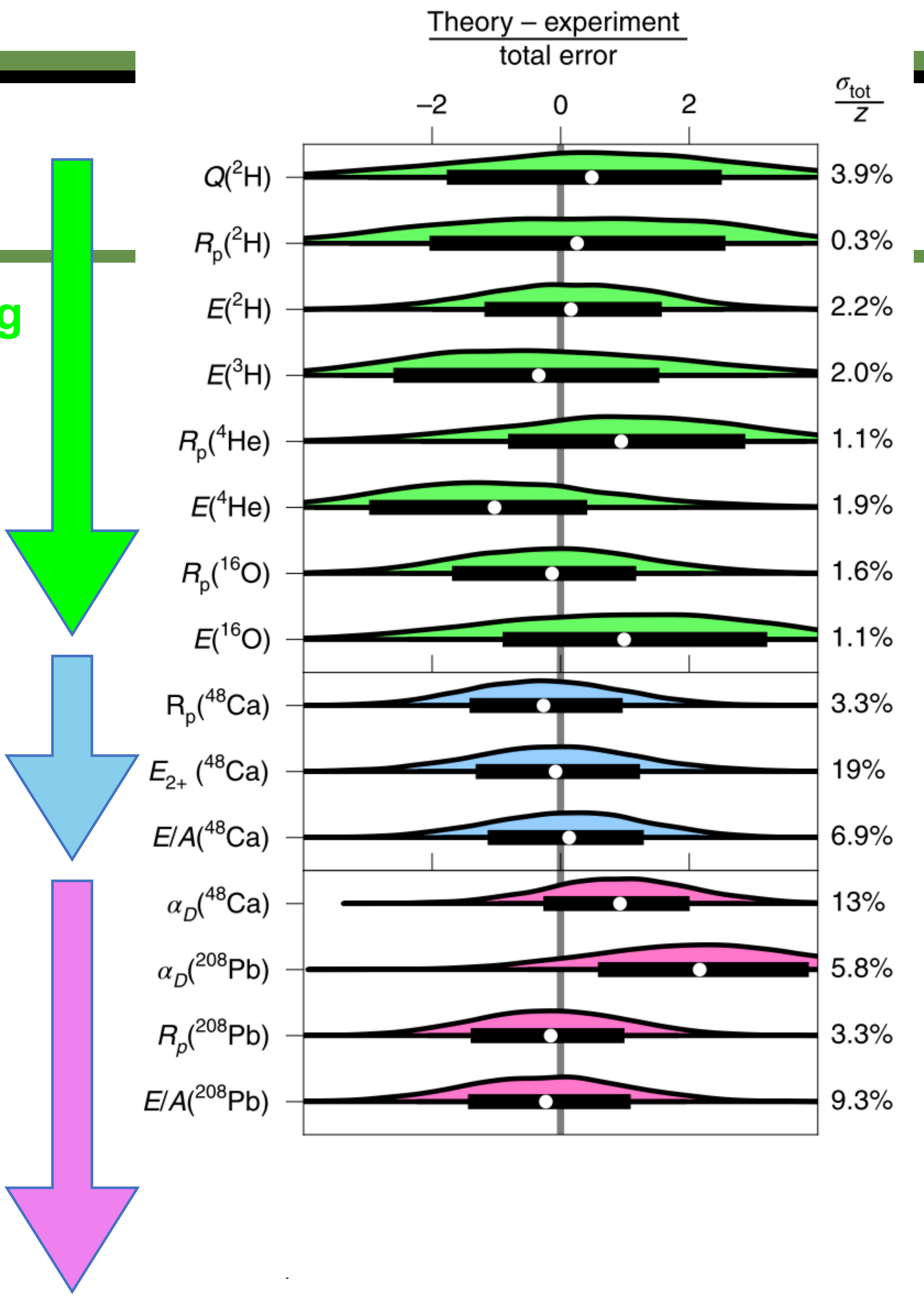
- Validation & prediction:
  - ✦ The weighted samples are approximately equivalent to the samples extracted from p(θ|D).

$$\text{PPD} = \{\mathcal{O}_{\text{target}}(\theta) : \theta \sim P(\theta|^{48}\text{Ca})\}$$



History matching

Calibration

Validation
Prediction

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

Neutron skin thickness of ^{208}Pb

- Calibration process:
    - ✦ Assign weights according to the reproduction of ^{48}Ca data, known as importance resampling method.
- Validation & prediction:
    - ✦ With the weights, 34 samples are approximately equivalent the 34 samples extracted from p(θ|D).

Neutron skins

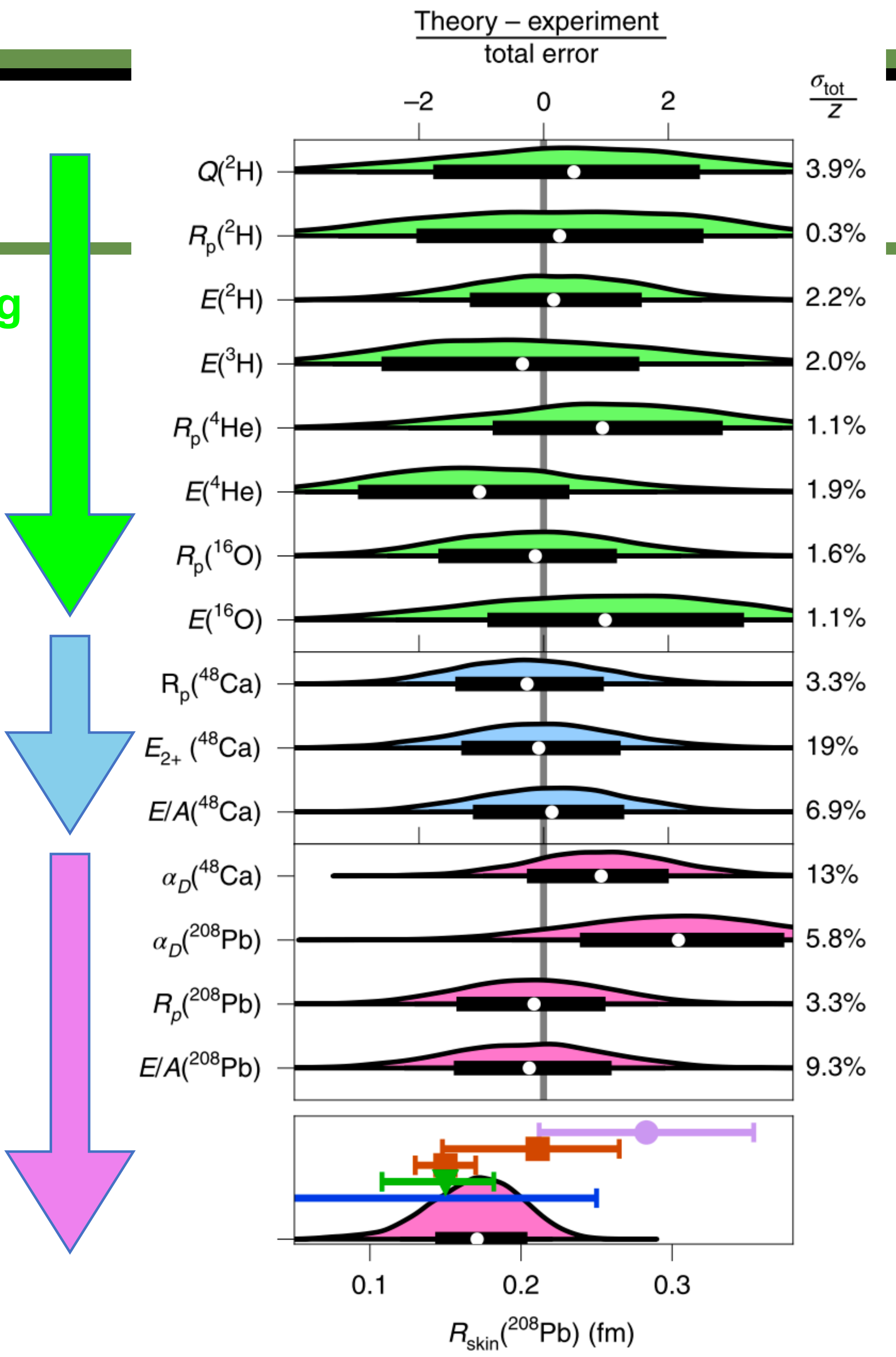
Observable	median	68% CR	90% CR
$R_{\mathrm{skin}}(^{48}\mathrm{Ca})$	0.164	$[0.141, 0.187]$	$[0.123, 0.199]$
$R_{\mathrm{skin}}(^{208}\mathrm{Pb})$	0.171	$[0.139, 0.200]$	$[0.120, 0.221]$

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

History matching

Calibration

Validation
Prediction



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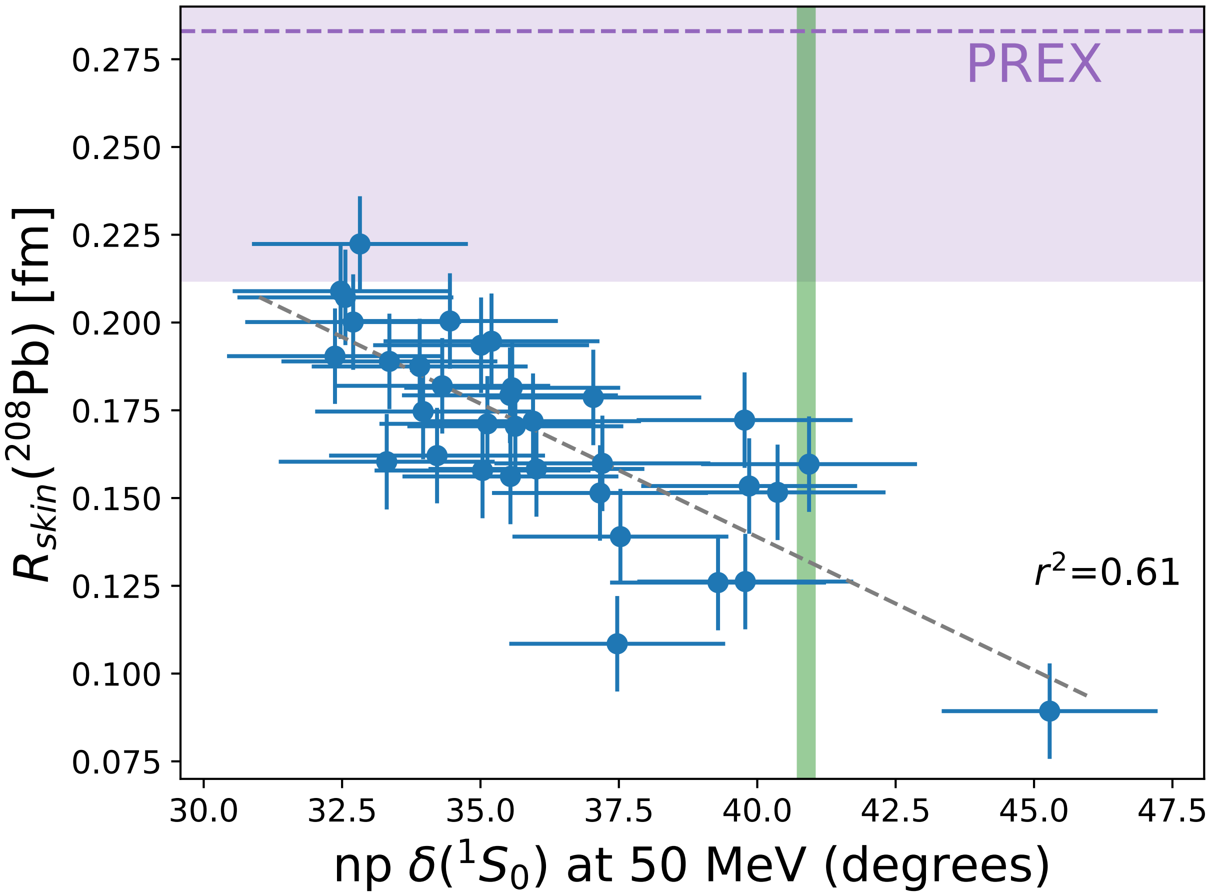

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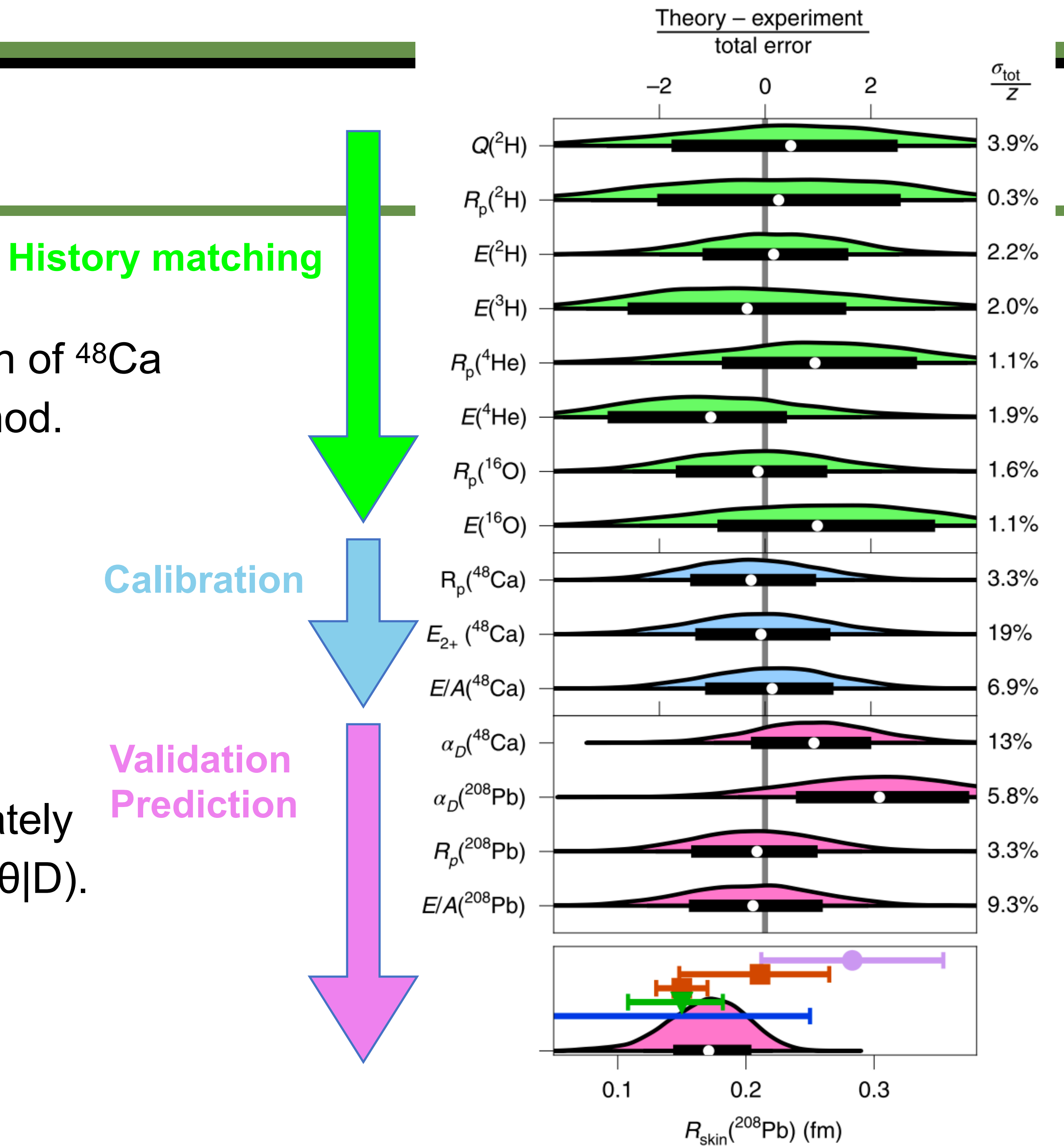
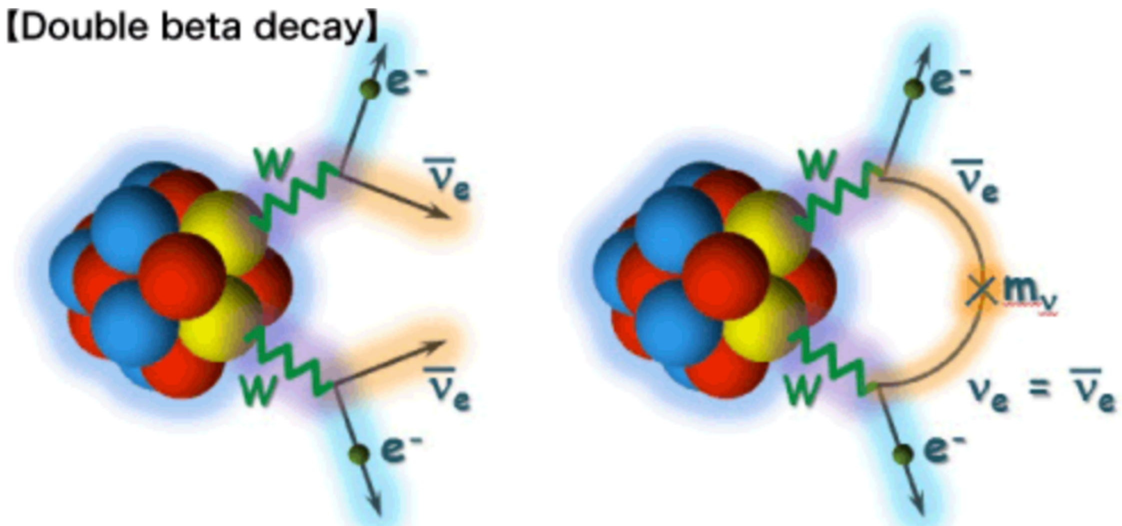
θ|D).



Neutrinoless double-beta decay

- Hypothetic process: it can happen only if the neutrino is its own antiparticle.
- Lepton number violation: 2n → 2p + 2e (0 → 2)
- Nature of neutrino

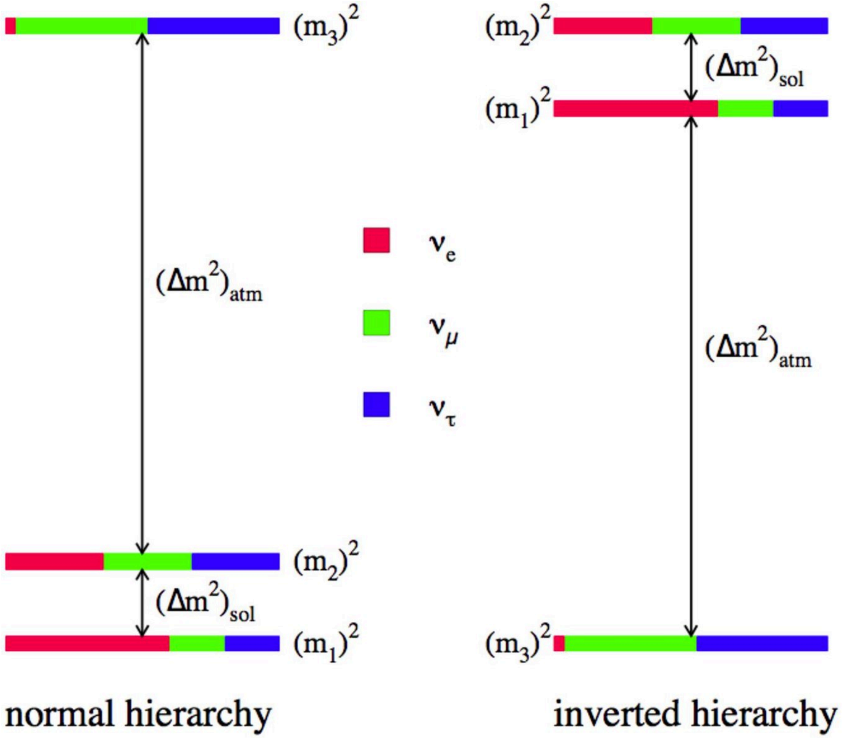
$\Delta m_{21}^2 \sim 7.5 \times 10^{-5}$ eV^2
$|\Delta m_{32}^2| \sim 2.4 \times 10^{-3}$ eV^2



Double beta decay
which emits anti-neutrinos

Neutrinoless
double beta decay

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



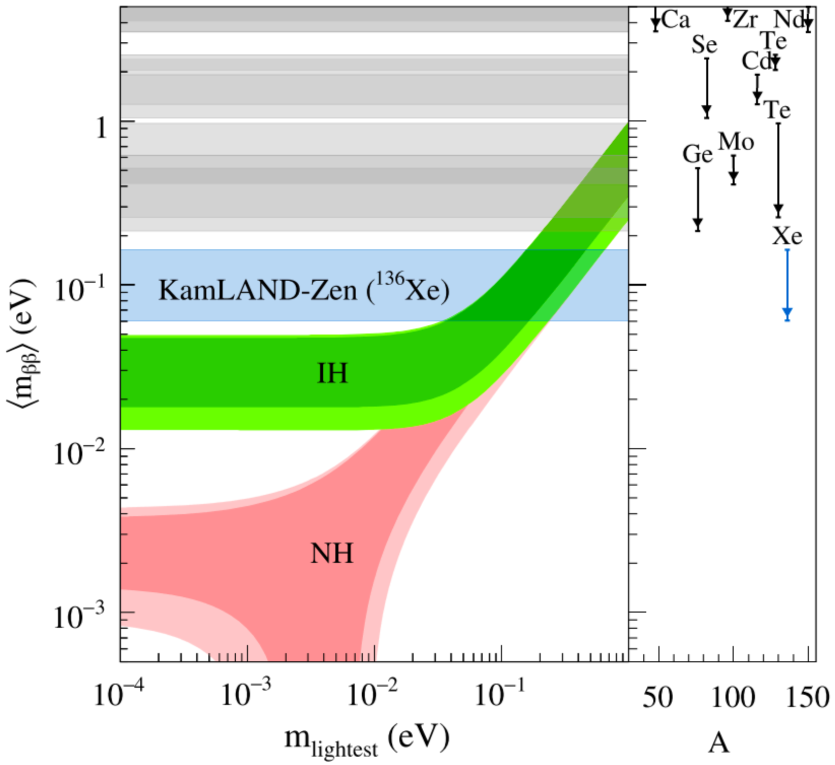
Neutrinoless double-beta decay

- Half-life formula:

$$(T^{0\nu\beta\beta})^{-1} = G^{0\nu}|M^{0\nu}|^2\langle m_{\beta\beta}\rangle^2, \quad \langle m_{\beta\beta}\rangle = \left|\sum_i U_{ei} m_i\right|$$

- $G^{0\nu}$: phase-space factor; known
- $M^{0\nu}$: nuclear matrix element; only theoretically available
- $<m_{\beta\beta}>$: absolute mass scale; unknown

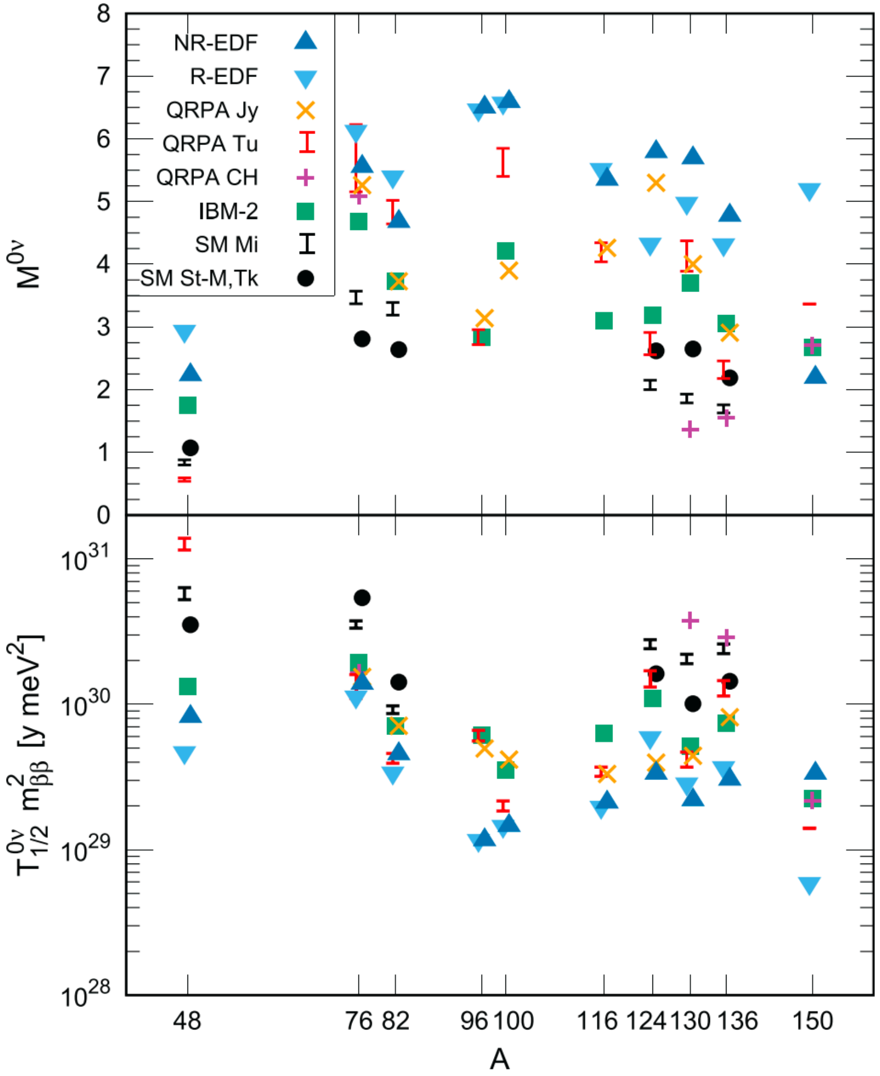
- We need $M^{0\nu}$ as precise as possible.



A. Gando et al., Phys. Rev. Lett. 117, 082503 (2016).

Nuclear Matrix Element (NME)

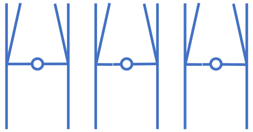
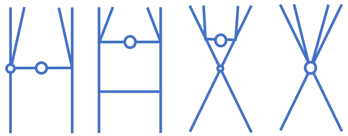
- Different theories provide different results
- Spread of theory results is factor 3
  - ✦ Meaning of the spread is unclear…
- A theoretical calculation with quantified uncertainty
  - ✤ Reasonable starting nuclear Hamiltonian(s)
  - ✤ Controllable many-body method(s)
  - ✤ Operators



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

Neutrinoless double-beta decay operator

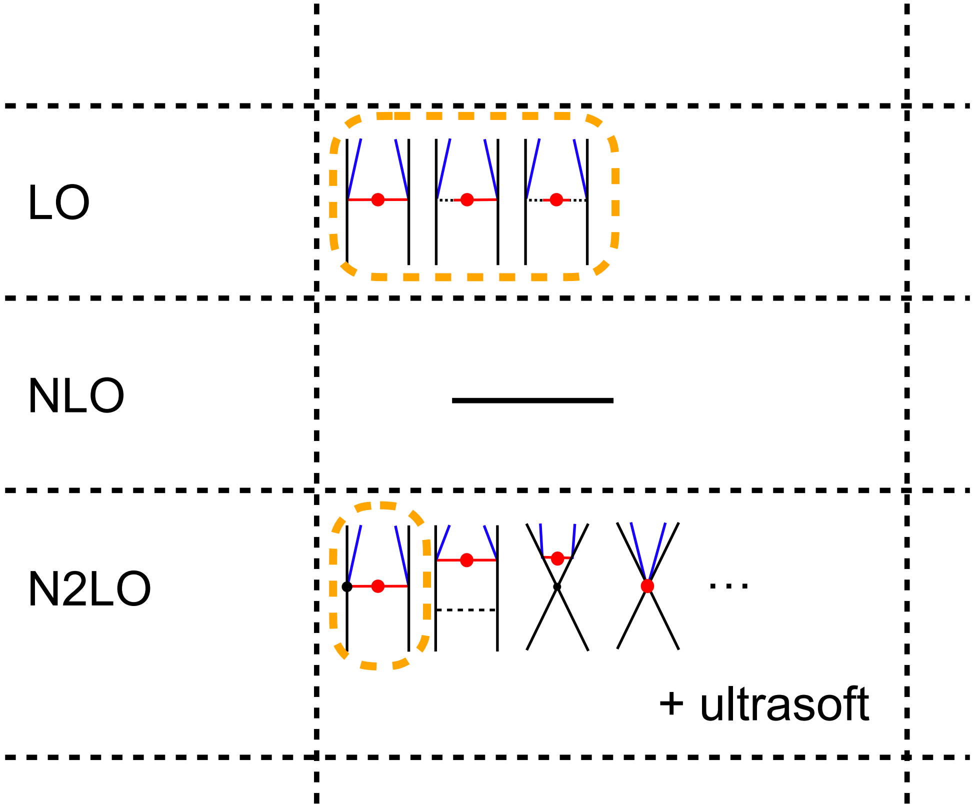
- Chiral EFT allows us a systematic expansion in lepton number violated sector.

LO	
NLO	—
N2LO	 ⋯ + ultrasoft

V. Cirigliano et al. Phys. Rev. C 97, 065501 (2018).

Neutrinoless double-beta decay operator

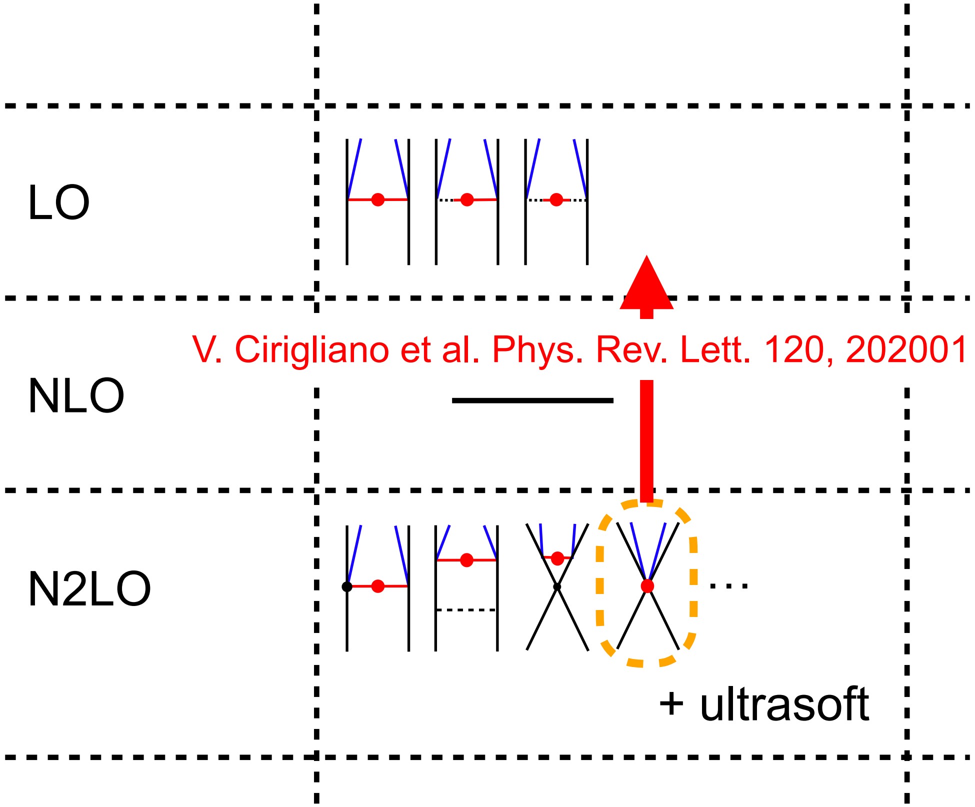
- Chiral EFT allows us a systematic expansion in lepton number violated sector.
  - Long-range contributions are the same as widely used contributions if the denominator energy is appropriately shifted.



V. Cirigliano et al. Phys. Rev. C 97, 065501 (2018).

Neutrinoless double-beta decay operator

- Chiral EFT allows us a systematic expansion in lepton number violated sector.
  - Long-range contributions are the same as widely used contributions if the denominator energy is appropriately shifted.
  - Short-range contact contribution

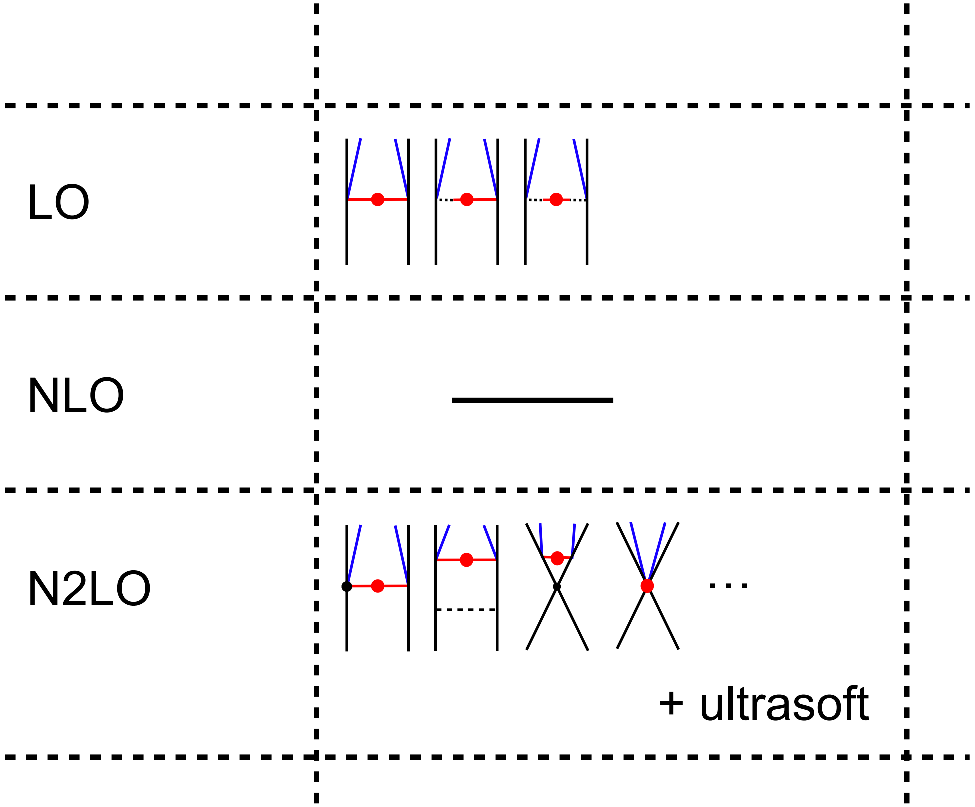


V. Cirigliano et al. Phys. Rev. Lett. 120, 202001 (2018).

V. Cirigliano et al. Phys. Rev. C 97, 065501 (2018).

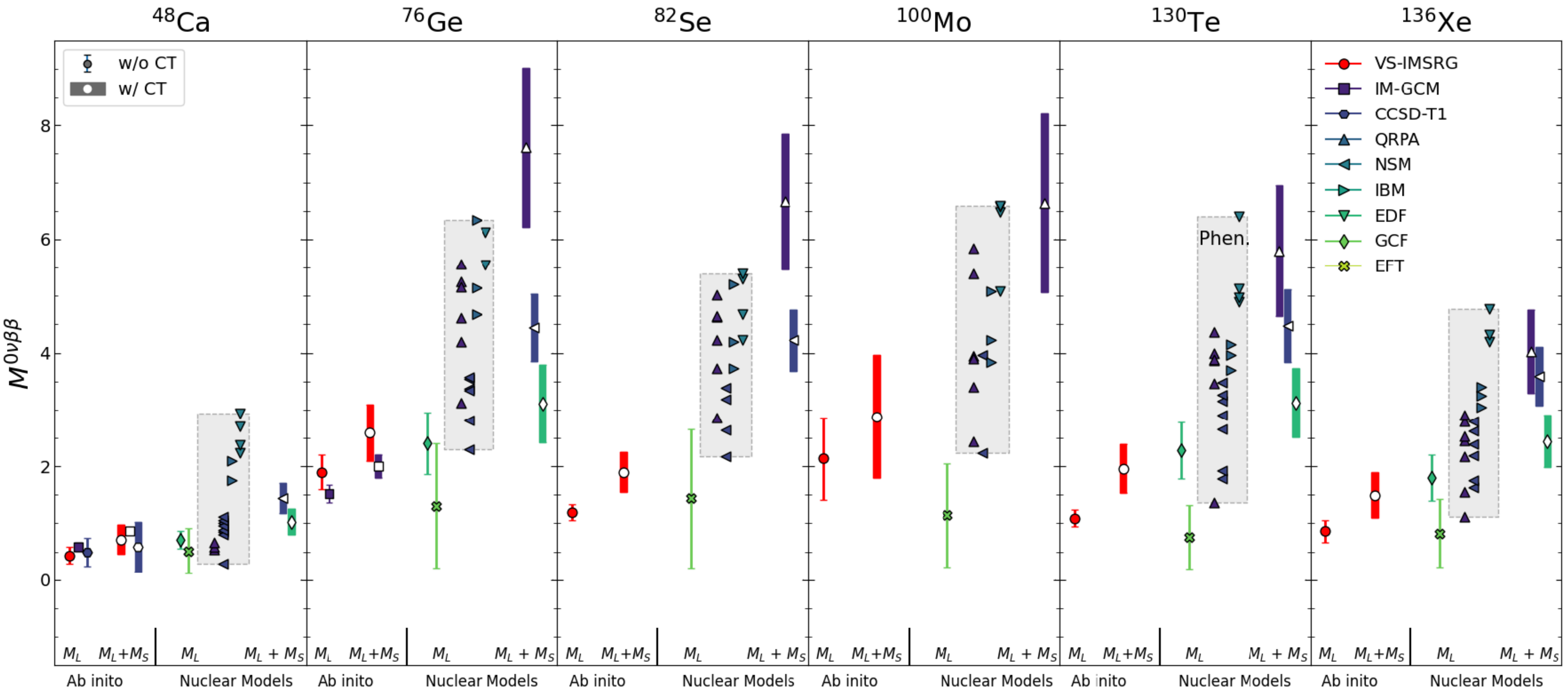
Neutrinoless double-beta decay operator

- Chiral EFT allows us a systematic expansion in lepton number violated sector.
  - Long-range contributions are the same as widely used contributions if the denominator energy is appropriately shifted.
  - Short-range contact contribution
  - Loop contributions that cannot be absorbed into corrections of form factors.
  - Ultrasoft contributions depends on structure of the intermediate nucleus.



V. Cirigliano et al. Phys. Rev. C 97, 065501 (2018).

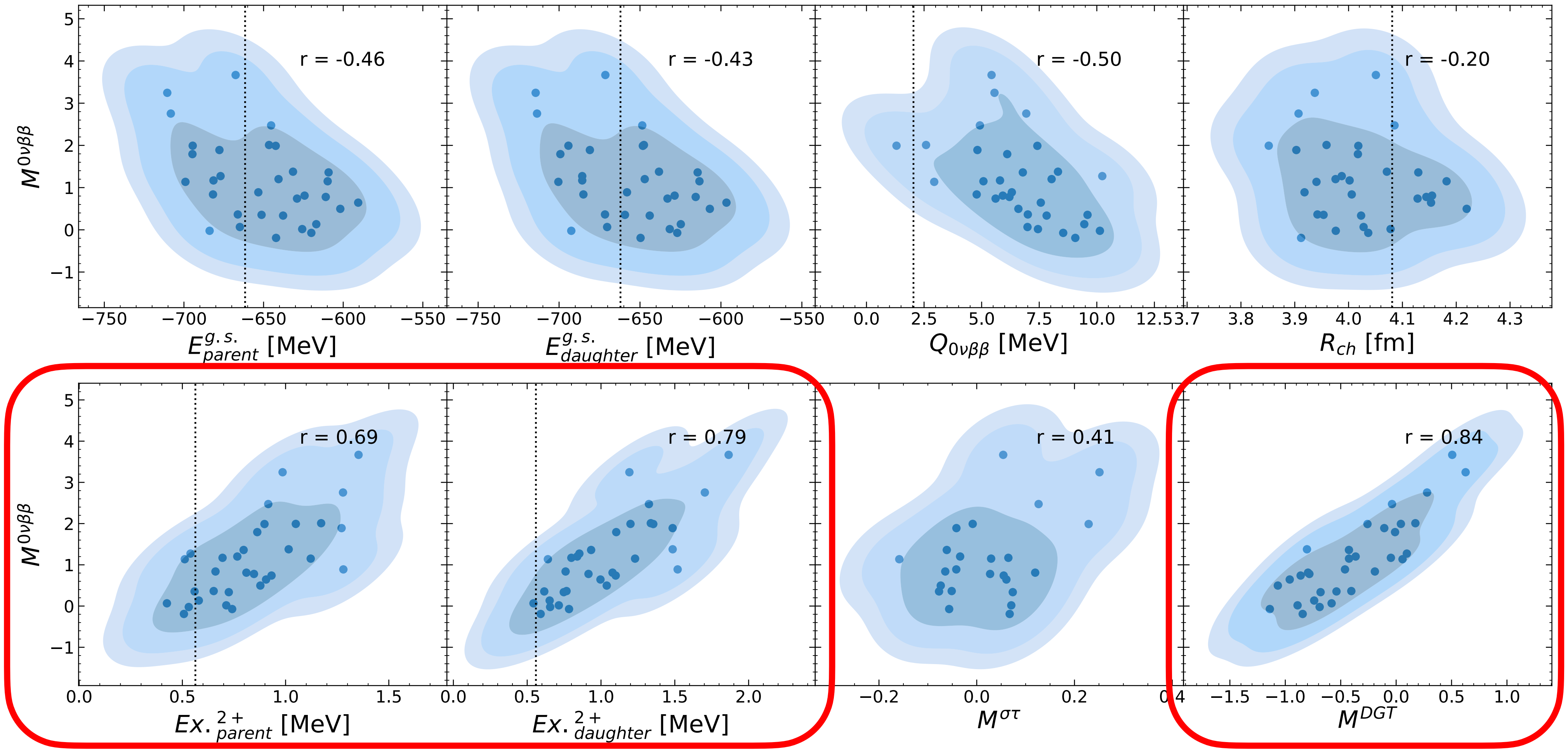
Computed NME



A Belley et al., arXiv:2307.15156.

*Uncertainty is not fully quantified

Correlation: different interaction parameter sets

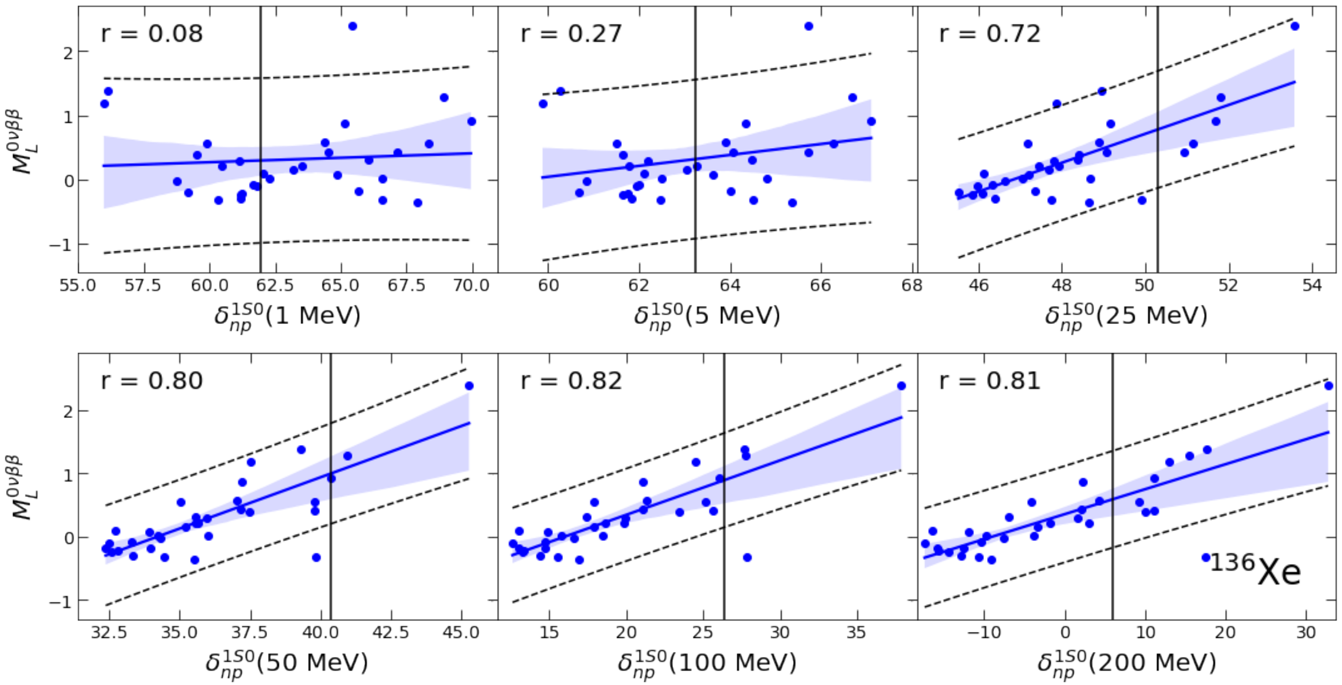


^{76}Ge

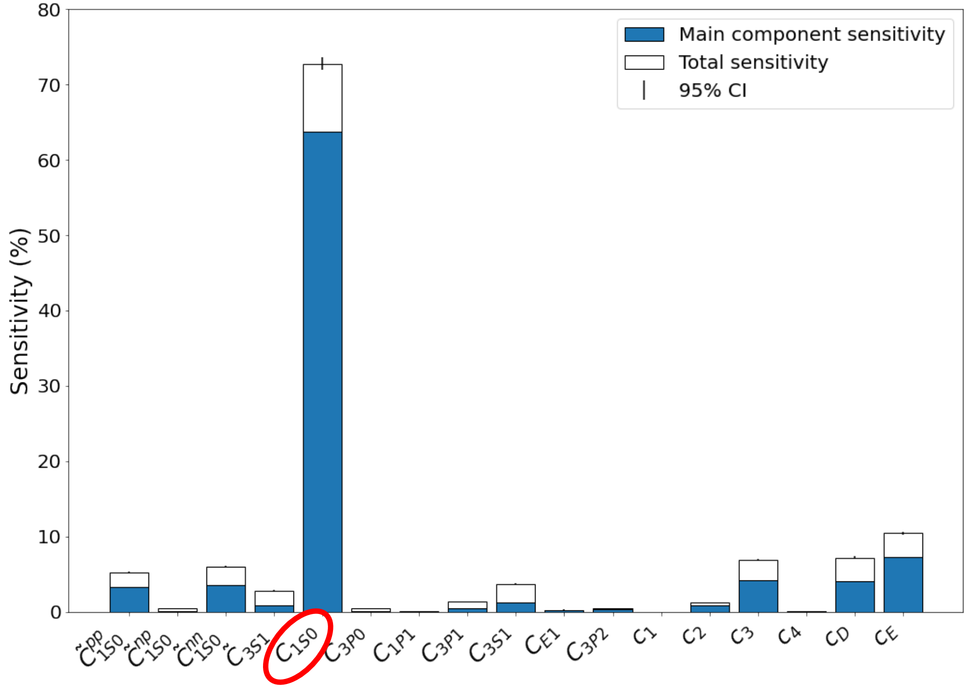
* correlation with 2^{+} energy is so far only seen in ^{76}Ge case.

A. Belley et al., arXiv: 2210.05809

Correlation: different interaction parameter sets



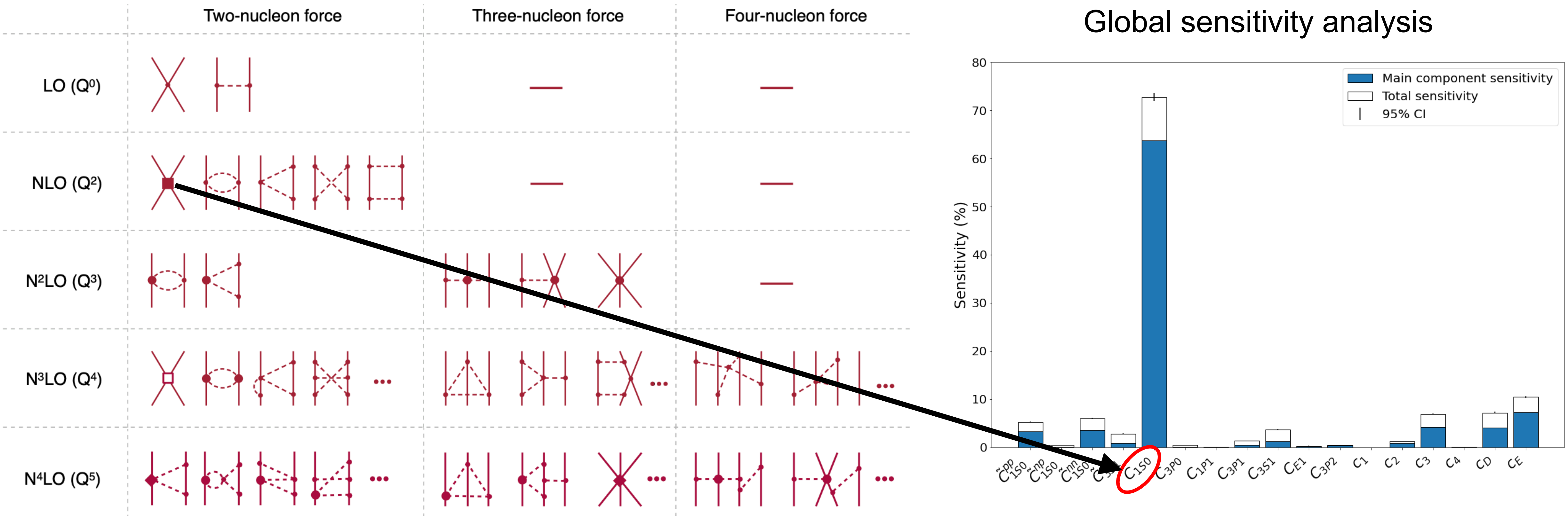
Global sensitivity analysis



Intermediate-energy phase shift can constrain the NME.

A. Belley et al., Phys. Rev. C 113, 014319 (2026).

Correlation: different interaction parameter sets

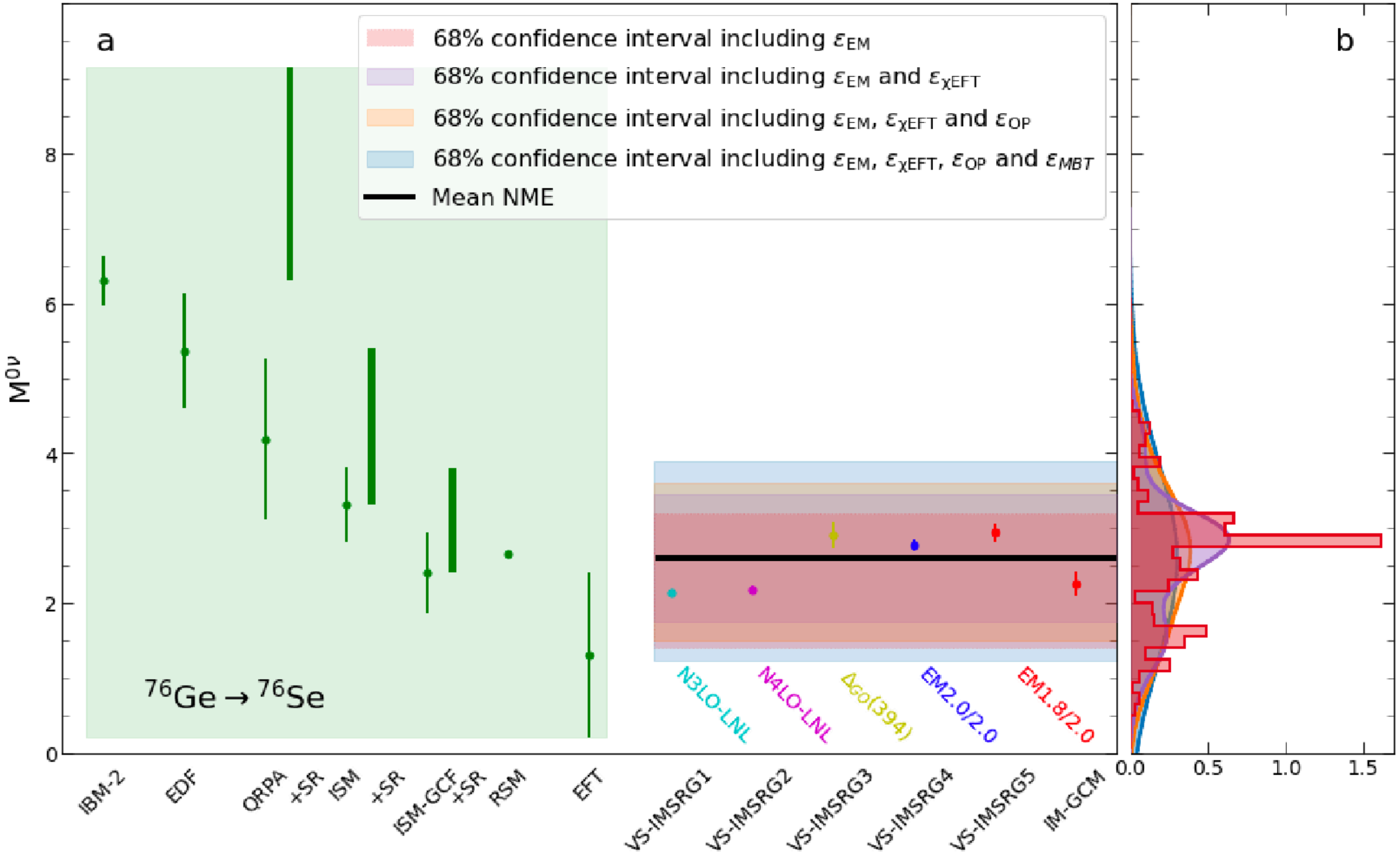


Intermediate-energy phase shift can constrain the NME.

A. Belley et al., Phys. Rev. C 113, 014319 (2026).

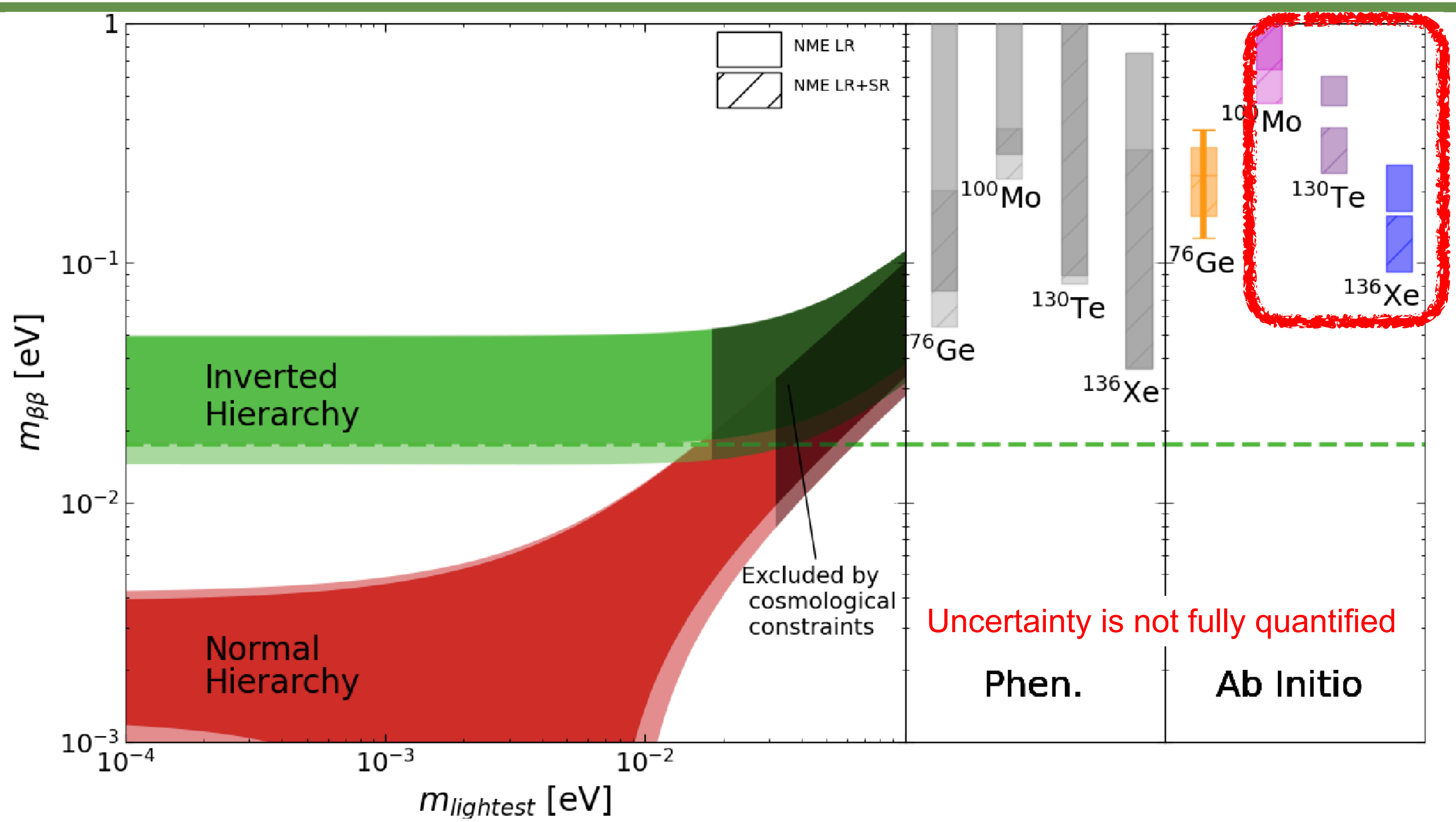
A better uncertainty quantification

- Uncertainties:
    - Interactions
        - Parameter uncertainty
        - EFT truncation
    - Operator
        - Closure approximation
        - Contact strength
    - Many-body methods
        - VS-IMSRG
        - IM-GCM
    - Emulator



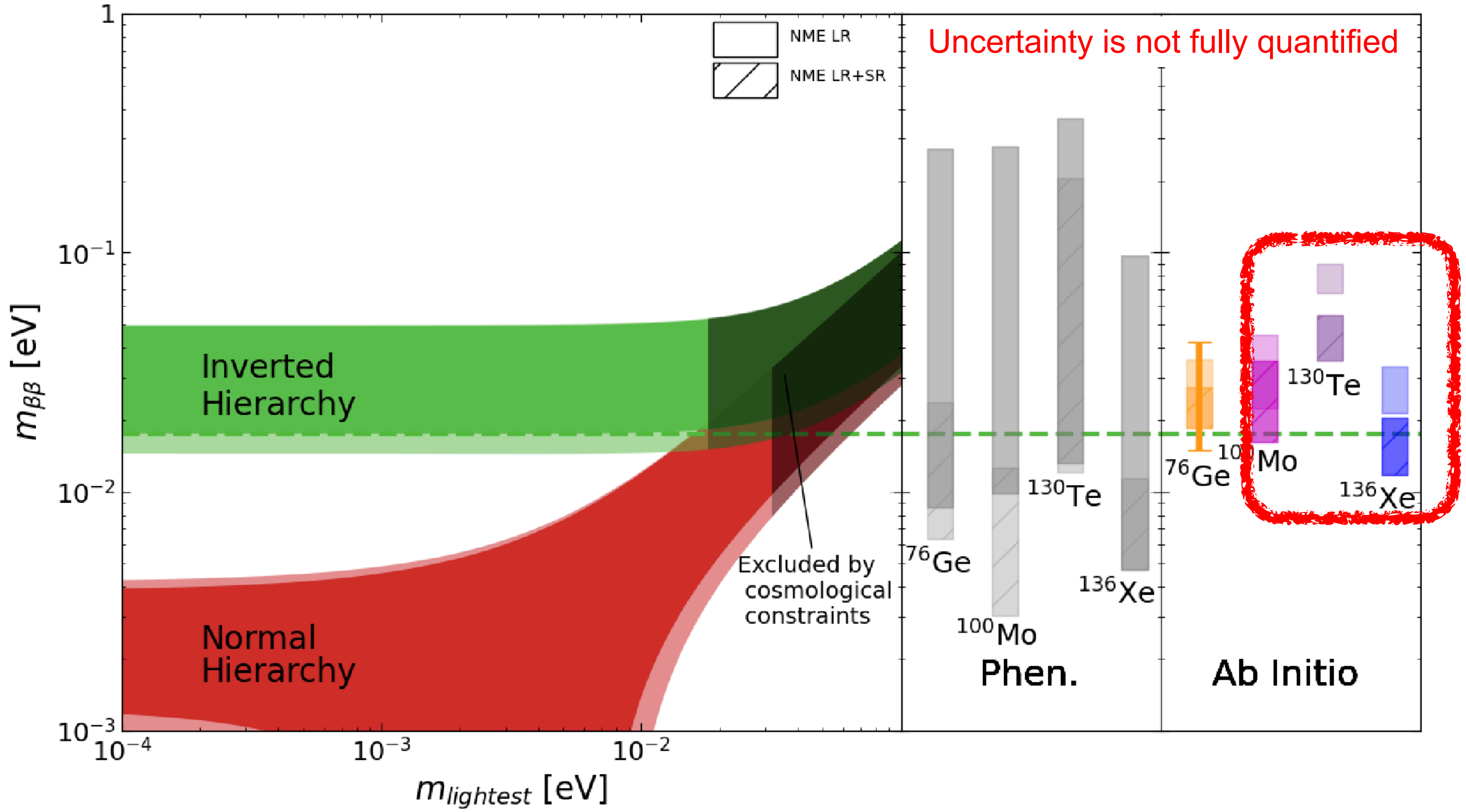
A. Belley et al., Phys. Rev. Lett. 132, 182502 (2024).

Effect on experimental limits



Experimental limits: GERDA (^{76}Ge) Phys. Rev. Lett. 125, 252502, CUPID-Mo (^{100}Mo) Eur. Phys. J. C 82 11, 1033 CUORE(^{130}Te) Nature 604, 53–58, and Kamland Zen (^{136}Xe) Phys. Rev. Lett. 130, 051801.

Effect on future research



Expected limits: LEGEND (^{76}Ge) arXiv:2107.11462,
CUPID (^{100}Mo) arXiv:1907.09376, SNO+(^{130}Te) arXiv:2104.11687and nEXO (^{136}Xe) J. Phys .G 49 1, 015104.

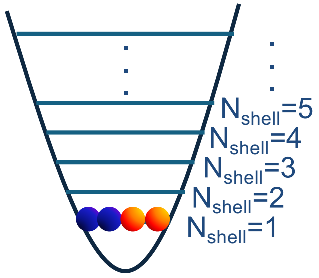
FCI activity @ Tsukuba

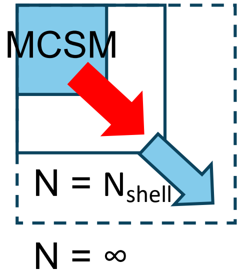
筑波大学
計算科学研究センター
Center for Computational Sciences

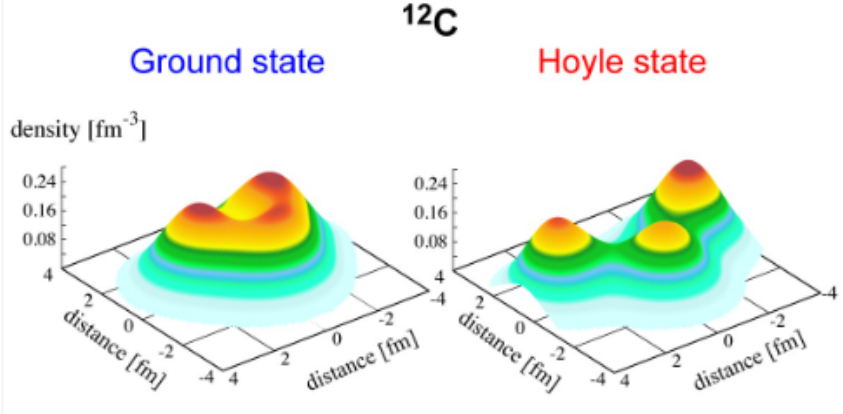
CC and IMSRG are not perfect → a benchmark with an exact method

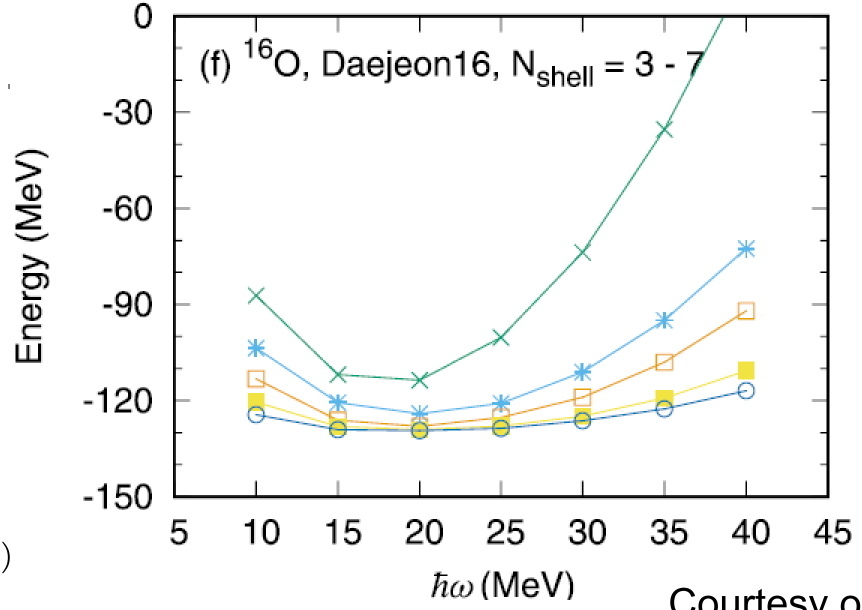
no-core Monte Carlo Shell Model (no-core MCSM)

- Full configuration interaction (FCI) approach
- Harmonic Oscillator basis, Nshell=7 and extrapolation to Nshell→ ∞
- light nuclei up to ^{20}Ne
- Daejeon16 / JISP16 interaction (soft 2-body interaction with minimizing 3-body-force effect).







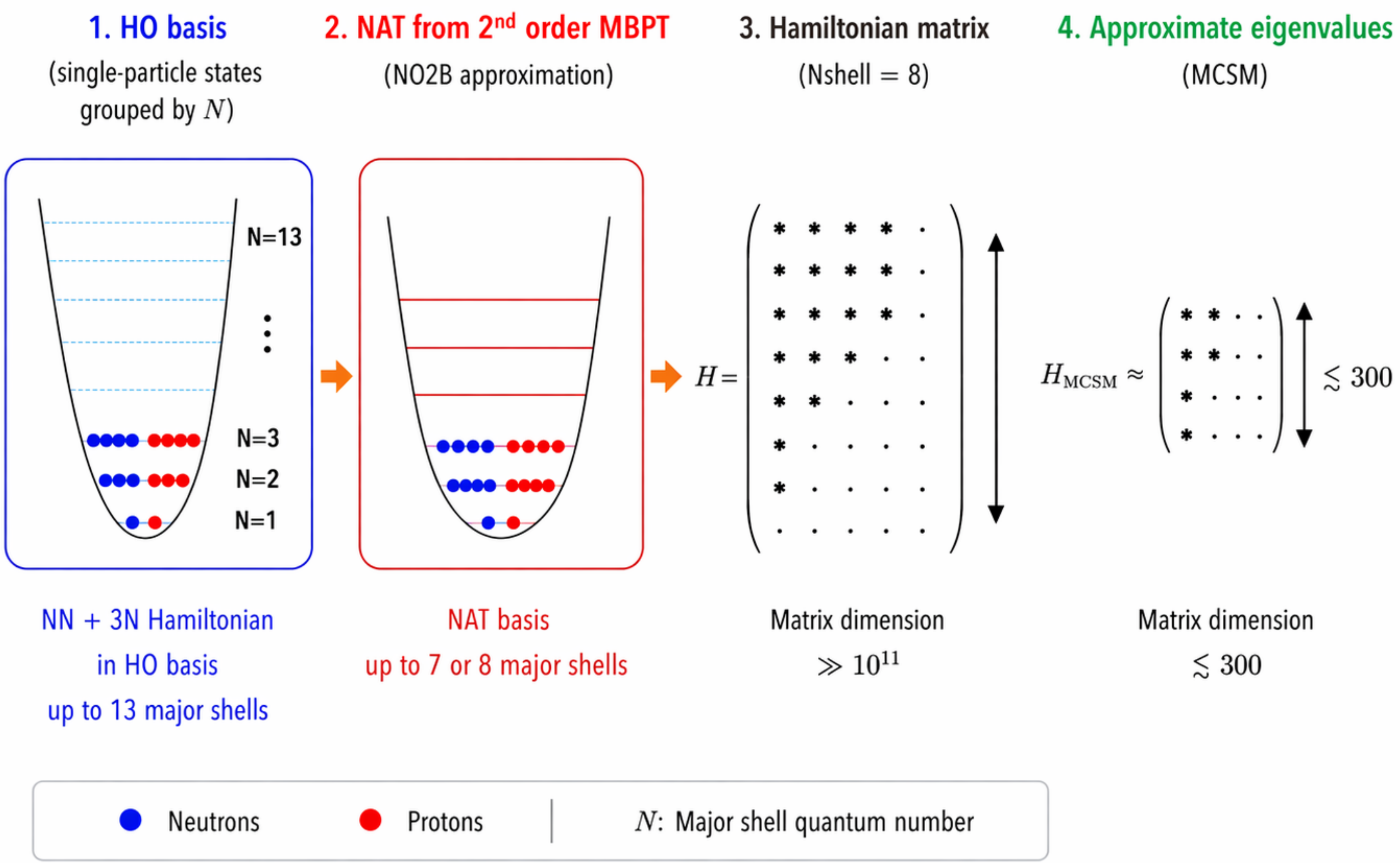


T. Abe, P. Maris *et al.,* Phys. Rev. C 104, 054315 (2021)
T. Otsuka, T. Abe *et al.,* Nat. Comm. 13, 2234 (2022)

Courtesy of N. Shimizu

FCI activity @ Tsukuba

Natural orbitals + no-core MCSM procedure



1. HO basis
(single-particle states grouped by N)

2. NAT from 2nd order MBPT
(NO2B approximation)

3. Hamiltonian matrix
(Nshell = 8)

4. Approximate eigenvalues
(MCSM)

NN + 3N Hamiltonian
in HO basis
up to 13 major shells

NAT basis
up to 7 or 8 major shells

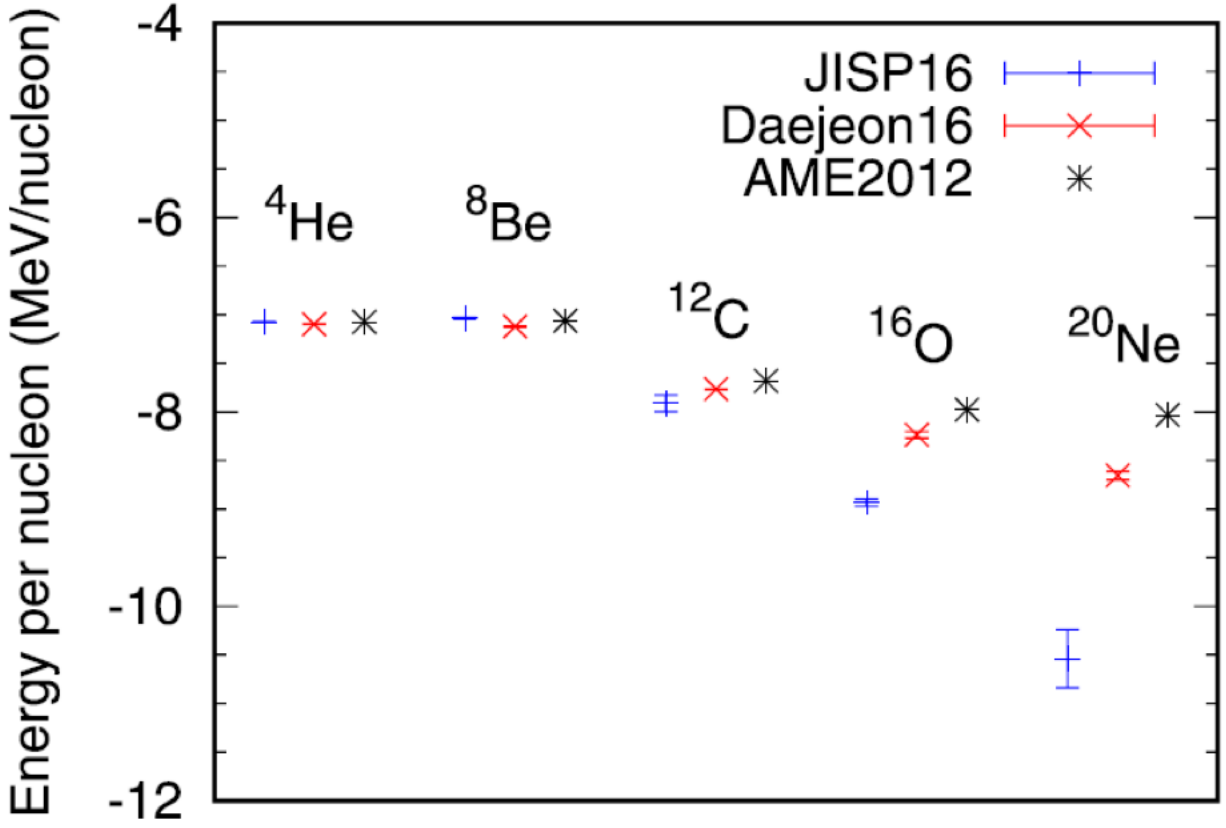
Matrix dimension
$\gg 10^{11}$

Matrix dimension
$\lesssim 300$

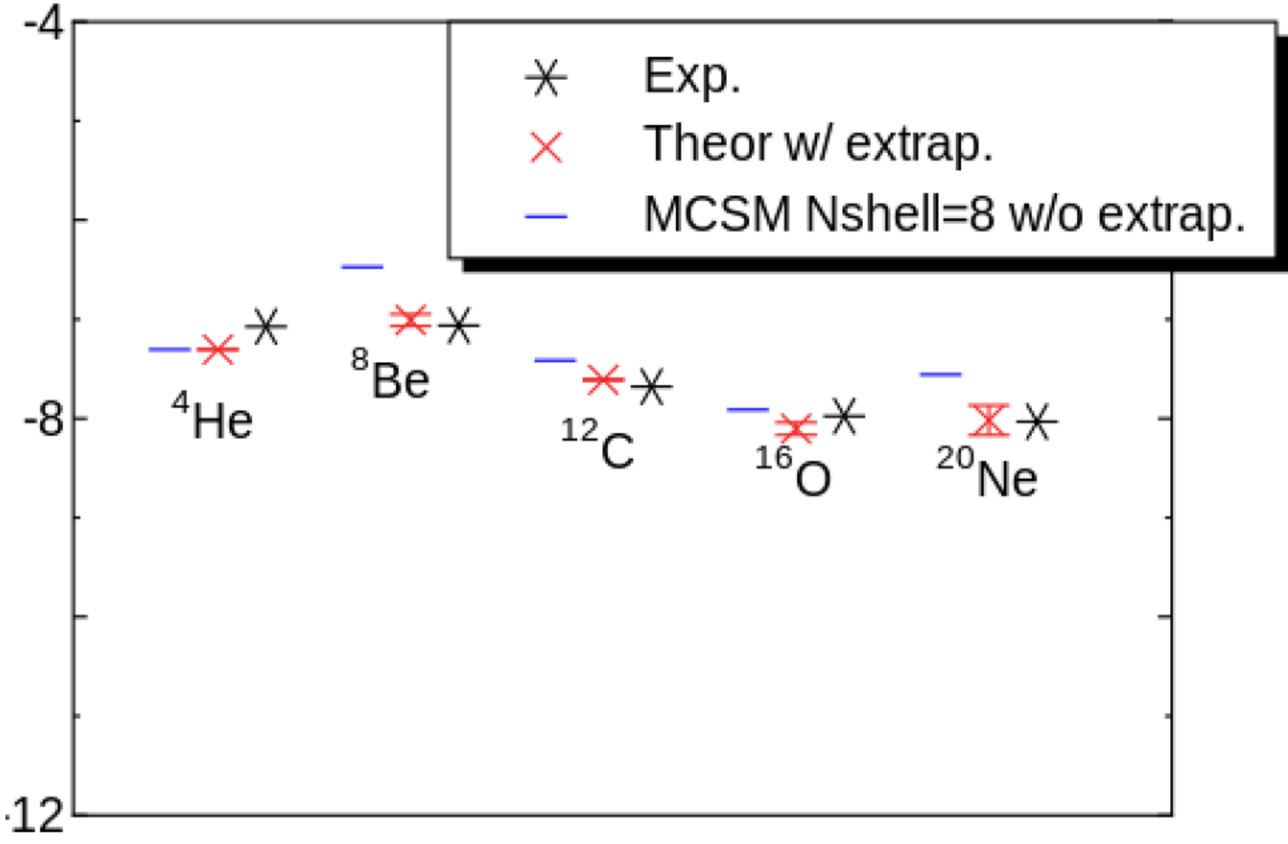
FCI activity @ Tsukuba

Daejeon16 and JISP16

T. Abe *et al.*, Phys. Rev. C 104, 054315 (2021)



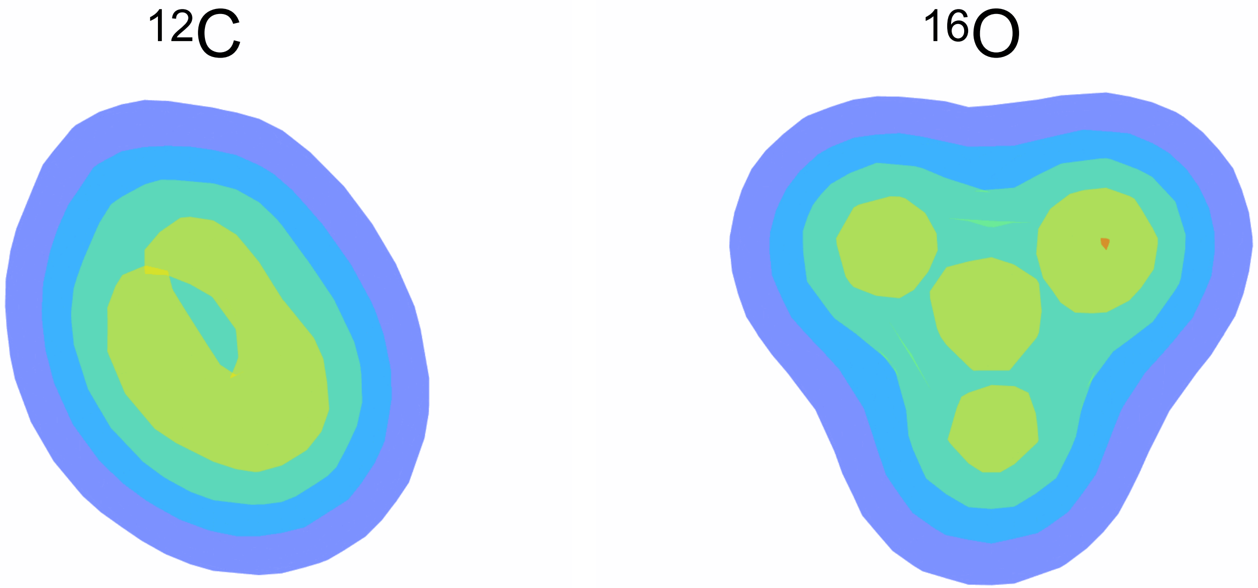
Present : chiral EFT 1.8/2.0 (EM) + NO2B approx.



Visualization MCSM density

- MCSM yields a good angular momentum state, and the shape would look like spherical (Lab frame w.f.)
- Intrinsic w. f.: $|\Phi_{\mathrm{intr}}\rangle \equiv \sum_{n=1}^{N_{\mathrm{basis}}} f_n R(\Omega_n)|\phi_n\rangle, \quad f_n \quad : \text{diagonalization coefficient}, \quad |\phi_n\rangle : \text{MCSM basis state}$
- The Euler's angle Ω_n

  → diagonalize Q-moment.
- Visualization of Intrinsic frame density



Visualization was done by Y. Tsunoda

N. Shimizu et al., PTEP, 01A205 (2012).
R. B. Wiringa et al., Phys. Rev. C 62, 014001 (2000).

Summary

- A reliable theoretical prediction is strongly desired
  - Uncertainty quantification is essential
  - A key ingredient is a (unbiased & strong) correlation between the target and calibration observables.

- Nuclear structure & electroweak observables to test a theory
  - Chiral EFT provides a consistent expansion in both Hamiltonian & operators

- Next challenges
  - Capturing physics for collective phenomena with VS-IMSRG
  - Calibrating BSM and astrophysics inputs with HIC data?
  - …

A. Kumar et al., Phys. Lett. B 874, 140184 (2026).

$$P(\tilde{D}|D, I) = \int d\boldsymbol{\theta} P(\tilde{D}|\boldsymbol{\theta}, I) P(\boldsymbol{\theta}|D, I)$$