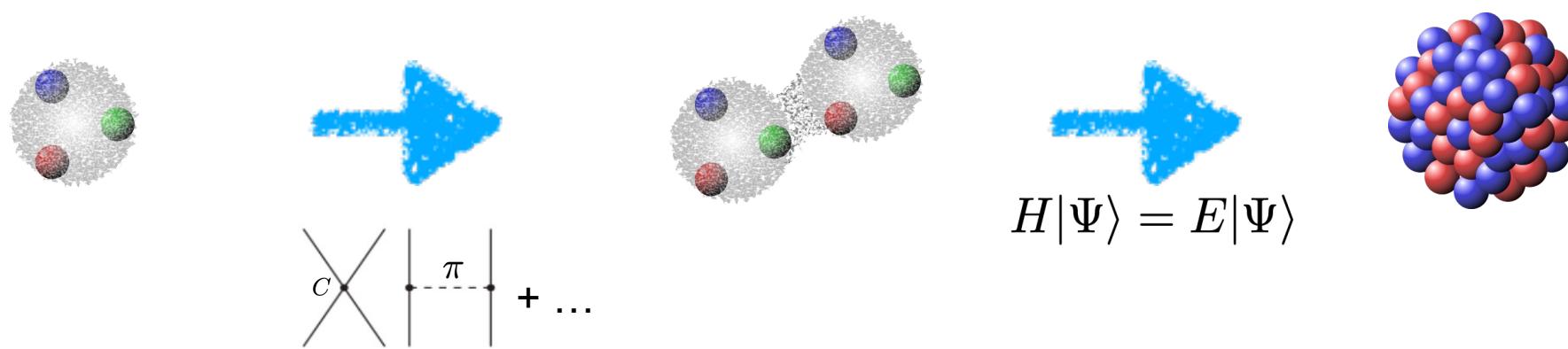


Recent advances in ab initio calculations of heavy nuclei



Supported by



Takayuki Miyagi

Collaborators



Chalmers University of Technology: **A. Ekström, C. Forssen**

Oak Ridge National Laboratory: **G. Hagen, Baishan Hu**

TRIUMF: **J. D. Holt, P. Navratil**

TU Darmstadt: **K. Hebeler**

University of Notre Dame: **S. R. Stroberg**

University of Mainz: **W. Jiang**

University of Tennessee: **T. Papenbrock, Z. Sun**

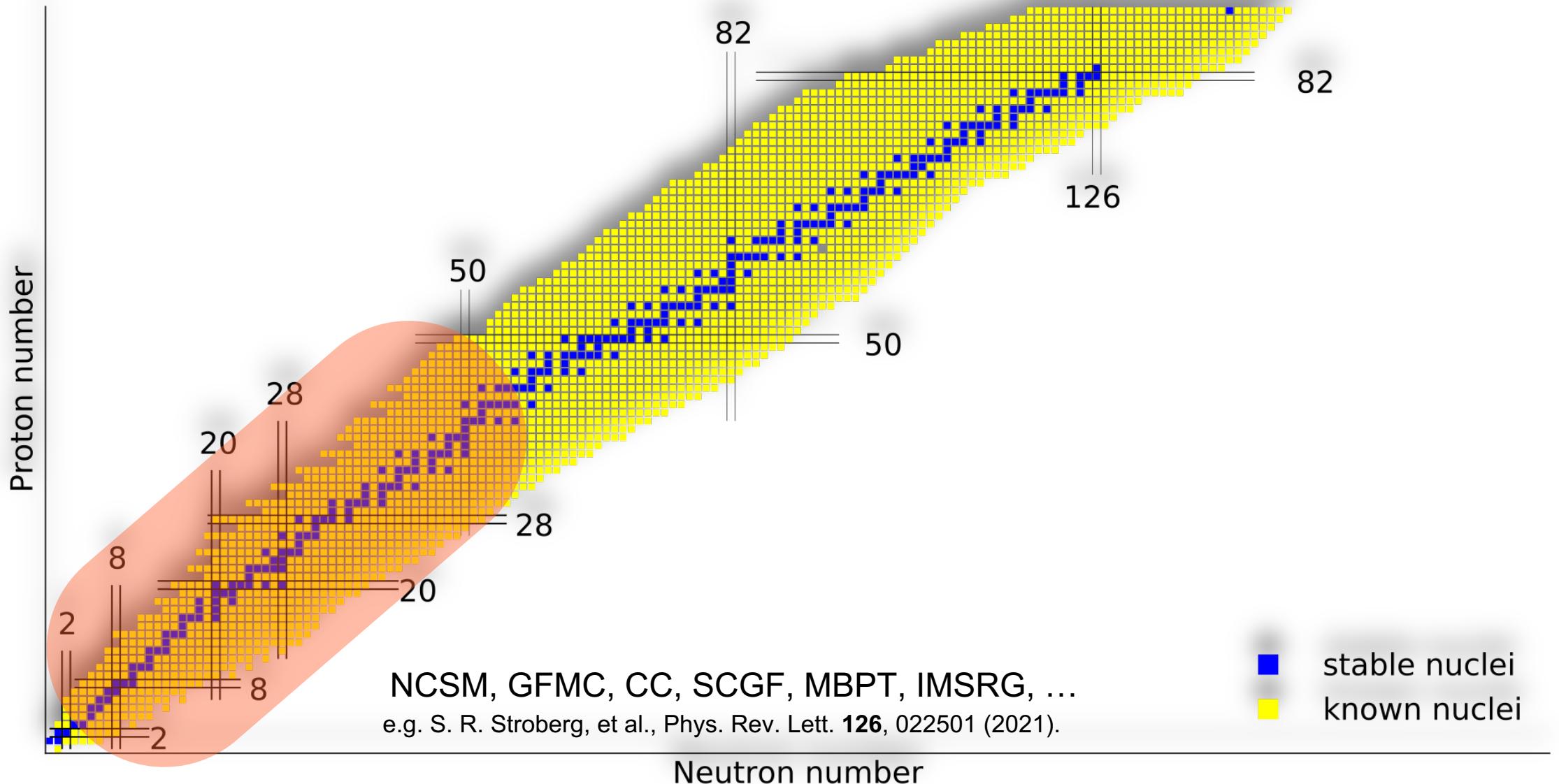
University of Durham: **I. Vernon**

Why heavy nuclei?

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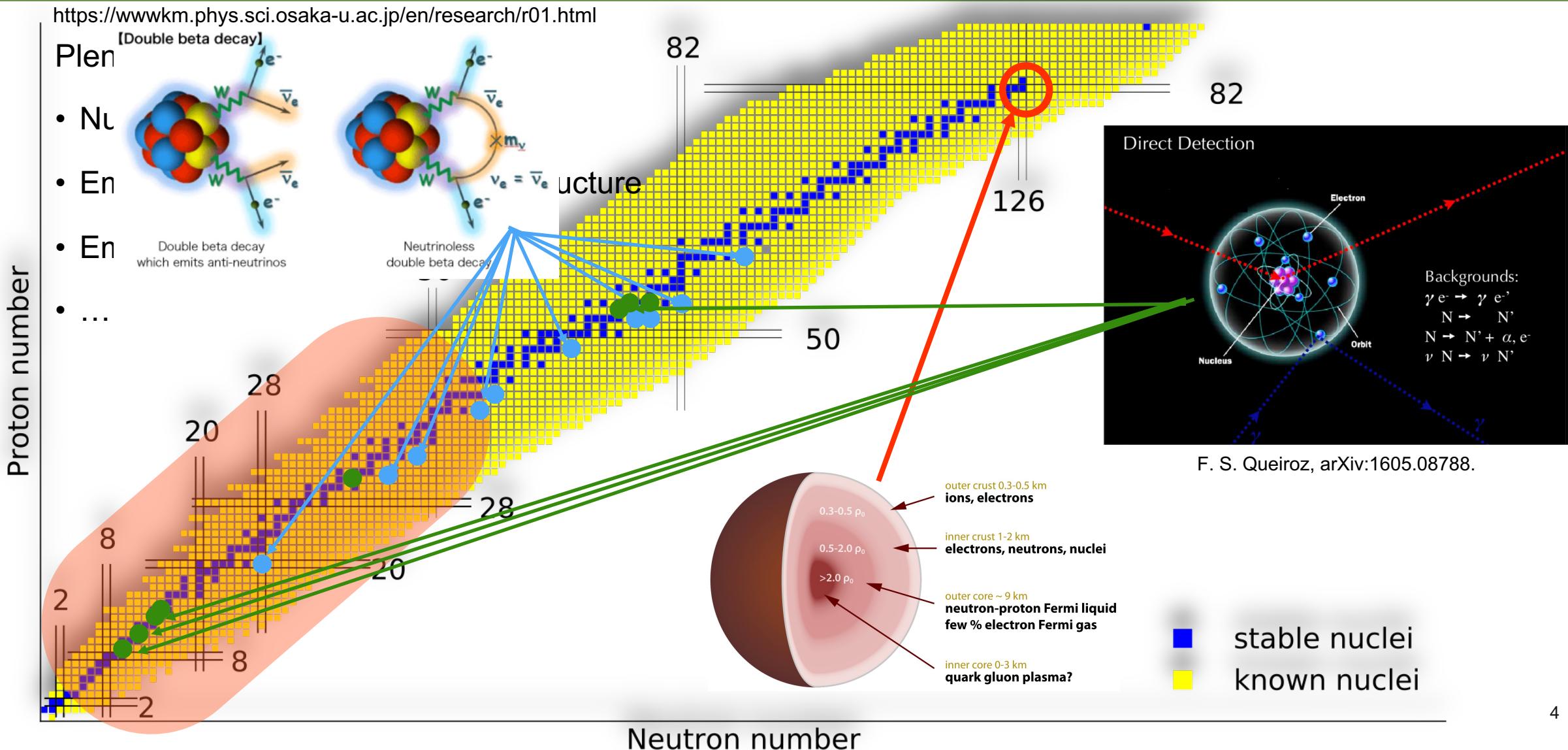
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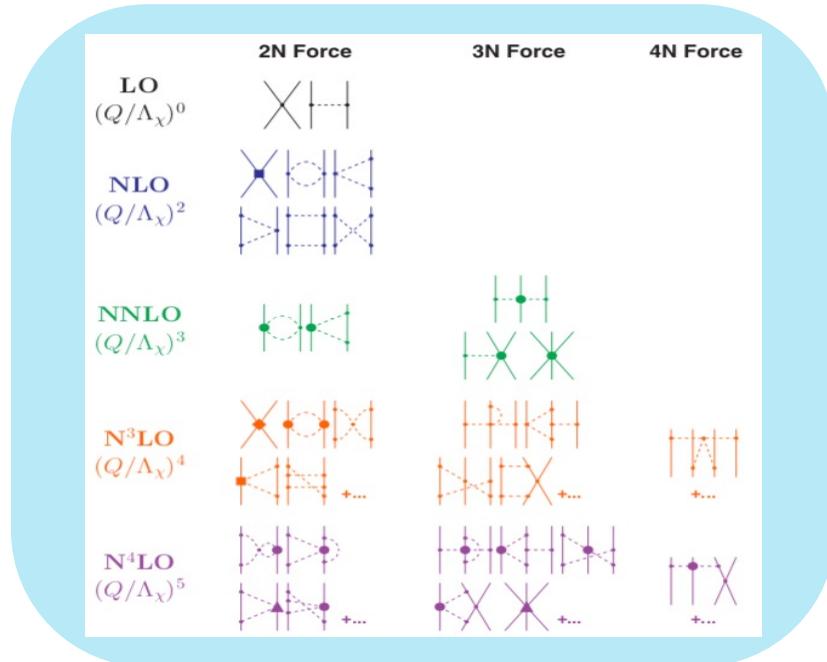
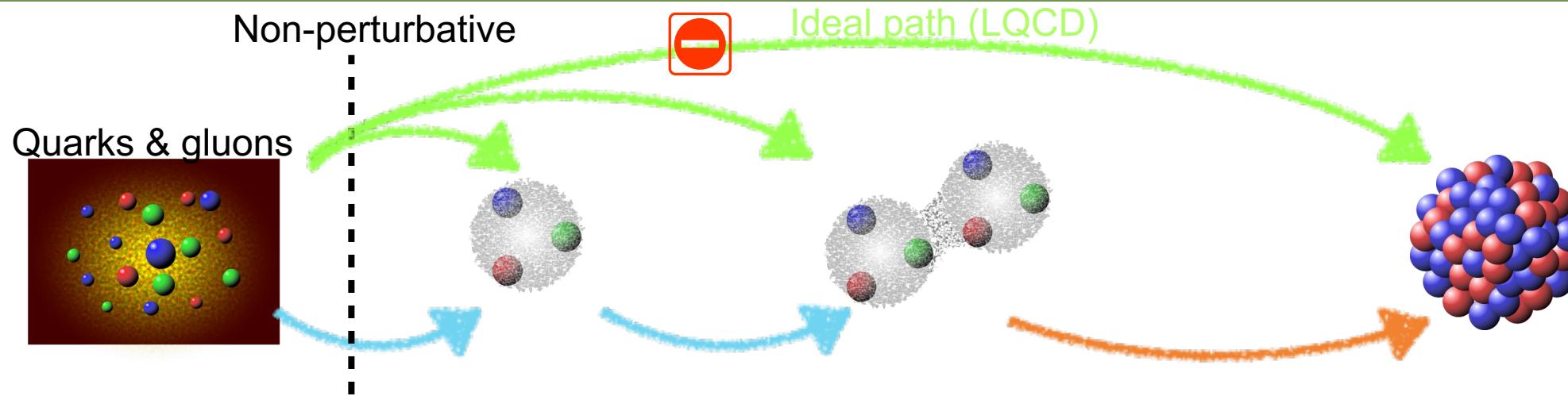
Why heavy nuclei?

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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

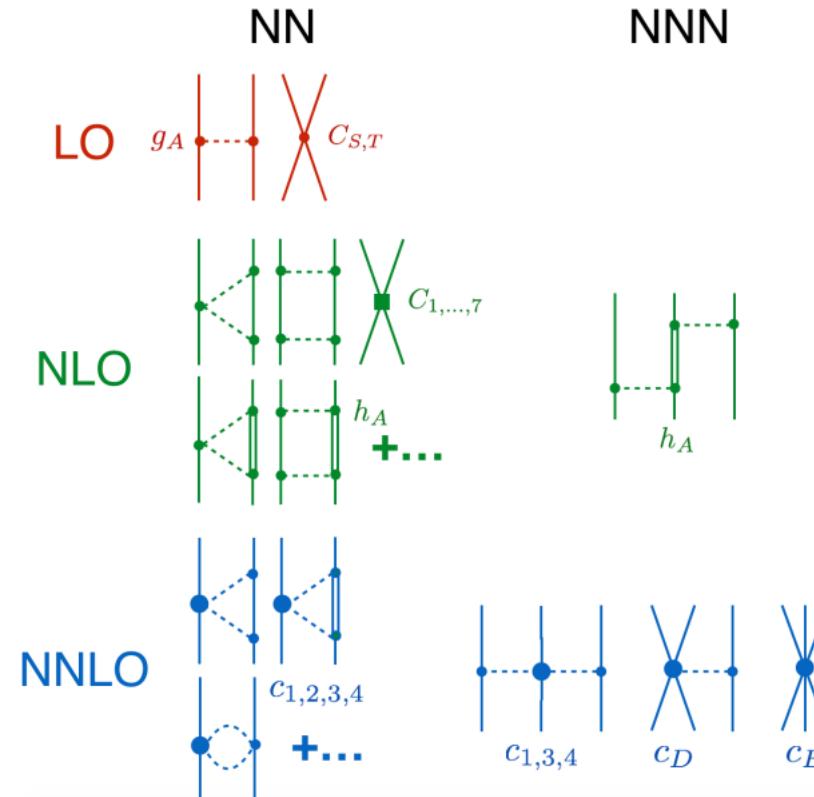
Weinberg, van Kolck, Kaiser, Epelbaum, Glöckle, Meißner, Entem, Machleidt, ...

Lagrangian construction

- ◆ Chiral symmetry
- ◆ Power counting

Systematic expansion

- ◆ Unknown LECs
- ◆ Many-body interactions
- ◆ Estimation of truncation error



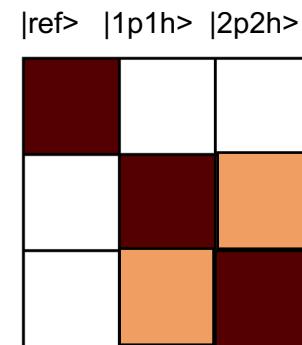
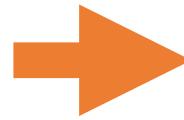
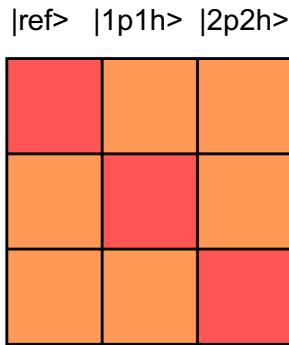
Taken from A. Ekström et al., Phys. Rev. C 97, 024332 (2018).

Many-body problem: similarity transformation methods

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Similarity transformation



How can we find Ω operator?

- ◆ Coupled-cluster method (CCM), in-medium similarity renormalization group (IMSRG), ...

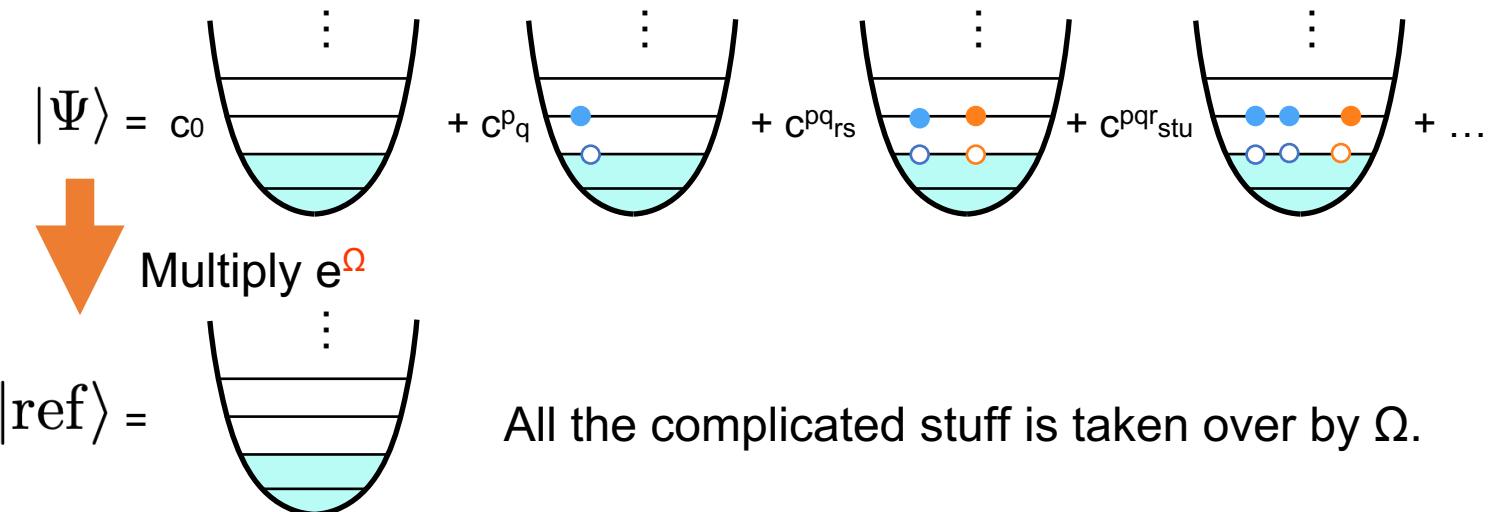
$$H|\Psi\rangle = E_{\text{g.s.}}|\Psi\rangle$$

$$e^{\Omega} H e^{-\Omega} e^{\Omega} |\Psi\rangle = E_{\text{g.s.}} e^{\Omega} |\Psi\rangle$$

$$\tilde{H}|\text{ref}\rangle = E_{\text{g.s.}}|\text{ref}\rangle$$

Multiply e^{Ω} to both side

Similarity transformation



In-medium similarity renormalization group approach

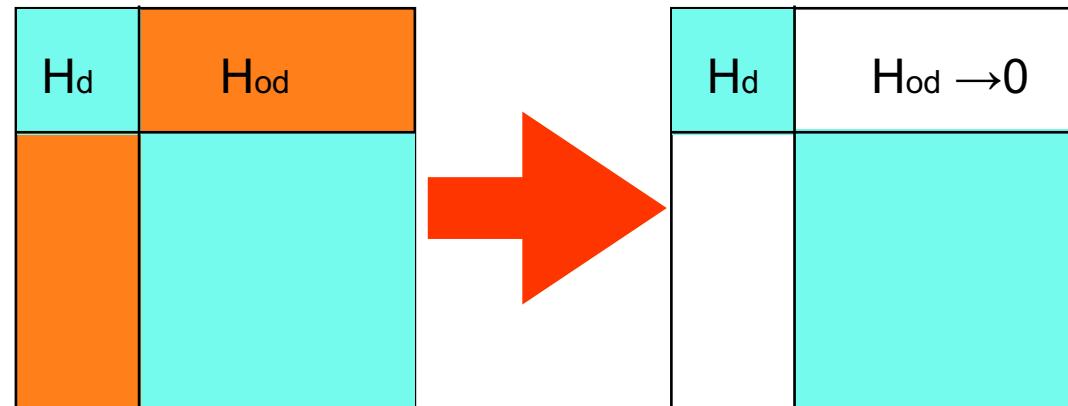
Similarity renormalization group

$$H(s) = U^\dagger(s) H(s=0) U(s)$$

$$\frac{dU(s)}{ds} = -\eta(s) U(s)$$

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

H. Hergert et al., Phys. Rep. 621, 165 (2016).
S. R. Stroberg et al., Annu. Rev. Nucl. Part. Sci. 69, 307 (2019).



The anti-Hermitian generator $\eta(s)$ is arbitrary.

How can we choose the functional form to suppress the off-diagonal MEs?

In-medium similarity renormalization group approach

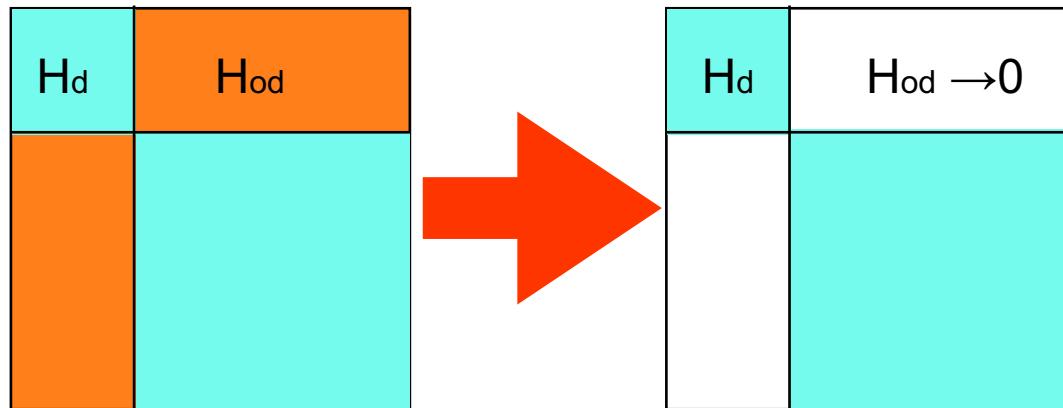
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S. R. Stroberg et al., Annu. Rev. Nucl. Part. Sci. 69, 307 (2019).



A simple example:

◆ 2 x 2 Hamiltonian

$$H(s) = \begin{pmatrix} c+z & x \\ x & c-z \end{pmatrix} = cI + z(s)\sigma_3 + x(s)\sigma_1 \quad \eta(s) = \frac{i}{2} \frac{x(s)}{z(s)} \sigma_2$$

$$\frac{dx(s)}{ds} = -x(s) \rightarrow x(s) = x(0) \exp(-s) \quad \text{Exponential decay of the off-diagonal ME.}$$

$$\text{note : } [\sigma_2, \sigma_3] = 2i\sigma_1$$

In-medium similarity renormalization group approach

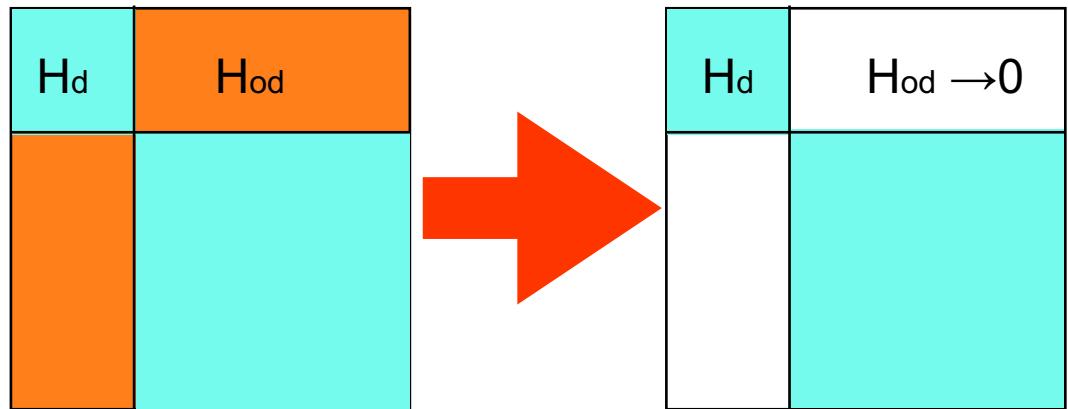
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An expect

$$\eta(s) = \frac{i}{2} \frac{x(s)\sigma_2}{z(s)}$$



Off-diagonal MEs need to be suppressed
Energy gap from the diagonal MEs

(Anti-Hermitian)

In-medium similarity renormalization group approach

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

$$H(s) = e^{\Omega(s)} H(s=0) e^{-\Omega(s)} \approx E(s) + \sum_{12} f_{12}(s) \{a_1^\dagger a_2\} + \frac{1}{4} \sum_{1234} \Gamma_{1234}(s) \{a_1^\dagger a_2^\dagger a_4 a_3\}$$

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

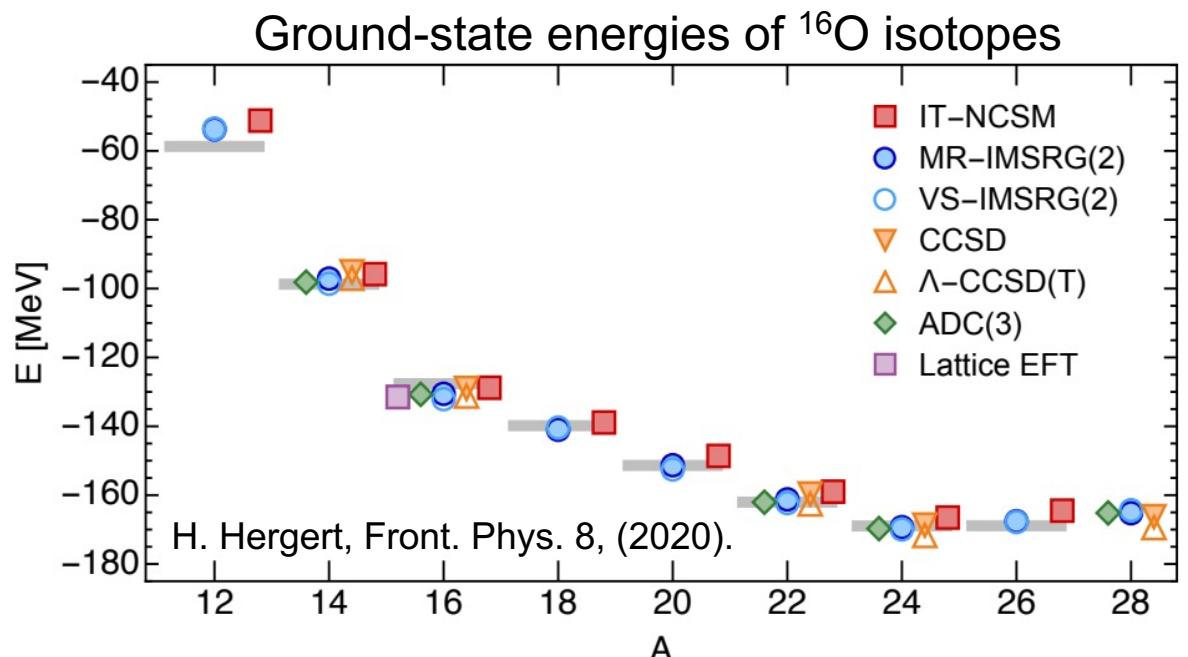
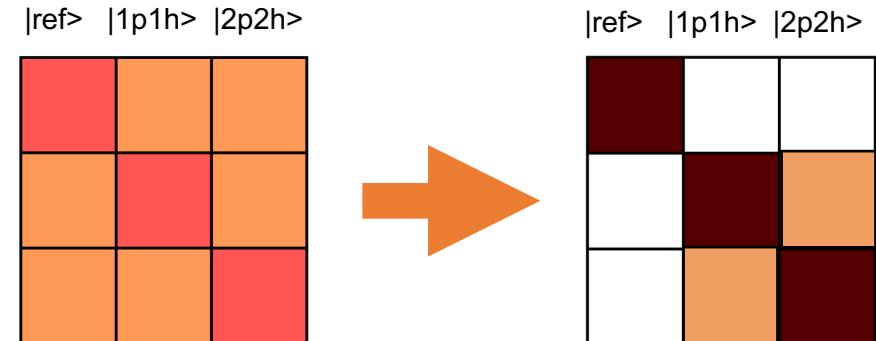
$$\eta_{12} = \frac{1}{2} \arctan \left(\frac{2f_{12}}{f_{11} - f_{22} + \Gamma_{1212}} \right)$$

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

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

Approximation:

- ◆ $H(s)$ and $\eta(s)$ are two-body operators.
- ◆ A few % error in the ground-state energy and radius



In-medium similarity renormalization group approach

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

$$H(s) = e^{\Omega(s)} H(s=0) e^{-\Omega(s)} \approx E(s) + \sum_{12} f_{12}(s) \{a_1^\dagger a_2\} + \frac{1}{4} \sum_{1234} \Gamma_{1234}(s) \{a_1^\dagger a_2^\dagger a_4 a_3\}$$

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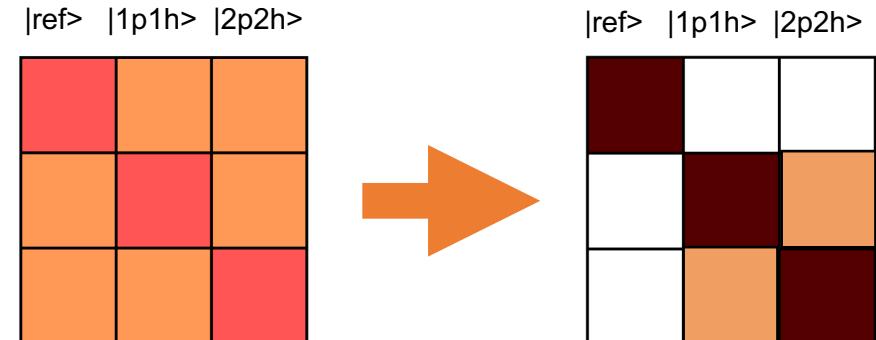
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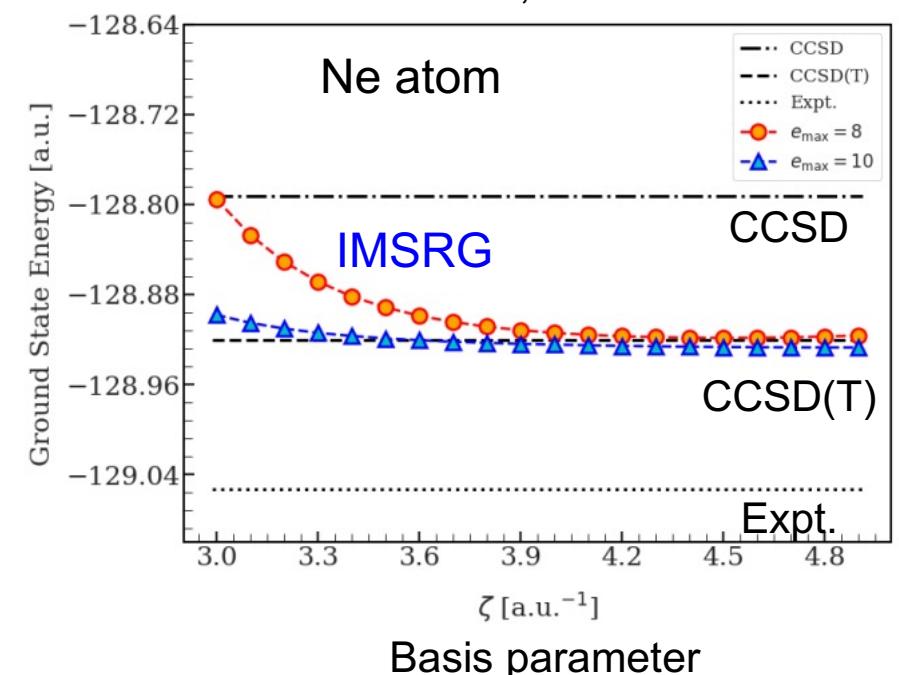
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G. Tenkila et al., arXiv:2212.08188



Towards heavy nuclei

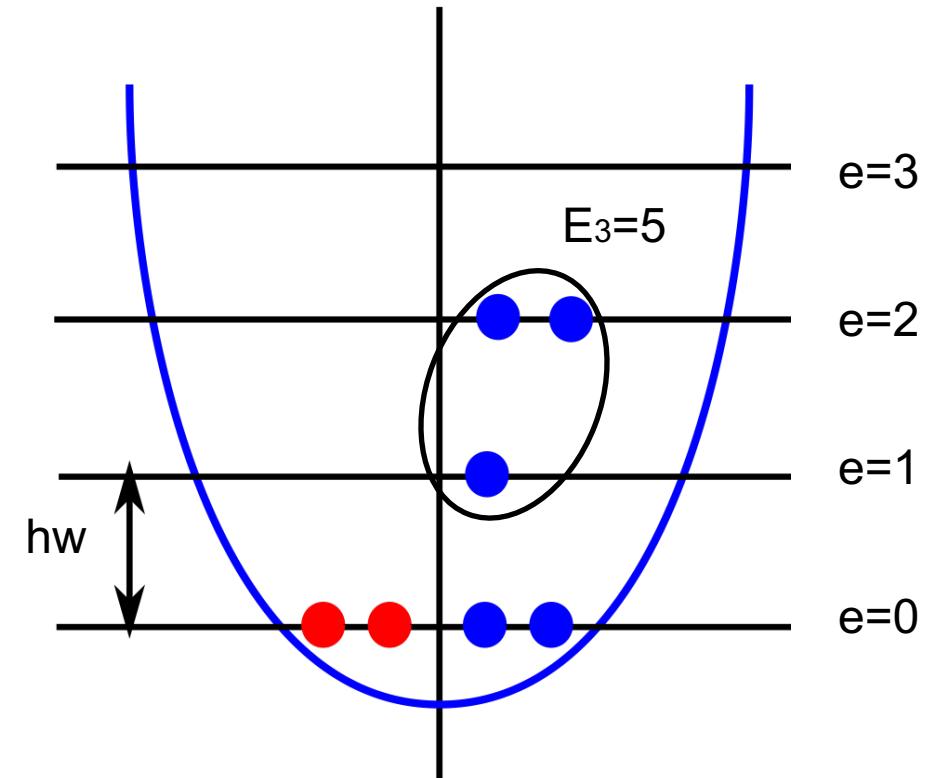
NN+3N Hamiltonian (harmonic oscillator basis)

Parameters controlling numerical calculations

- ◆ Frequency (hw)
- ◆ e_{max} (number of major shells)
- ◆ E_{3max} (sum of 3B HO quanta)

One has to increase e_{max} and E_{3max} until results converge!

Limited E_{3max} does not allow to access heavy systems.



Towards heavy nuclei

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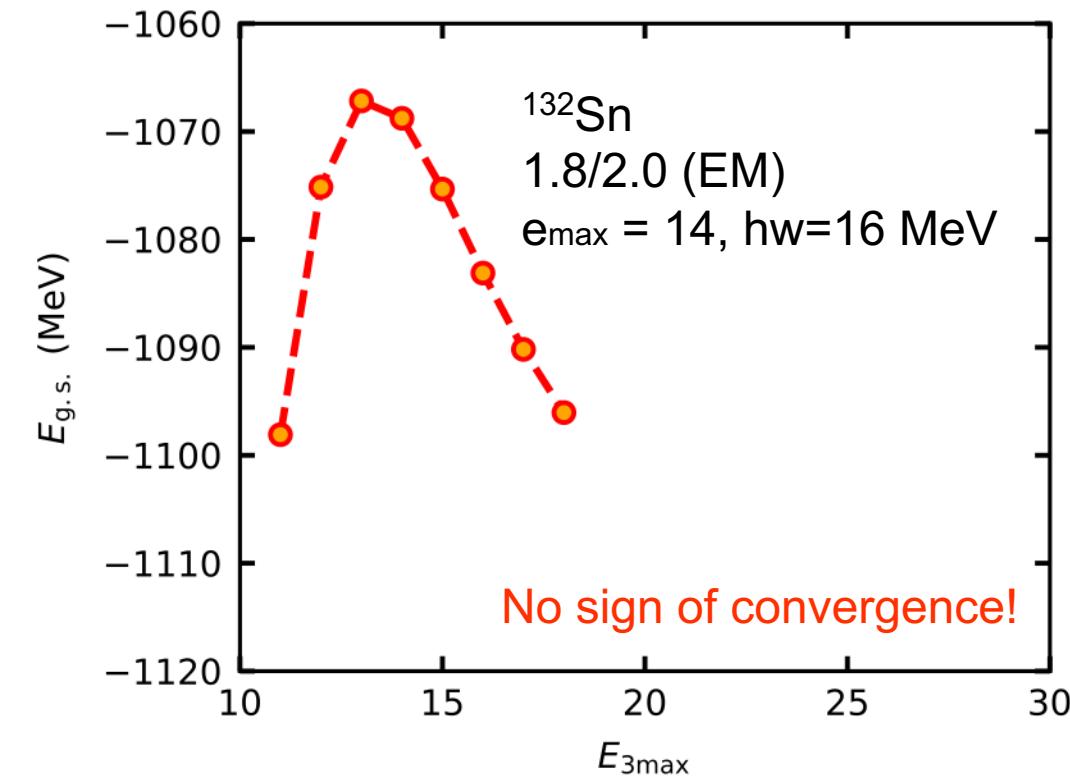
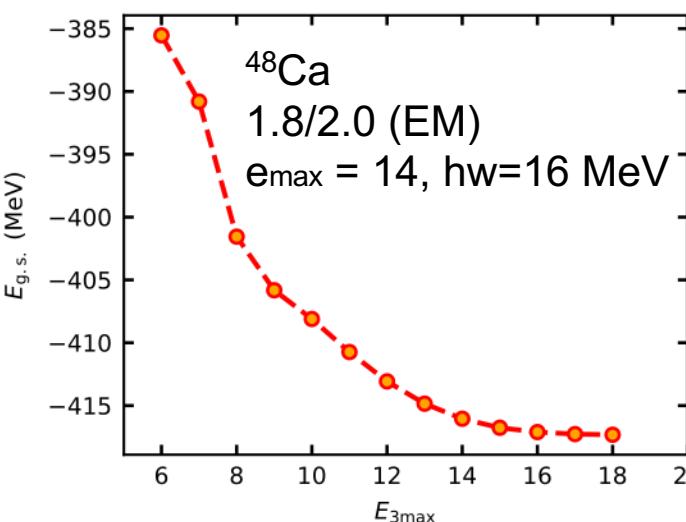
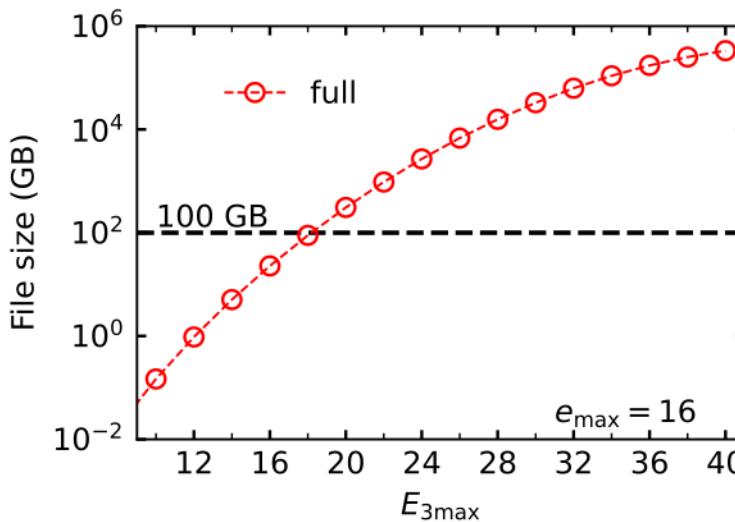
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NN+3N Hamiltonian (harmonic oscillator basis)

Parameters controlling numerical calculations

- ◆ Frequency ($\hbar\omega$)
- ◆ e_{\max} (number of major shells)
- ◆ $E_{3\max}$ (sum of 3B HO quanta)



Residual interactions



Hamiltonian: $H = \sum_{p'p} t_{p'p} c_{p'}^\dagger c_p + \frac{1}{4} \sum_{p'q'pq} v_{p'q'pq} c_{p'}^\dagger c_{q'}^\dagger c_q c_p + \frac{1}{36} \sum_{p'q'r'pqr} v_{p'q'r'pqr} c_{p'}^\dagger c_{q'}^\dagger c_{r'}^\dagger c_r c_q c_p$

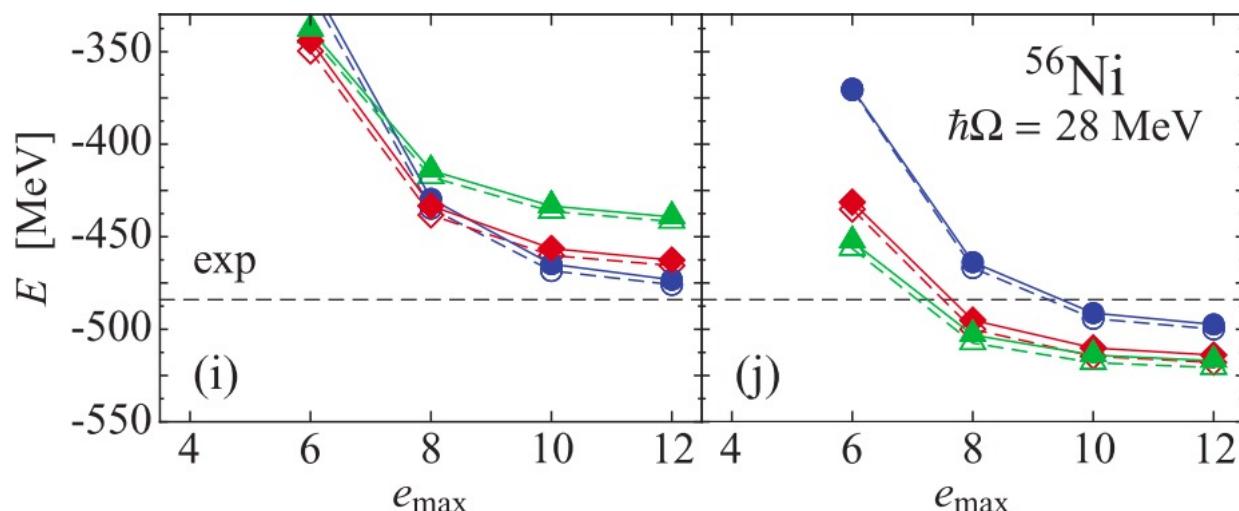
Normal ordering

$$H = E_0 + \sum_{p'p} f_{p'p} :c_{p'}^\dagger c_p: + \frac{1}{4} \sum_{p'q'pq} \Gamma_{p'q'pq} :c_{p'}^\dagger c_{q'}^\dagger c_q c_p: + \frac{1}{36} \sum_{p'q'r'pqr} W_{p'q'r'pqr} :c_{p'}^\dagger c_{q'}^\dagger c_{r'}^\dagger c_r c_q c_p:$$

Input of post mean-field calc. (NO2B)

Effect of residual 3N

CC calculations from S. Binder et al., Phys. Rev. C 87, 021303 (2013).



Solid: with W term
Dashed: without W term

W term: only $\sim 1\%$ of the total gs energy!

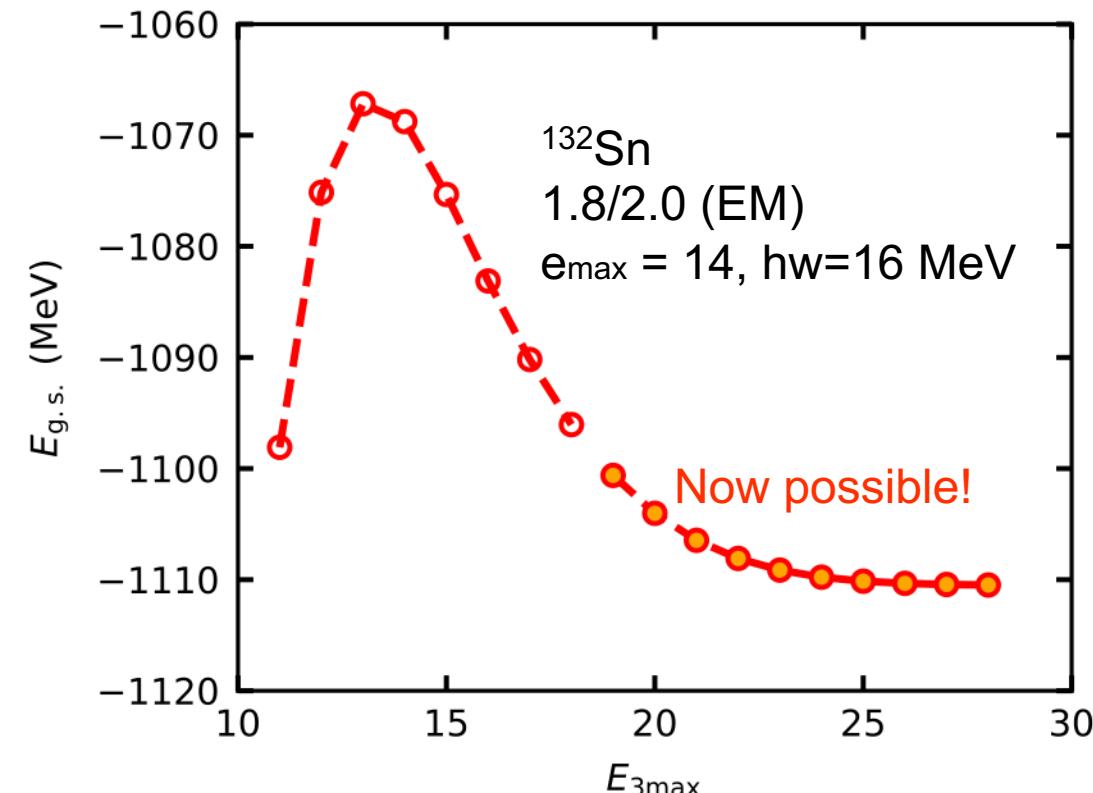
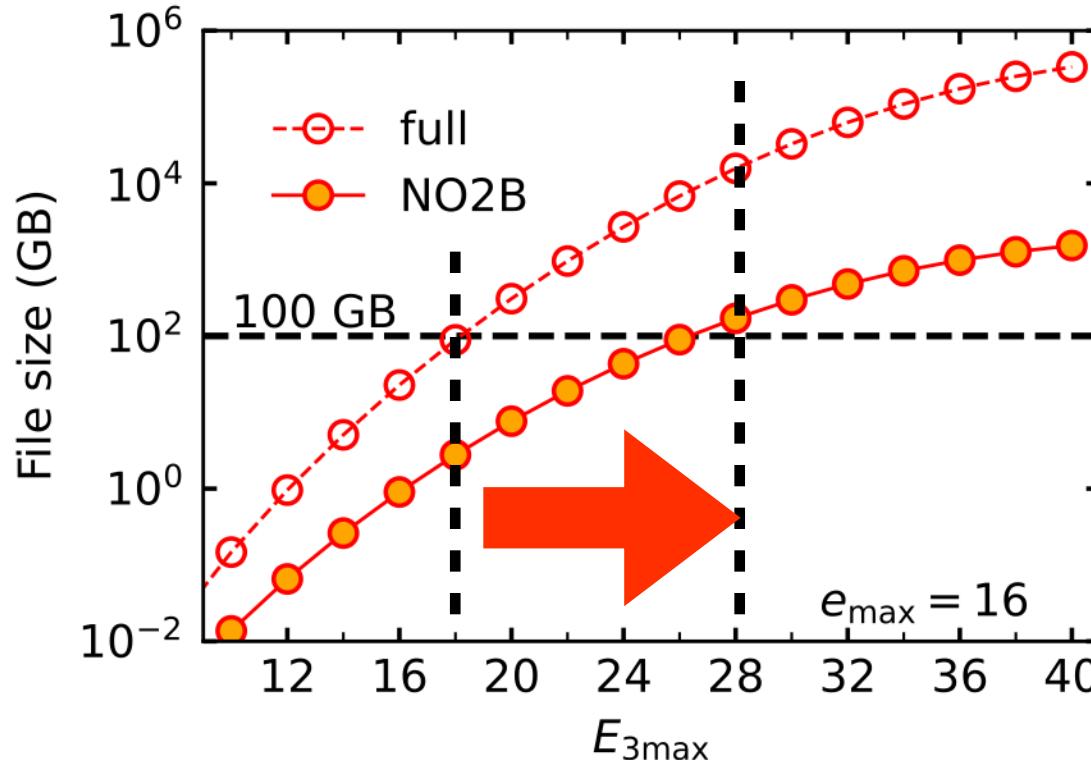
NO2B approximation (neglect W term)

NO2B 3N storage scheme

Store only the matrix elements entering NO2B approximation.

$$V_{p'q'r'pqr}^{\text{NO2B}} = V_{p'q'r'pqr} \tilde{\delta}_{r'r}$$

Determined by symmetry of one-body density matrix
c.f. parity and rotational symmetry for a spherical reference



Extrapolation

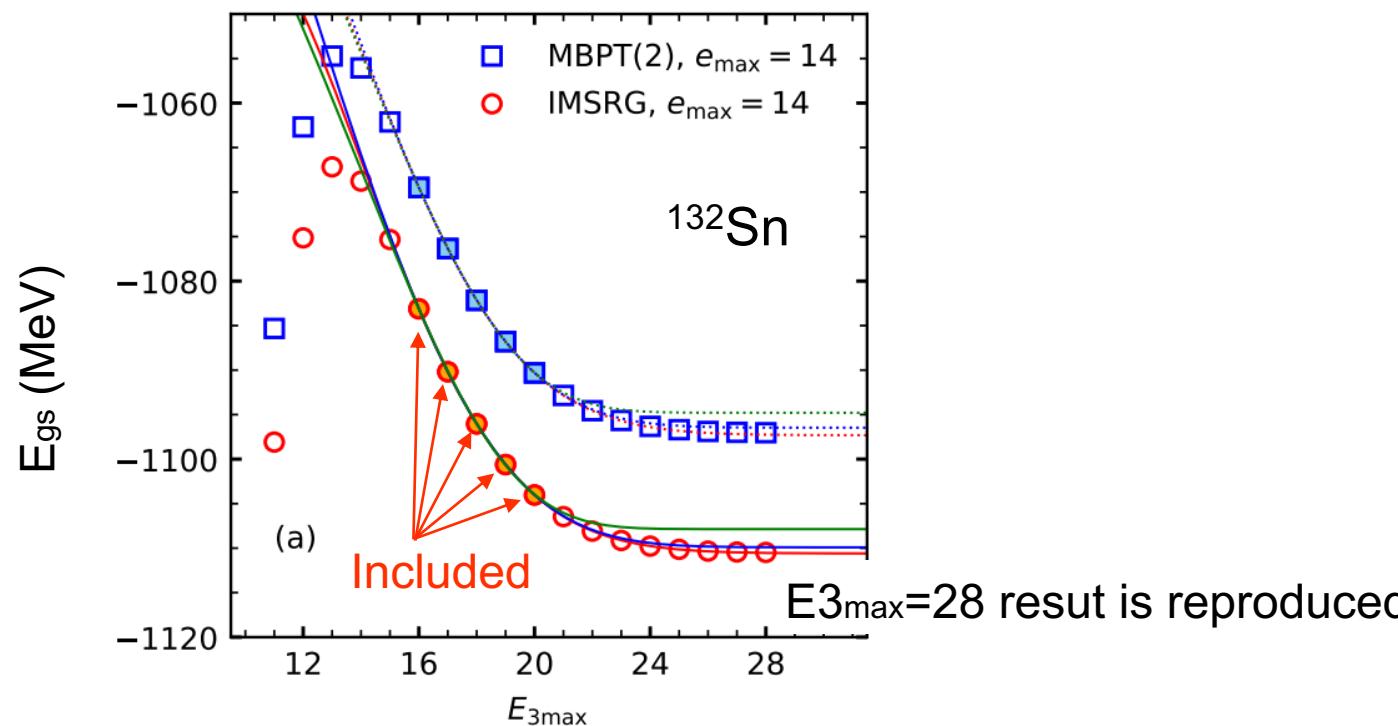
Asymptotic behavior expected from the 2nd order MBPT.

$$E(E_{3\max}) = A \gamma_{\frac{2}{n}} \left[\left(\frac{E_{3\max} - \mu}{\sigma} \right)^n \right] + C$$

Fitting parameters

$$\mu \approx 3(2n_F + l_F)$$

The same form can be expected for any operators dominated by one-body part, e.g., radius



Extrapolation

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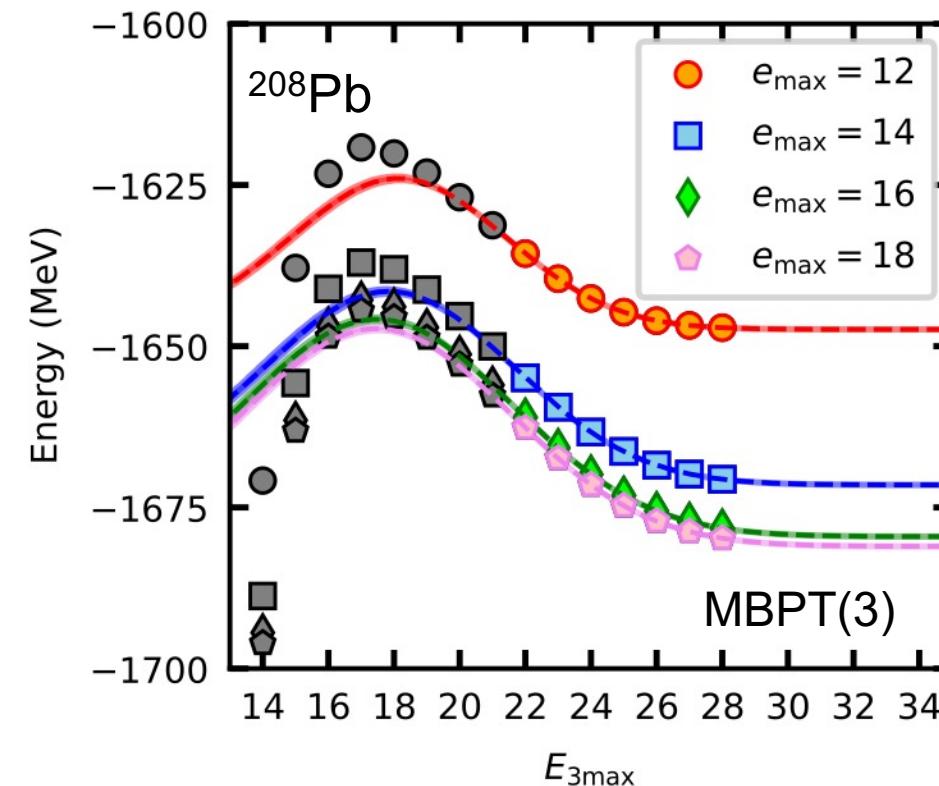
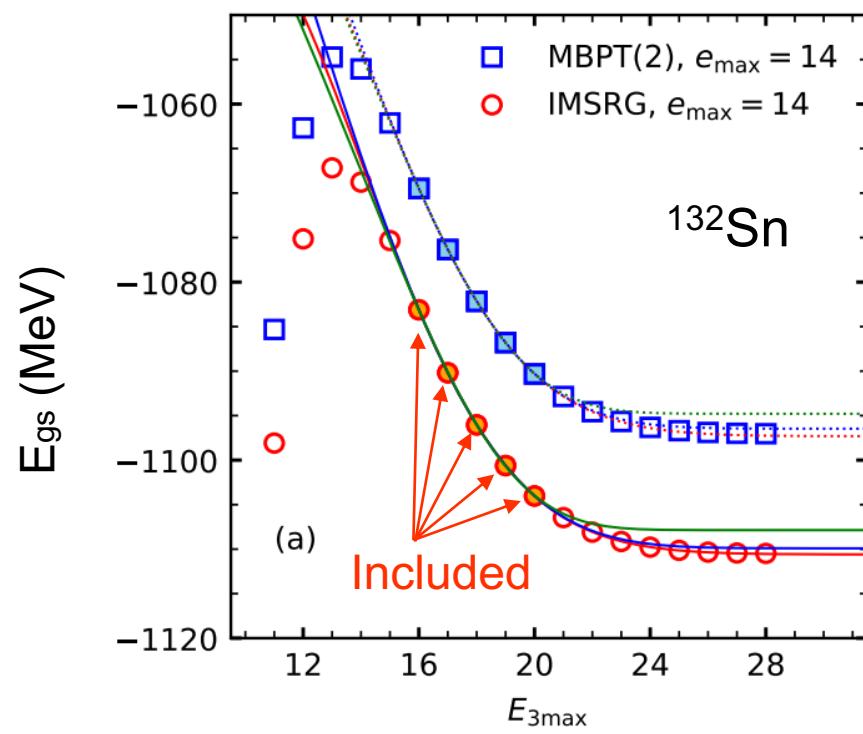
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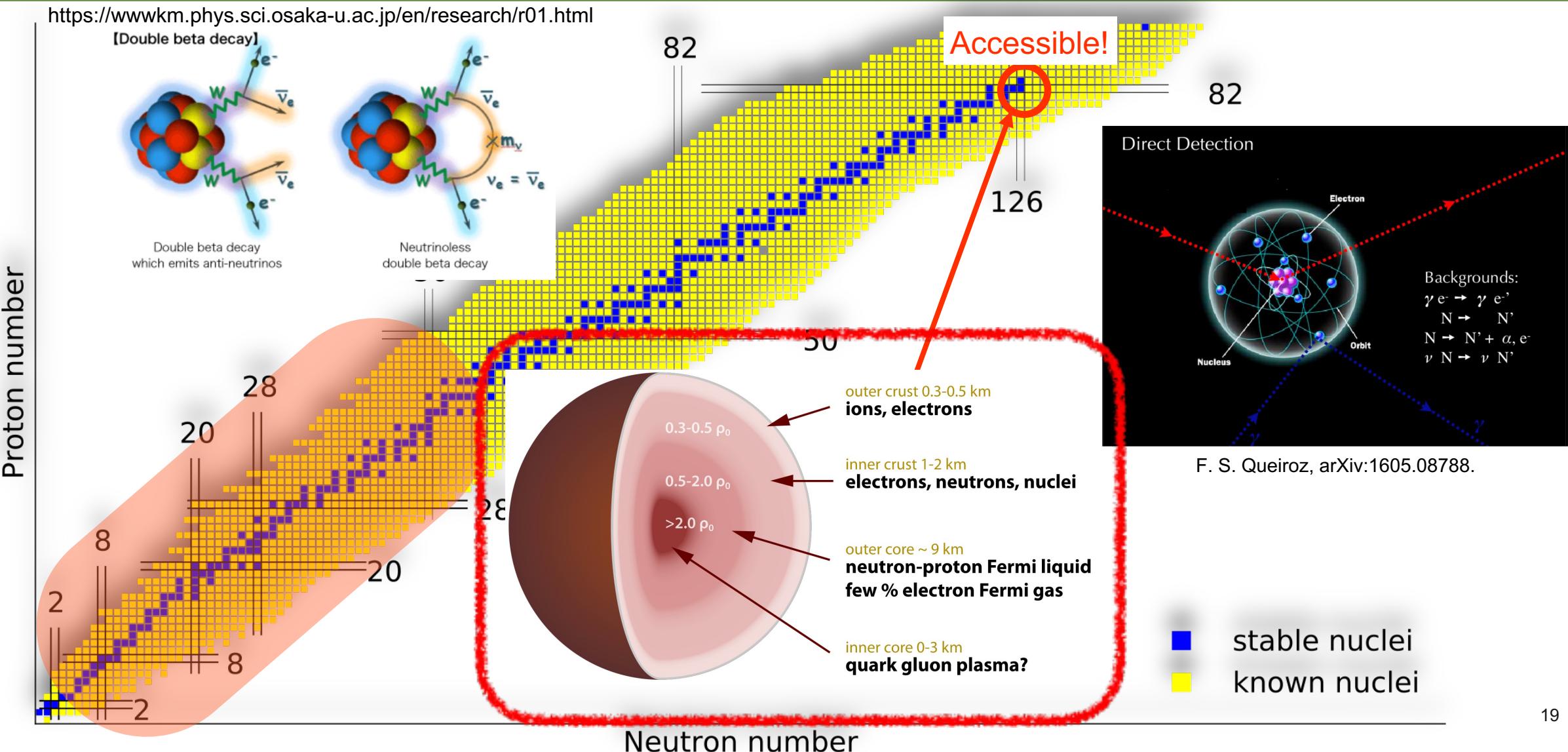


Why heavy nuclei?

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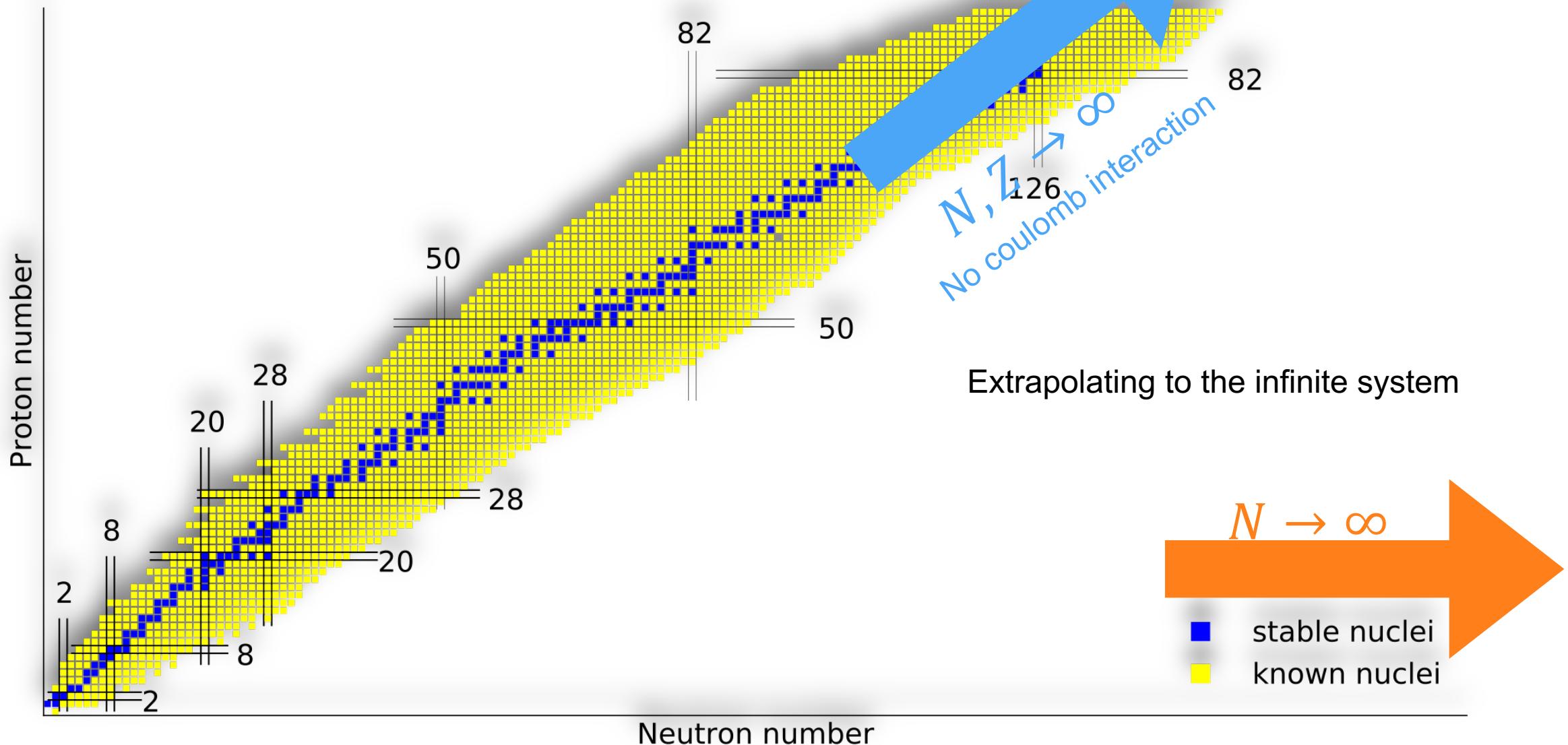


Infinite nuclear matter & neutron star

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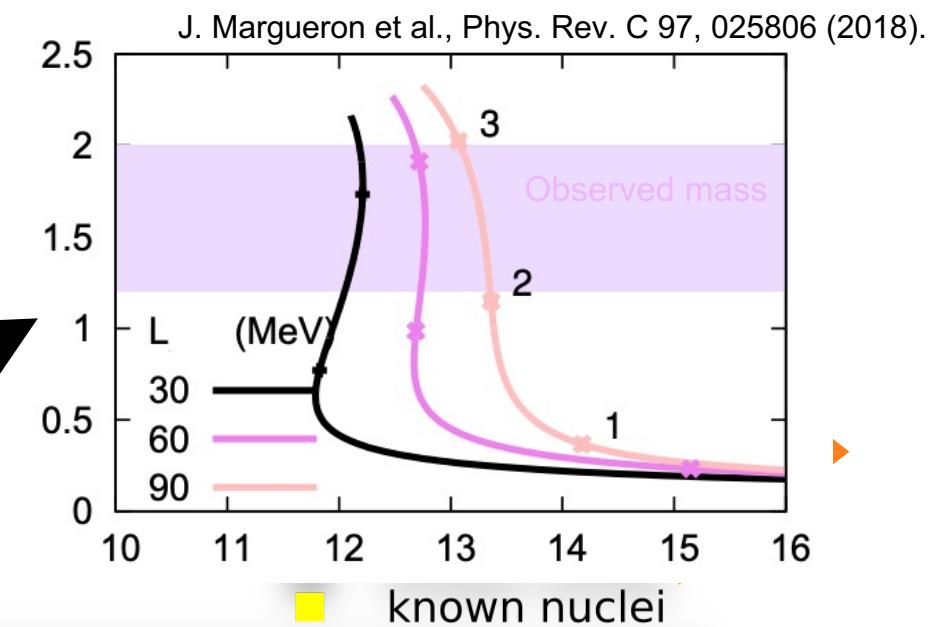
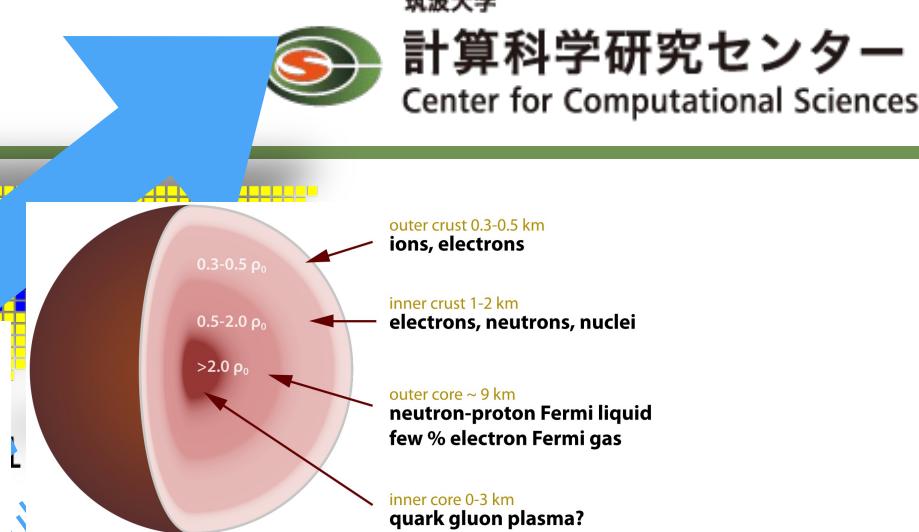
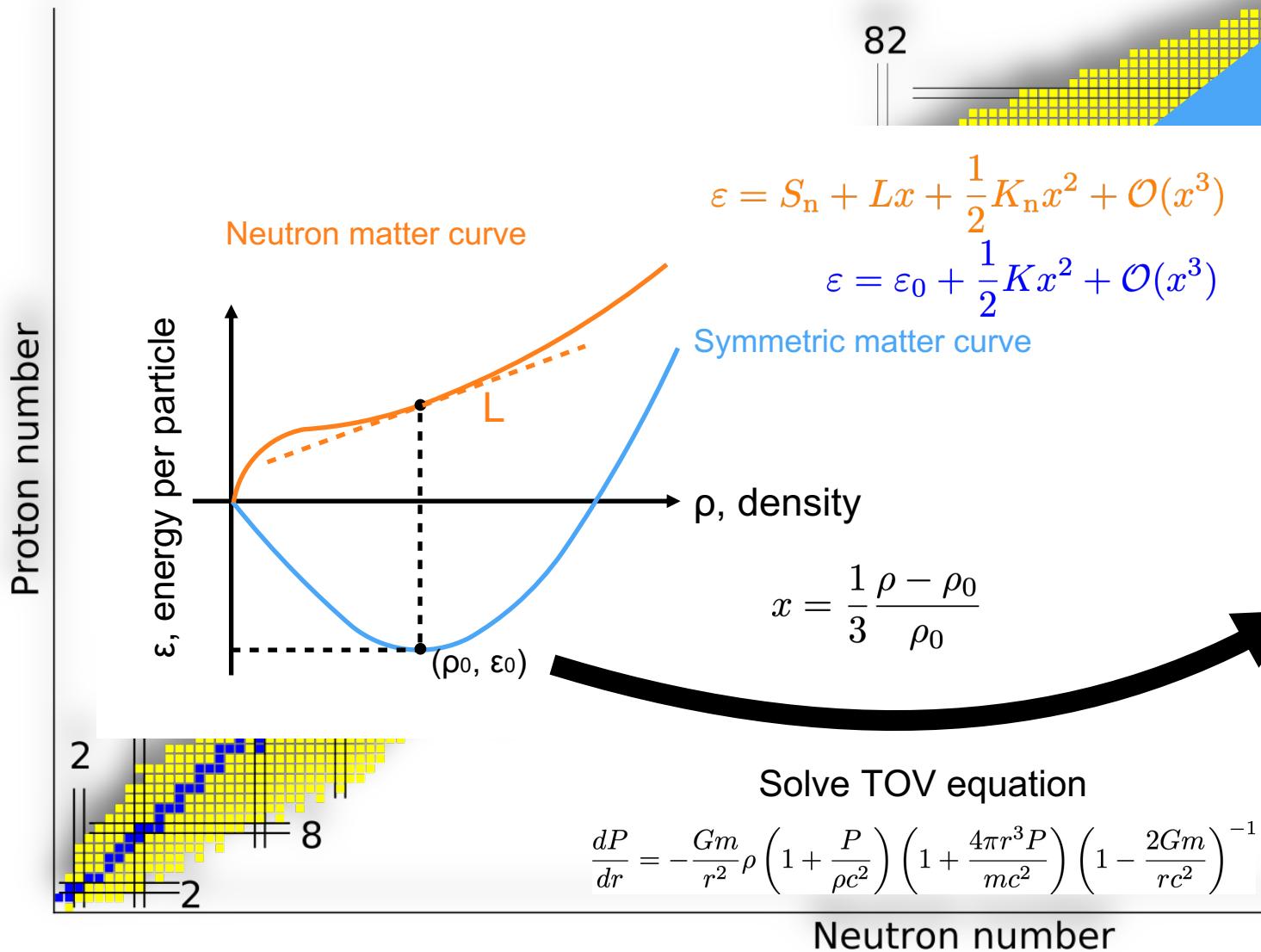
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Infinite nuclear matter & neutron star

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Correlation connecting finite and infinite systems

Correlation from MF calculations

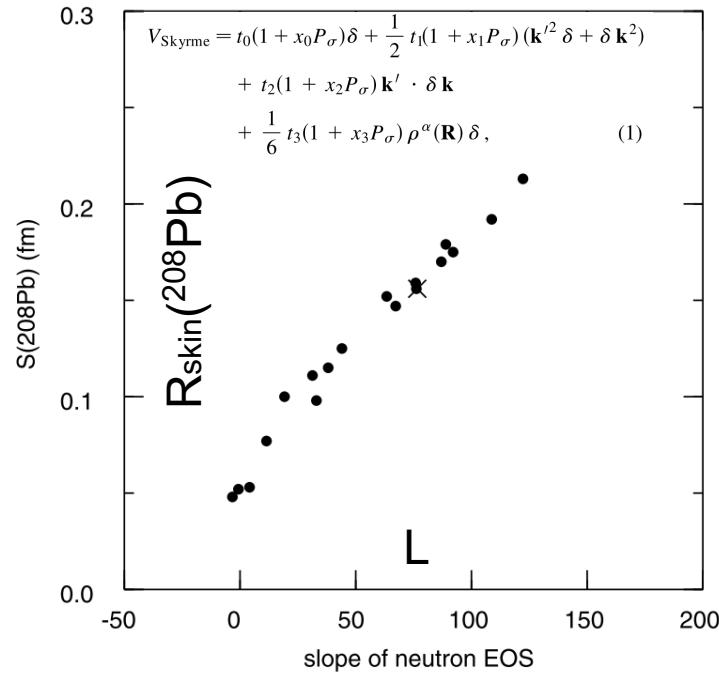
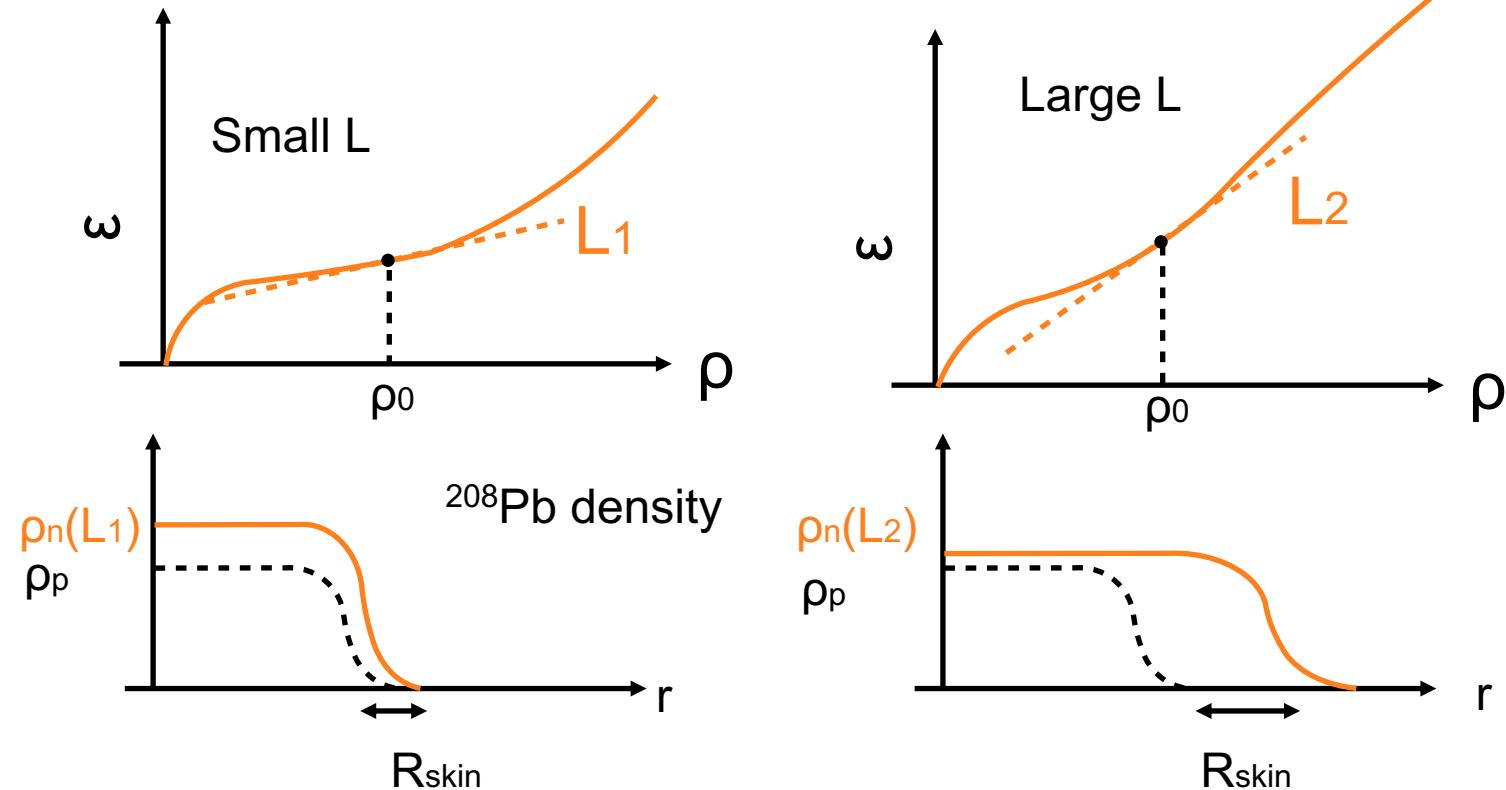


Figure taken from B. Alex Brown, Phys. Rev. Lett. 85, 5296 (2000).

Motivation:

Robustness of the correlation

Narrower prediction of $R_{\text{skin}}(^{208}\text{Pb})$



For $L_1 < L_2$, $\rho_n(L_2) < \rho_n(L_1)$

$\rightarrow R_n(L_1) < R_n(L_2)$

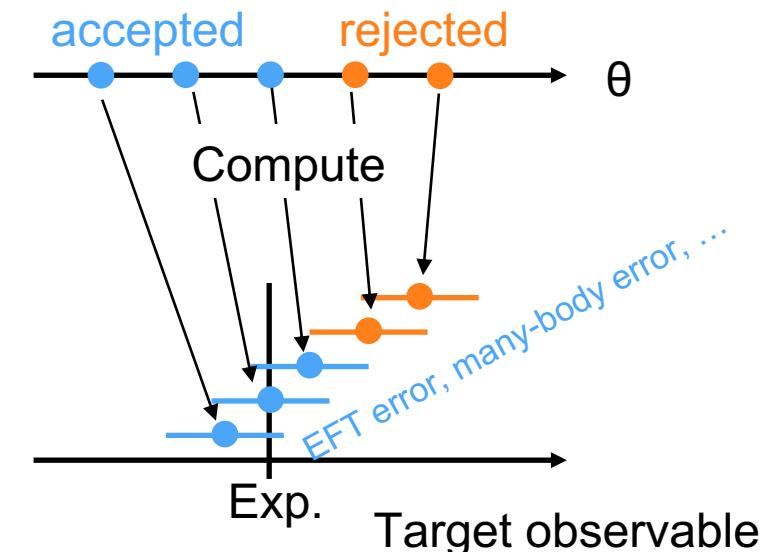
$\rightarrow r_{\text{skin}}(L_1) < r_{\text{skin}}(L_2)$

*Assumption: proton radius is fitted.

Sampling parameters

Non-imausible (NI) 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 $\sim 10^9$ parameter sets, 34 **non-imausible (NI)** interactions were found.

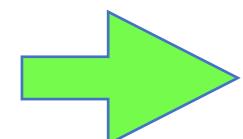
Neutron skin thickness of ^{208}Pb

History matching:

- Sampling 17 parameters in (delta-full) chiral EFT such that the parameter set is consistent with some selected data.

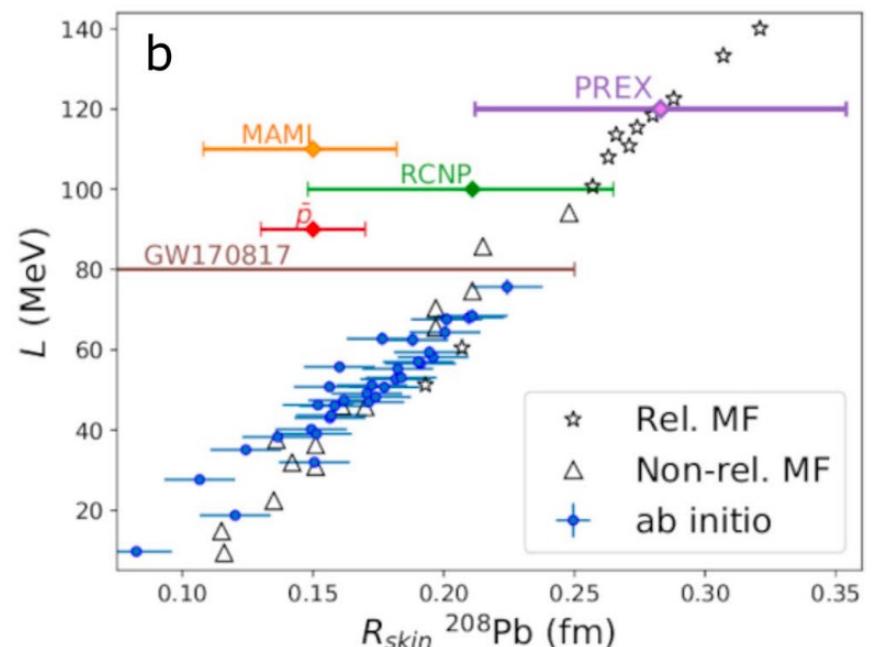
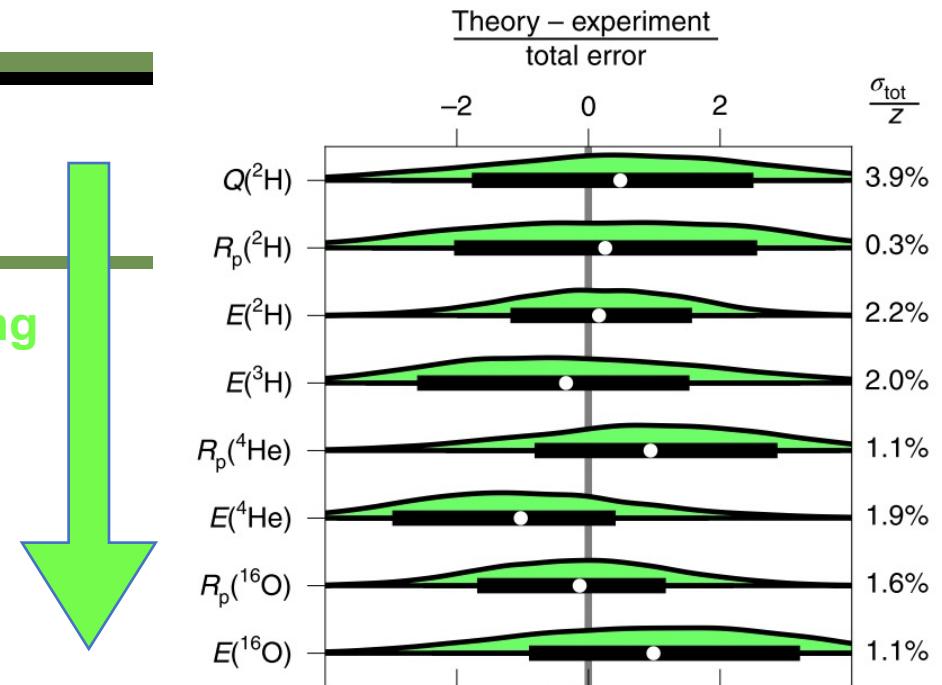
- Proton-neutron scattering phase shifts, $E(^2\text{H})$, $R_p(^2\text{H})$, $Q(^2\text{H})$, $E(^3\text{H})$, $E(^4\text{He})$, $R_p(^4\text{He})$, $E(^{16}\text{O})$, and $R_p(^{16}\text{O})$.

$\sim 10^9$ parameter sets



34 NI parameter sets

History matching



Neutron skin thickness of ^{208}Pb

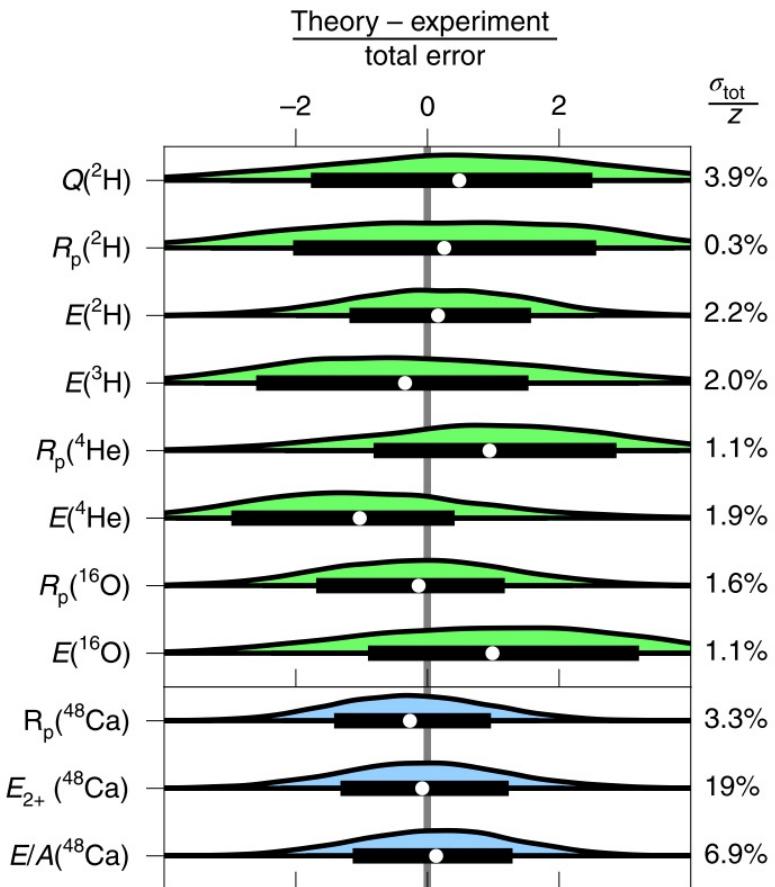
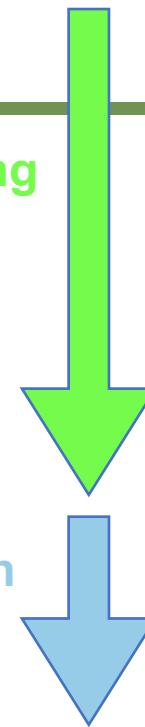
Calibration:

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

$$w_i = \frac{\mathcal{L}(D|\theta_i)}{\sum_{j=1}^{34} \mathcal{L}(D|\theta_j)},$$
$$\mathcal{L}(D|\theta_i) = \mathcal{N}(D, \sigma_{\text{exp}}^2 + \sigma_{\chi\text{EFT}}^2 + \sigma_{\text{MB}}^2)$$

History matching

Calibration



Neutron skin thickness of ^{208}Pb

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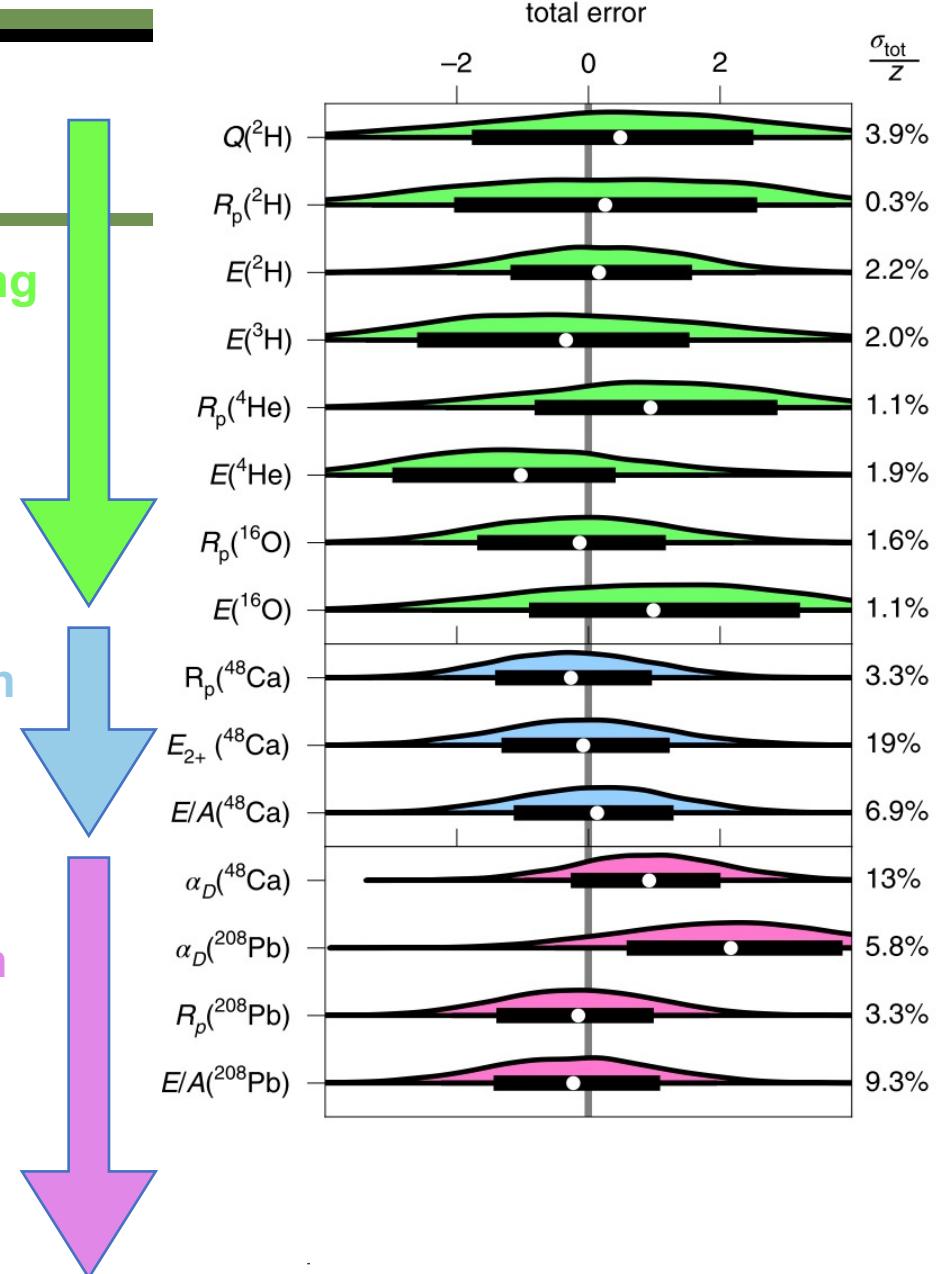
Validation & prediction:

- ◆ The weighted samples are approximately equivalent to the samples extracted from $p(\theta|D)$. $\text{PPD} = \{\mathcal{O}_{\text{target}}(\theta) : \theta \sim P(\theta|^{48}\text{Ca})\}$

History matching

Calibration

Validation Prediction



Neutron skin thickness of ^{208}Pb

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Validation & prediction:

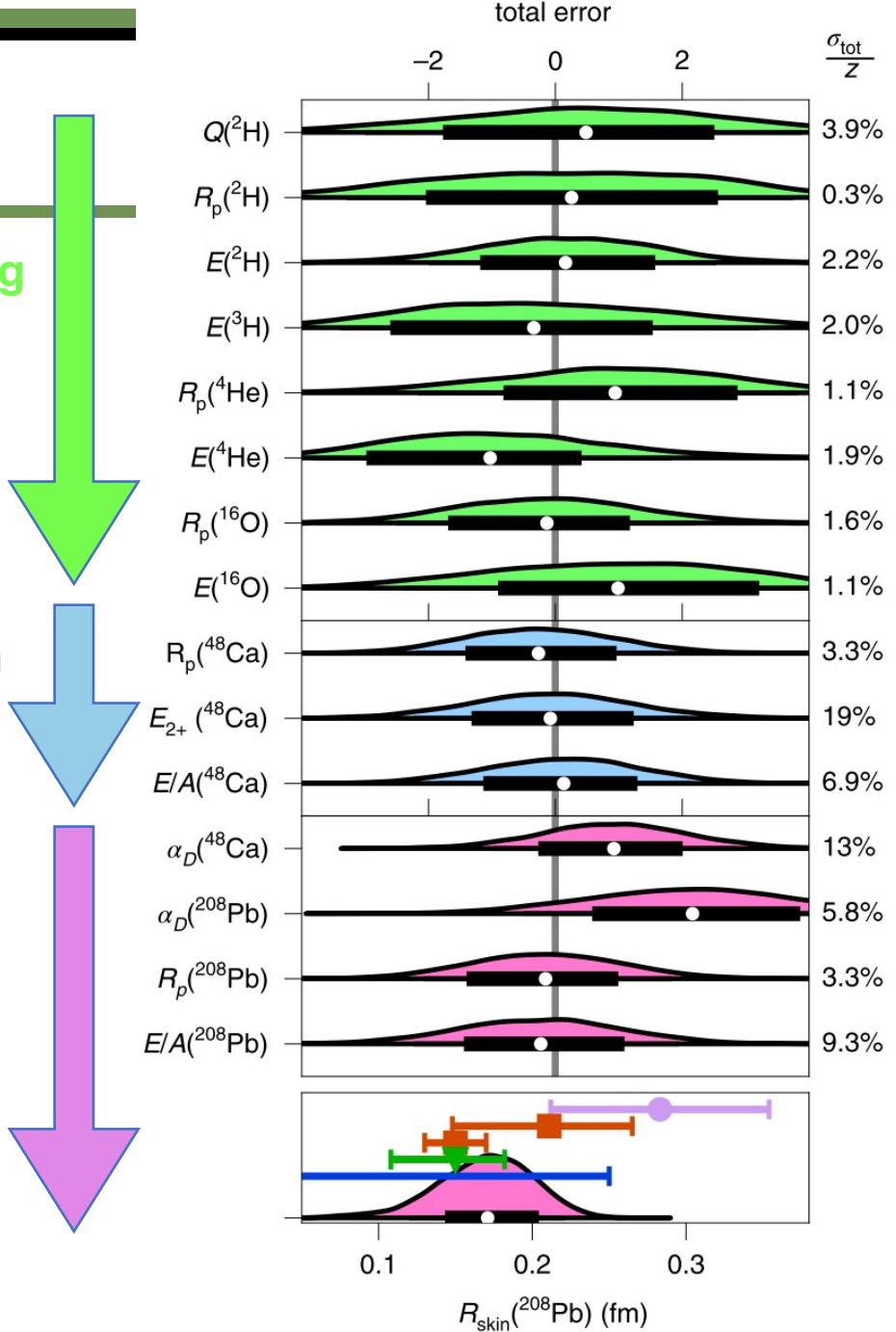
- ◆ The weighted samples are approximately

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

History matching

Calibration

Validation
Prediction



Neutron skin of ^{208}Pb

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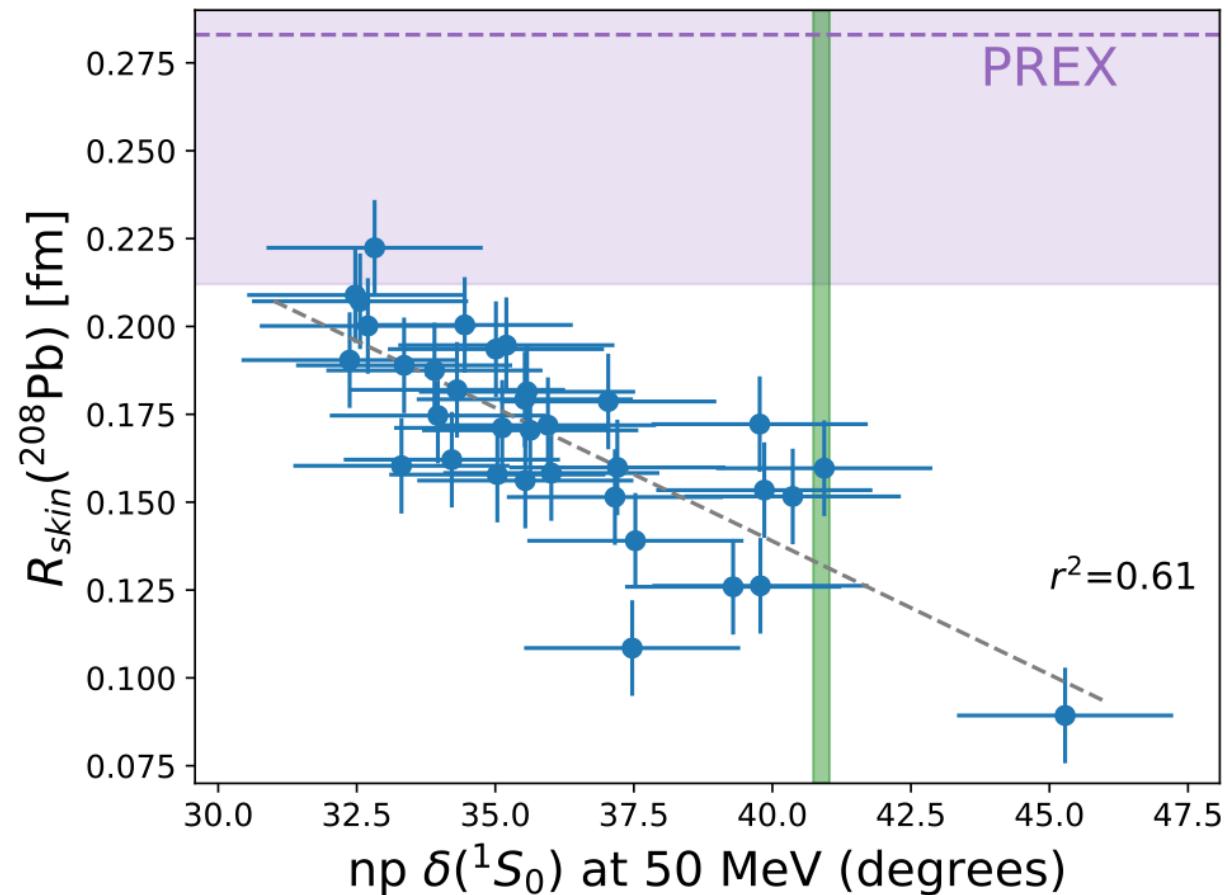


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Ab initio prediction $0.14 < R_{\text{skin}}(^{208}\text{Pb}) < 0.20$ is relatively narrow.

Constraining on S-wave scattering phase shift rules out thick $R_{\text{skin}}(^{208}\text{Pb})$.

Correlation connecting few- and many-body systems



Ongoing development

Construction of a fast and accurate emulator

- ◆ parametric matrix model P. Cook et al., arXiv: 2401.11694

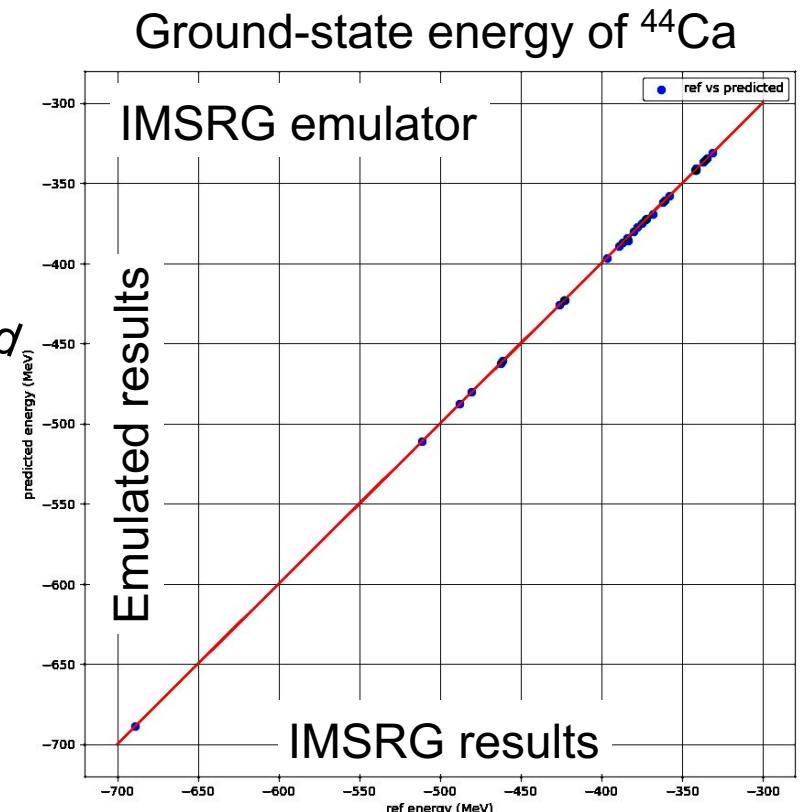
Data-driven eigenvector continuation-like method*
~ 10⁶⁻⁹ times speed up!

With the emulator, one can explore

- ❖ Impact of 3N interaction in medium-mass nuclei
- ❖ Observables to further constrain LECs in ChEFT



Hang Yu



* See S. Yoshida's talk for the details of the eigenvector continuation

Summary & outlook

The nuclear ab initio calculations of heavy nuclei are becoming feasible.

We combined the state-of-the-art techniques to predict the neutron skin of ^{208}Pb , including the possible uncertainties.

The well-known $R_{\text{skin}}(^{208}\text{Pb})$ vs L correlation can be found in ab initio calculations.

NN scattering phase-shift is crucial to constrain $R_{\text{skin}}(^{208}\text{Pb})$.

More things need to be done.

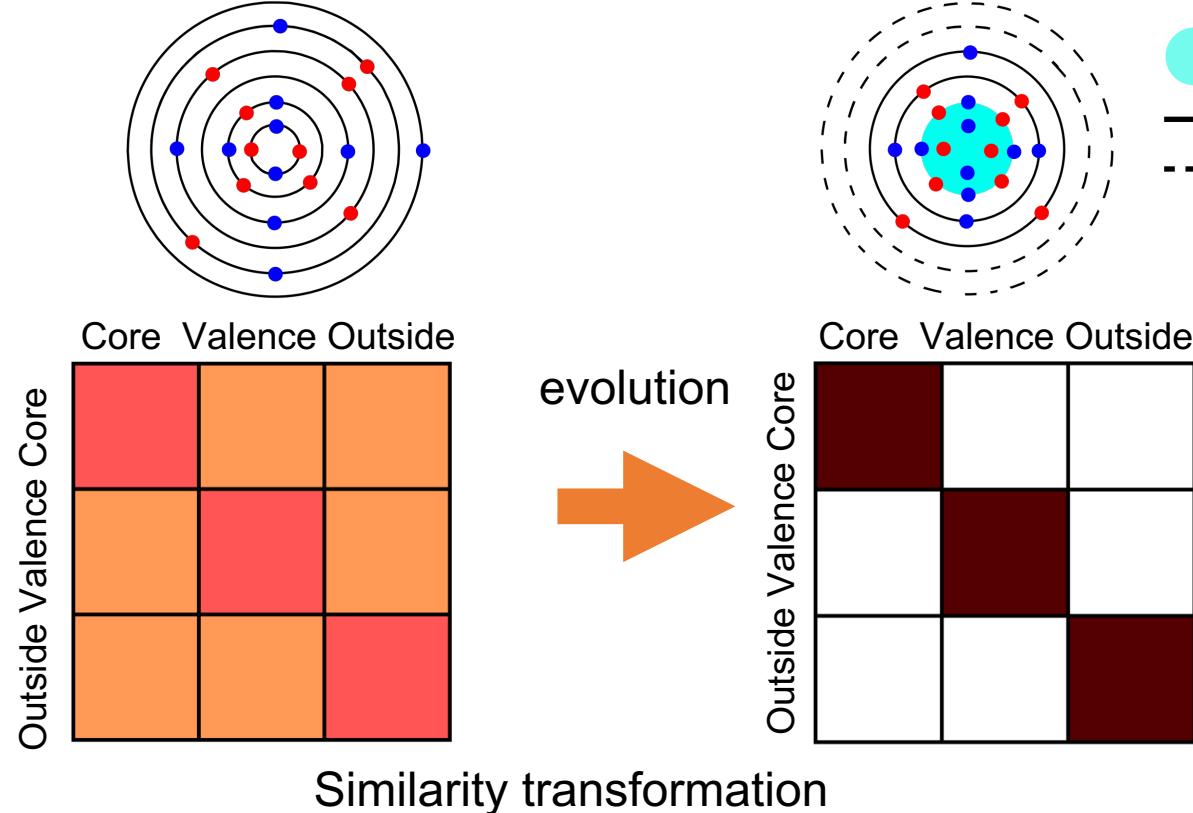
- ◆ Better quantified uncertainty, Cutoff independence, CREX vs PREX, ...

The same strategy can be applied to other research.

- ◆ 0vbb decay, WIMP-nucleus scattering, electric dipole moment, ...

Backup slides

Valence-space in-medium similarity renormalization group



H

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

s: flow parameter

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

- : frozen core
- : valence
- : outside

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

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

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

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

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

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

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

Normal ordering wrt a single Slater determinant

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

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

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

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

- ◆ Normal ordered two-body (NO2B) approximation:
$$H \approx E_0 + \sum_{pq} f_{pq} \{a_p^\dagger a_q\} + \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} \{a_p^\dagger a_q^\dagger a_s a_r\}$$

E3max extrapolation

One has to make sure that HF results are well converged.

Assuming that the employed nuclear interaction is soft enough: $E_{\text{corr}} \approx E_{\text{MBPT}}^{[2]}$

$$\Gamma_{abij} = V_{abij}^{\text{NN}} + \sum_k V_{abkijk}^{\text{3N}} n_k$$

With an optimal frequency, MP(2) energy can be approximated as $E_{\text{MBPT}}^{[2]} \approx \frac{1}{4\hbar\Omega} \sum_{abij} \frac{\Gamma_{ijab}\Gamma_{abij}}{e_i + e_j - e_a - e_b}$

- MP(2) enegy difference between E3max and E3max+1: $\Delta E_{\text{MBPT}}^{[2]} = \frac{1}{2\hbar\Omega} \sum_{ijk} \sum_{ab} \frac{V_{ijab}^{\text{NN}} V_{abkijk}^{\text{3N}}}{e_i + e_j + e_k - e_a - e_b - e_k} \delta_{E_{\text{3max}}, e_a + a_b + e_k}$
- Further assumption: $V_{abij}^{\text{NN}} \approx \bar{V}^{\text{NN}} \exp \left\{ - \left[\frac{m\epsilon_0(e_a + e_b - e_i - e_j)}{\Lambda_{\text{NN}}^2} \right]^n \right\}$, $V_{abkijk}^{\text{3N}} \approx \bar{V}^{\text{3N}} \exp \left\{ - \left[\frac{m\epsilon_0(e_a + e_b + e_k - e_i - e_j - e_k)}{\Lambda_{\text{3N}}^2} \right]^n \right\}$

One finds:

$$\Delta E_{\text{MBPT}}^{[2]} \approx AX \exp \left[-\frac{X^n}{\sigma^n} \right], \quad X = E_{\text{3max}} - \mu, \quad \frac{1}{\sigma^n} = m^n \epsilon_0^n \left(\frac{1}{\Lambda_{\text{NN}}^{2n}} + \frac{1}{\Lambda_{\text{3N}}^{2n}} \right)$$

After integrating the above, one obtains:

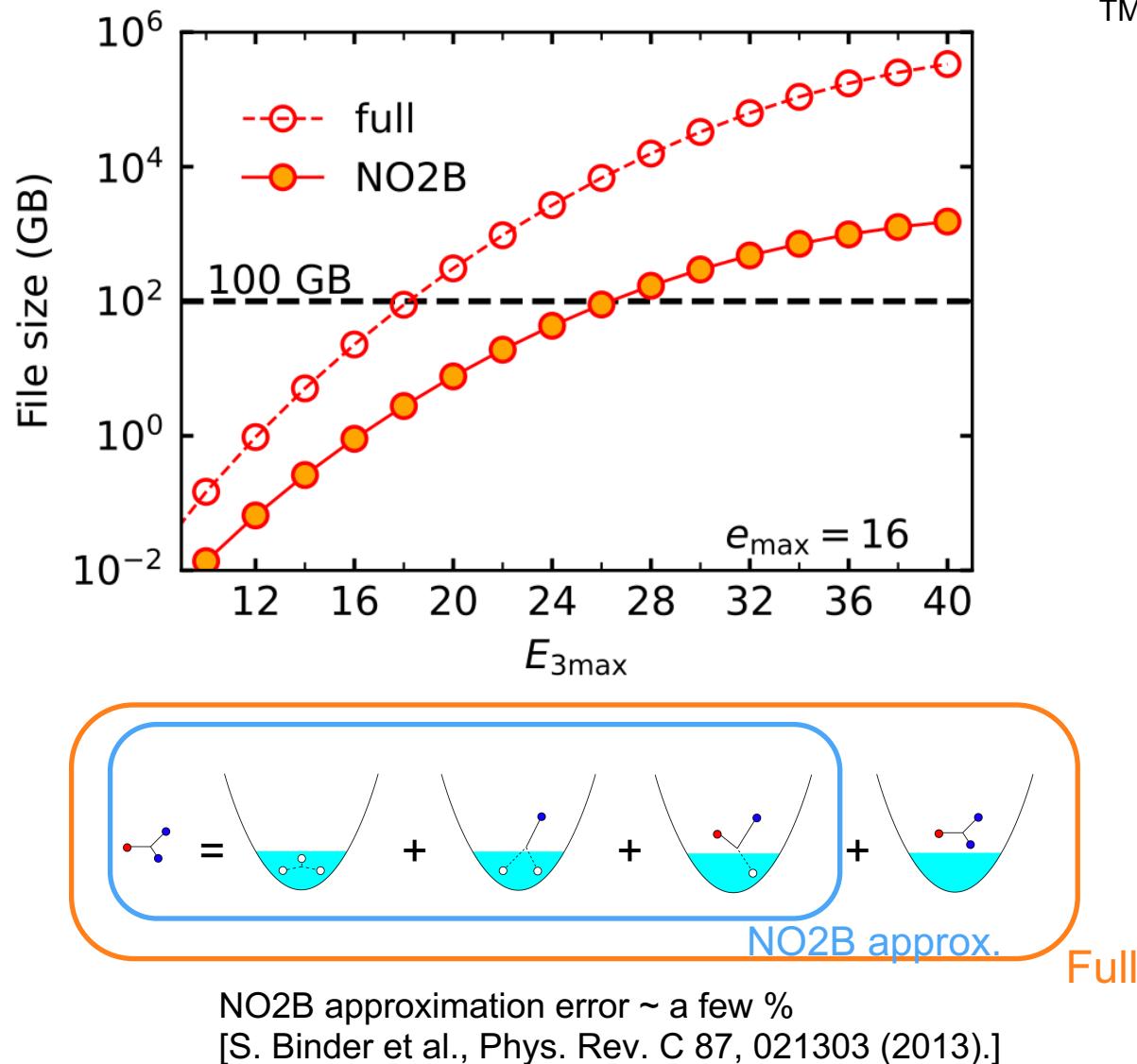
$$E(E_{\text{3max}}) = A \gamma_{\frac{2}{n}} \left[\left(\frac{E_{\text{3max}} - \mu}{\sigma} \right)^n \right] + C$$

$E_{3\max}$ convergence in heavy nuclei

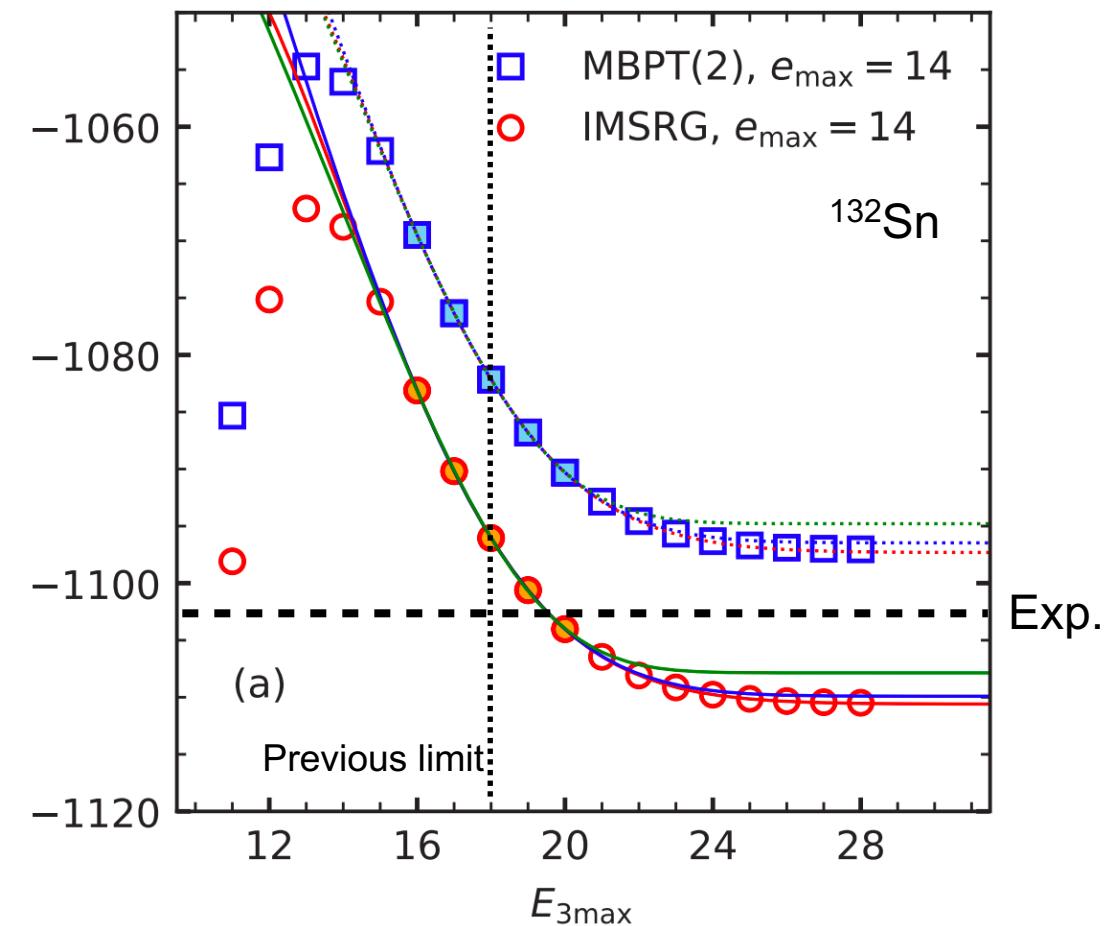
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TM, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt, Phys. Rev. C 105, 014302 (2022).



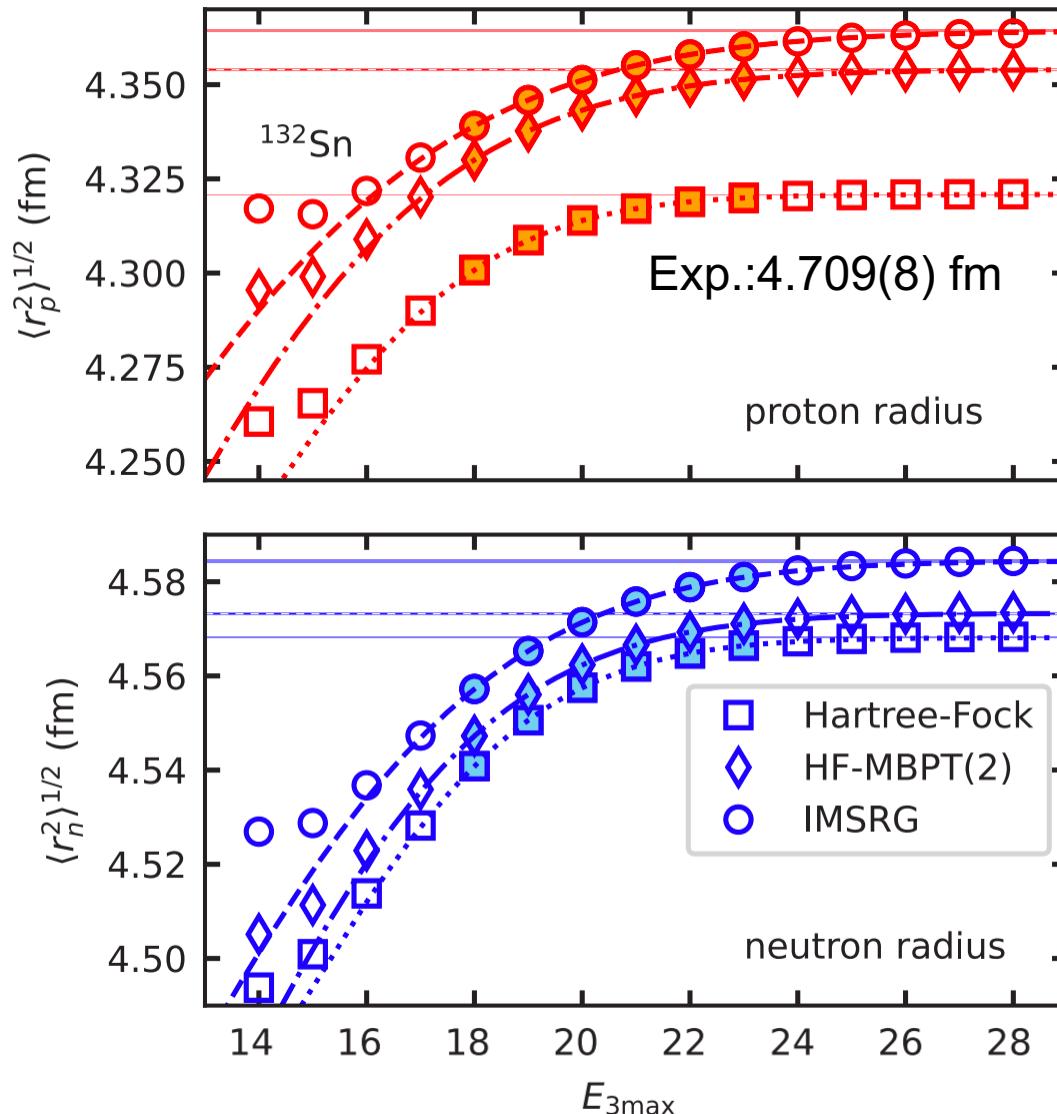
Asymptotic form: $E \approx A \gamma_{\frac{2}{n}} \left[\left(\frac{E_{3\max} - \mu}{\sigma} \right)^n \right] + E_\infty$

Radii

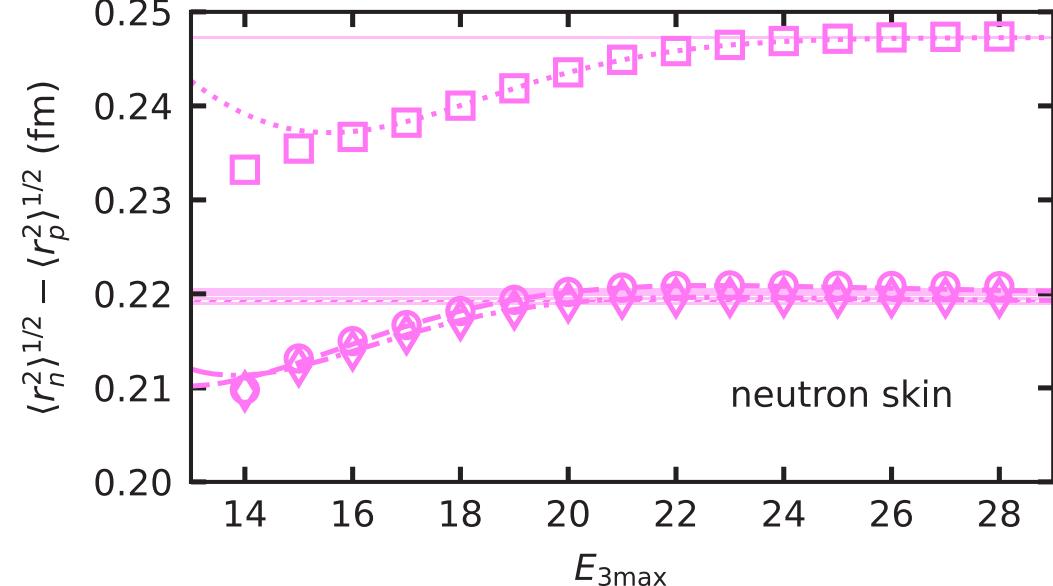
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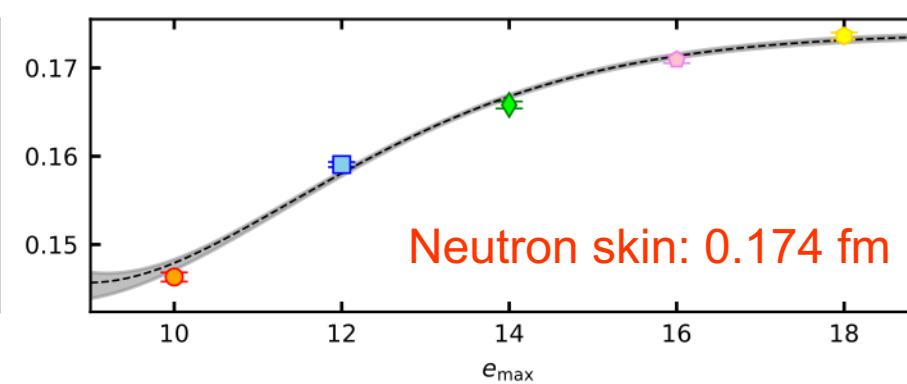
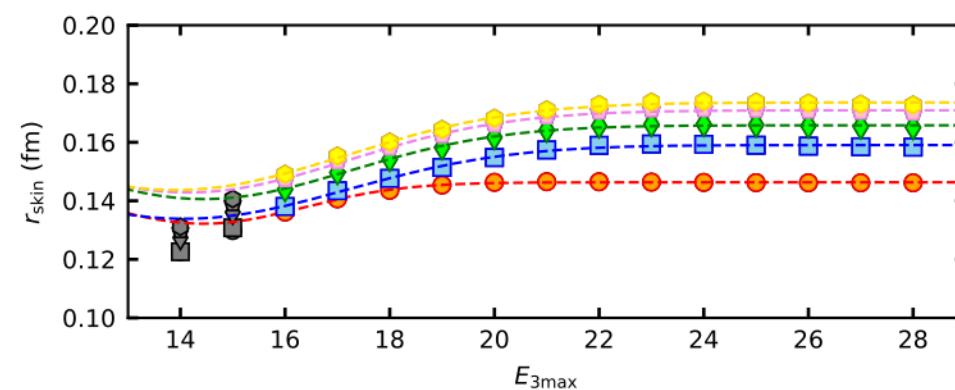
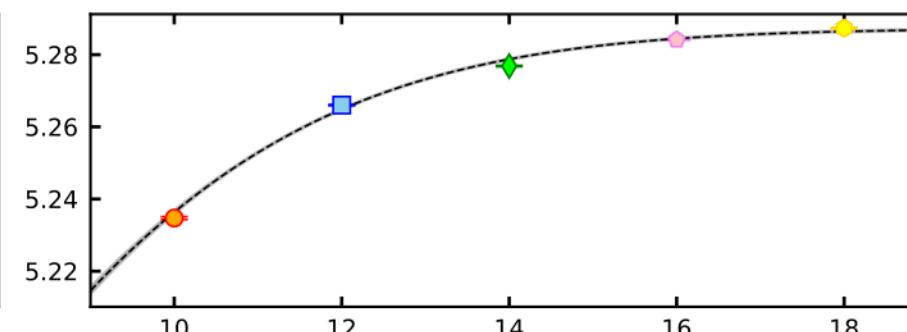
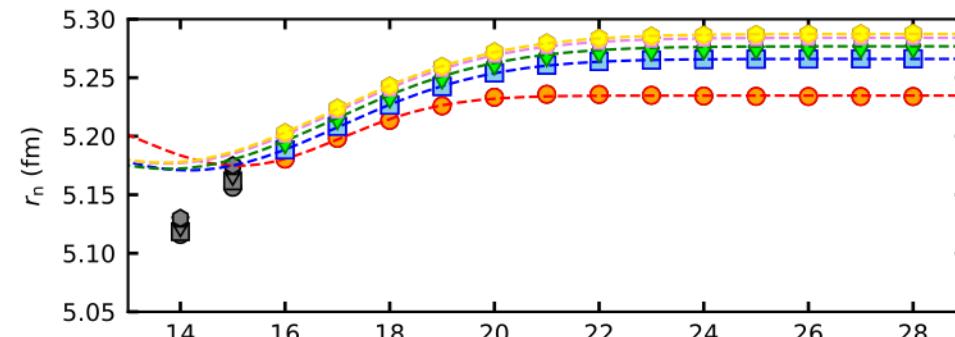
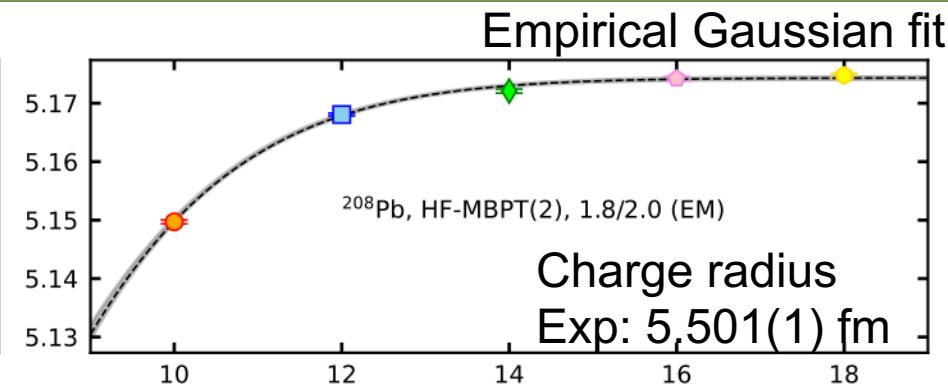
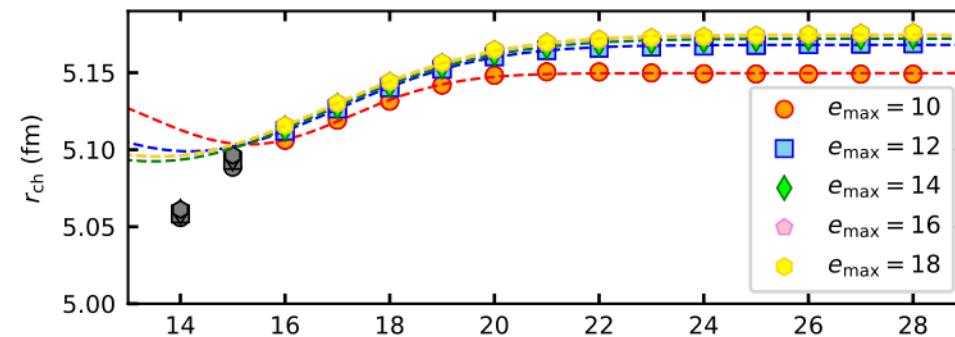
Asymptotic form: $\langle r^2 \rangle \approx A \gamma_{\frac{2}{n}} \left[\left(\frac{E_{3\text{max}} - \mu}{\sigma} \right)^n \right] + \langle r^2 \rangle_\infty$

Radii

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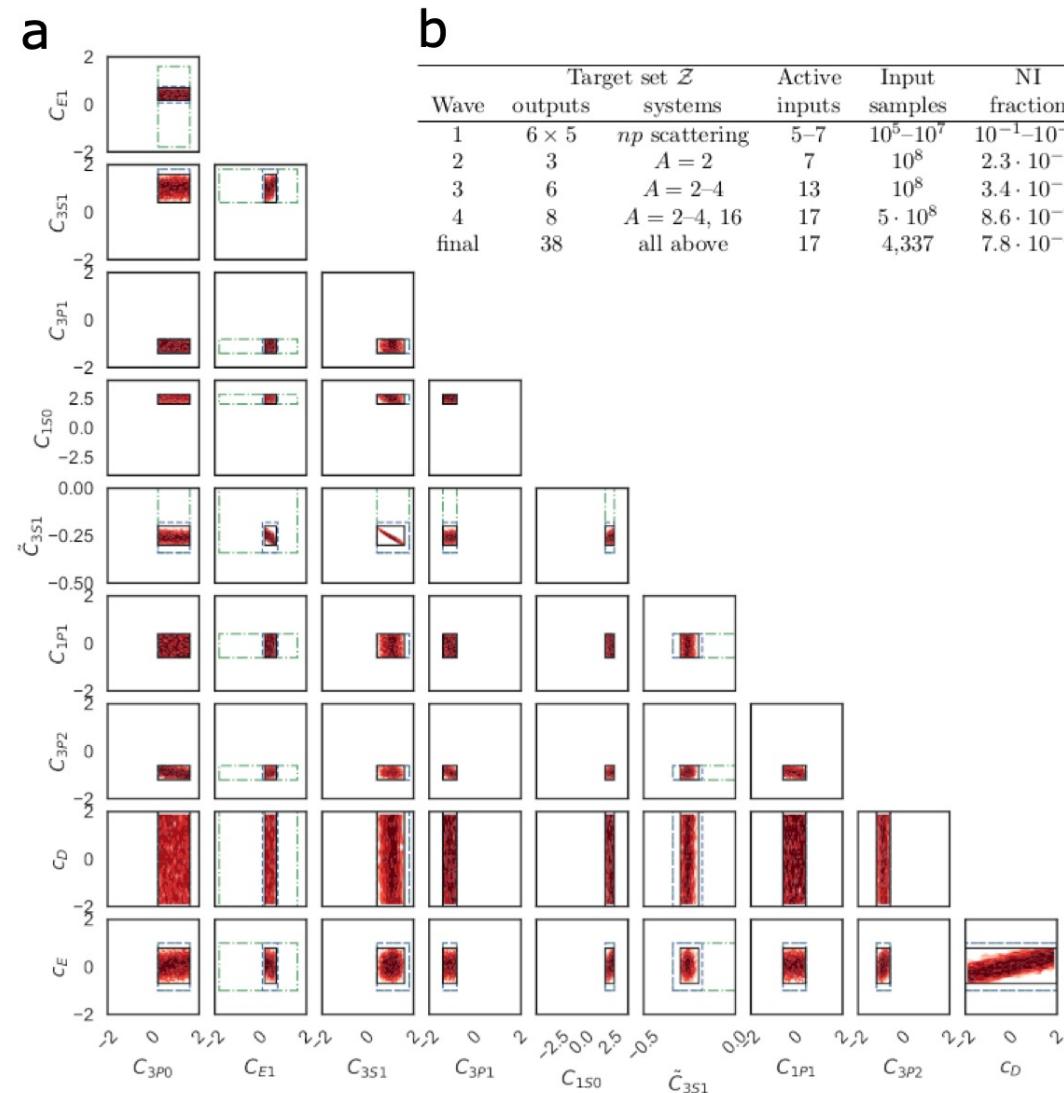
Non-imausible interactions

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- Sequentially rule out the possibility:



Error assignments

History-matching observables						
Observable	z	ε_{exp}	$\varepsilon_{\text{model}}$	$\varepsilon_{\text{method}}$	ε_{em}	PPD
$E(^2\text{H})$	-2.2246	0.0	0.05	0.0005	0.001%	$-2.22^{+0.07}_{-0.07}$
$R_p(^2\text{H})$	1.976	0.0	0.005	0.0002	0.0005%	$1.98^{+0.01}_{-0.01}$
$Q(^2\text{H})$	0.27	0.01	0.003	0.0005	0.001%	$0.28^{+0.02}_{-0.02}$
$E(^3\text{H})$	-8.4821	0.0	0.17	0.0005	0.01%	$-8.54^{+0.34}_{-0.37}$
$E(^4\text{He})$	-28.2957	0.0	0.55	0.0005	0.01%	$-28.86^{+0.86}_{-1.01}$
$R_p(^4\text{He})$	1.455	0.0	0.016	0.0002	0.003%	$1.47^{+0.03}_{-0.03}$
$E(^{16}\text{O})$	127.62	0.0	1.0	0.75	0.5%	$-126.2^{+3.0}_{-2.8}$
$R_p(^{16}\text{O})$	2.58	0.0	0.03	0.01	0.5%	$2.57^{+0.06}_{-0.06}$

Calibration observables						
Observable	z	ε_{exp}	$\varepsilon_{\text{model}}$	$\varepsilon_{\text{method}}$	ε_{em}	PPD
$E/A(^{48}\text{Ca})$	-8.667	0.0	0.54	0.25	—	$-8.58^{+0.72}_{-0.72}$
$E_{2+}(^{48}\text{Ca})$	3.83	0.0	0.5	0.5	—	$3.79^{+0.86}_{-0.96}$
$R_p(^{48}\text{Ca})$	3.39	0.0	0.11	0.03	—	$3.36^{+0.14}_{-0.13}$

Validation observables						
Observable	z	ε_{exp}	$\varepsilon_{\text{model}}$	$\varepsilon_{\text{method}}$	ε_{em}	PPD
$E/A(^{208}\text{Pb})$	-7.867	0.0	0.54	0.5	—	$-8.06^{+0.99}_{-0.88}$
$R_p(^{208}\text{Pb})$	5.45	0.0	0.17	0.05	—	$5.43^{+0.21}_{-0.23}$
$\alpha_D(^{48}\text{Ca})$	2.07	0.22	0.06	0.1	—	$2.30^{+0.31}_{-0.26}$
$\alpha_D(^{208}\text{Pb})$	20.1	0.6	0.59	0.8	—	$22.6^{+2.1}_{-1.8}$

Error assignments

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