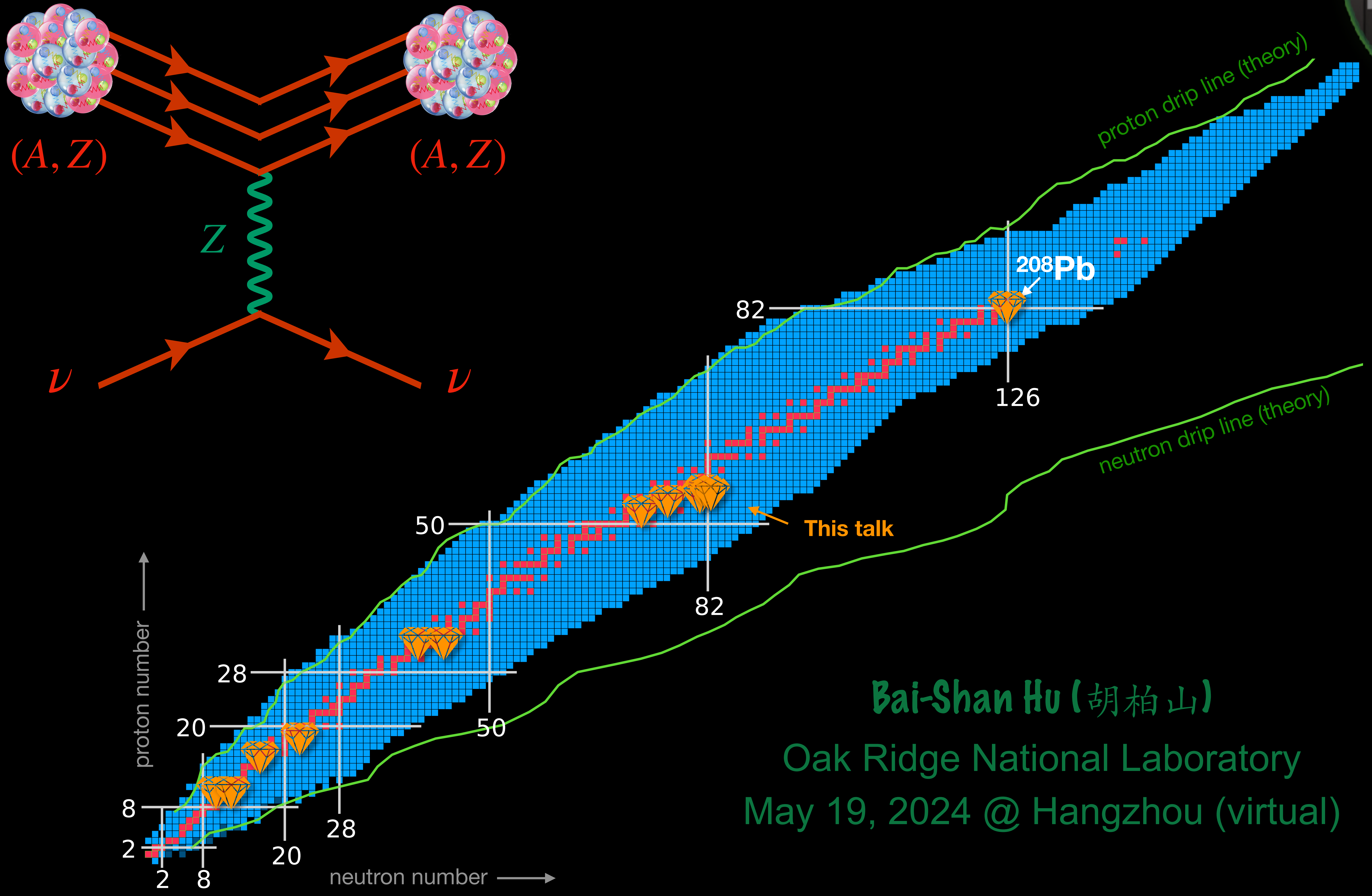
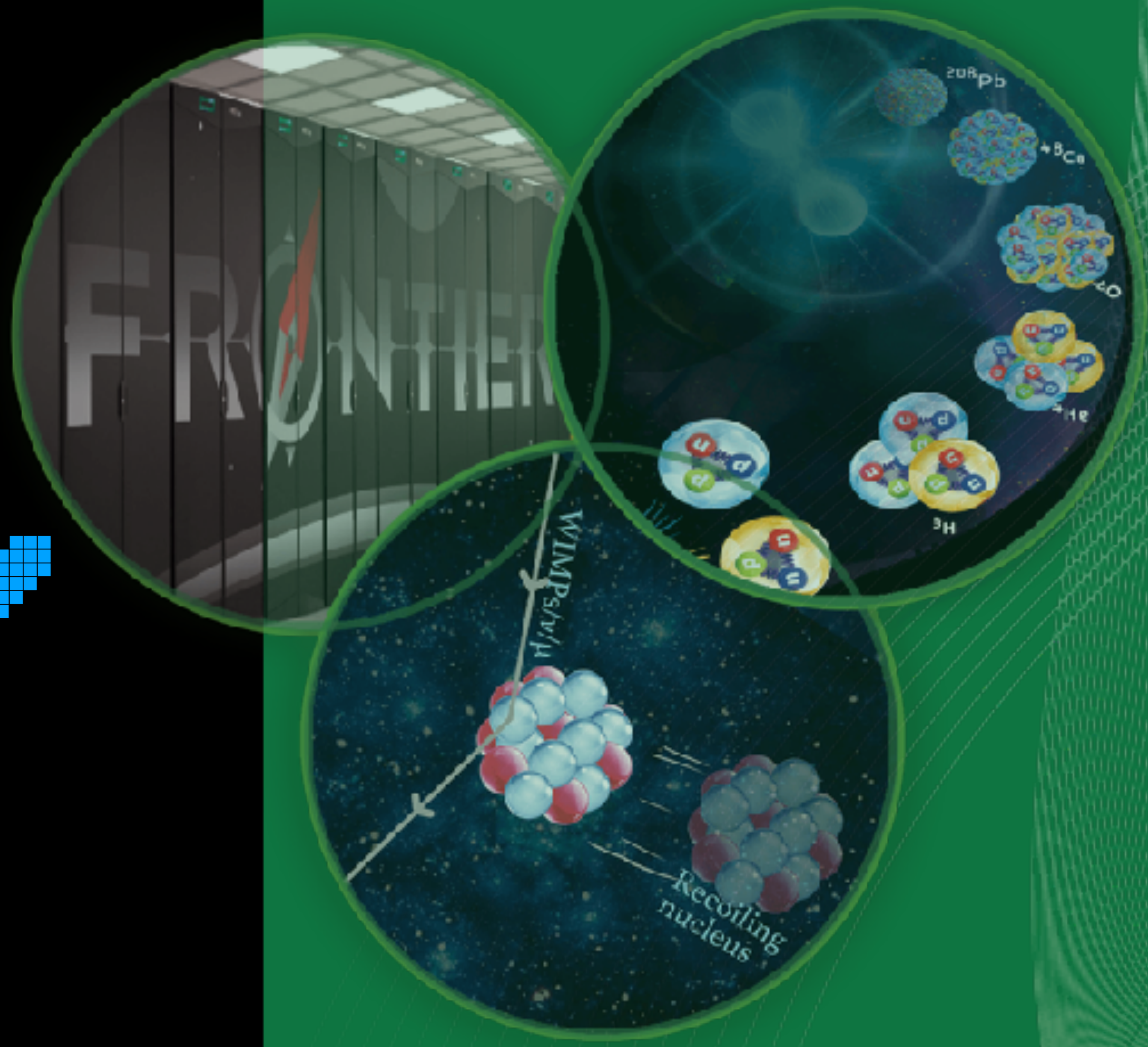
Ab initio Nuclear Theory for neutrino-nucleus scattering





Bai-Shan Hu (胡柏山)

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May 19, 2024 @ Hangzhou (virtual)

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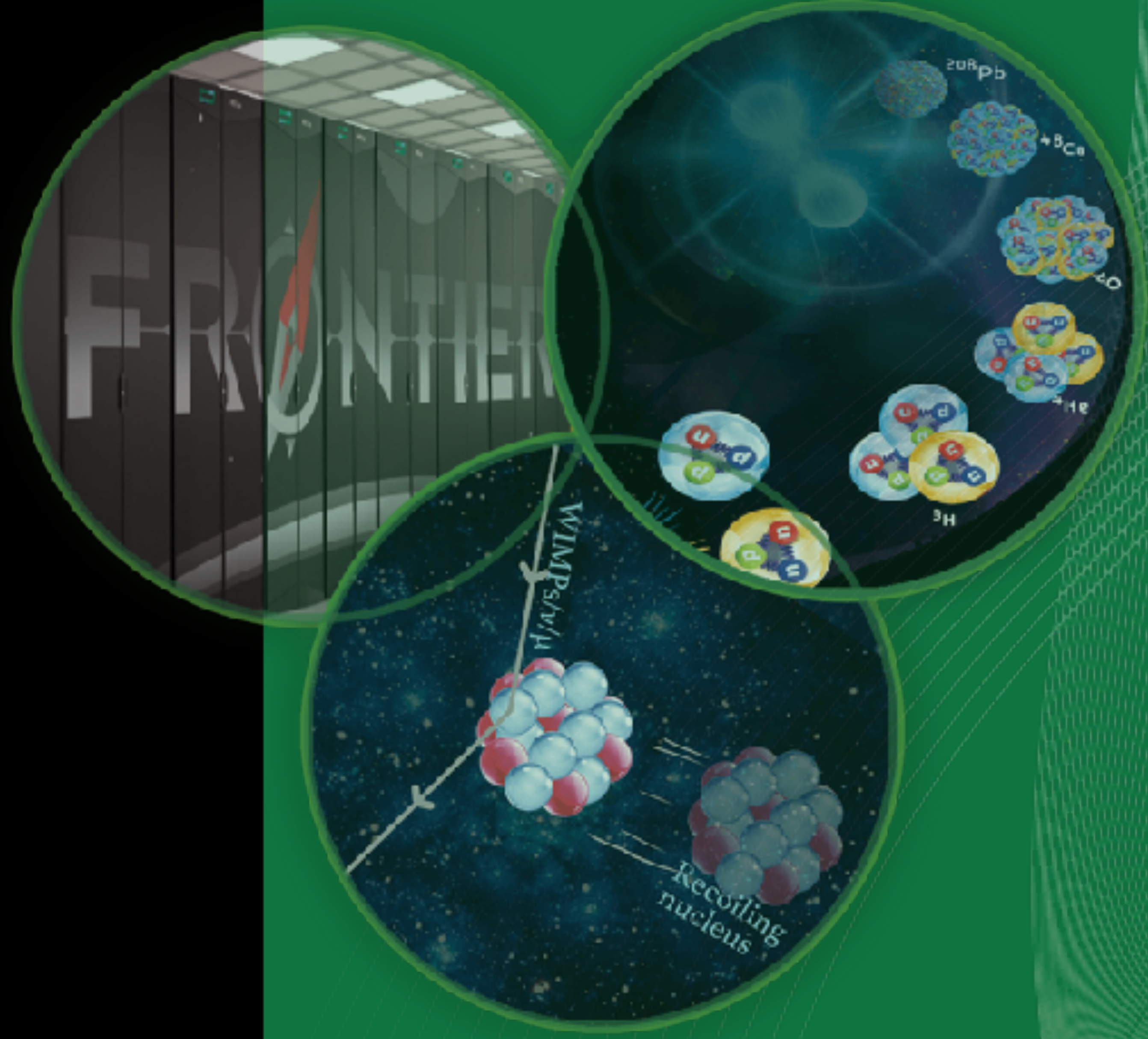

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Outline

What is *ab initio* nuclear calculation?

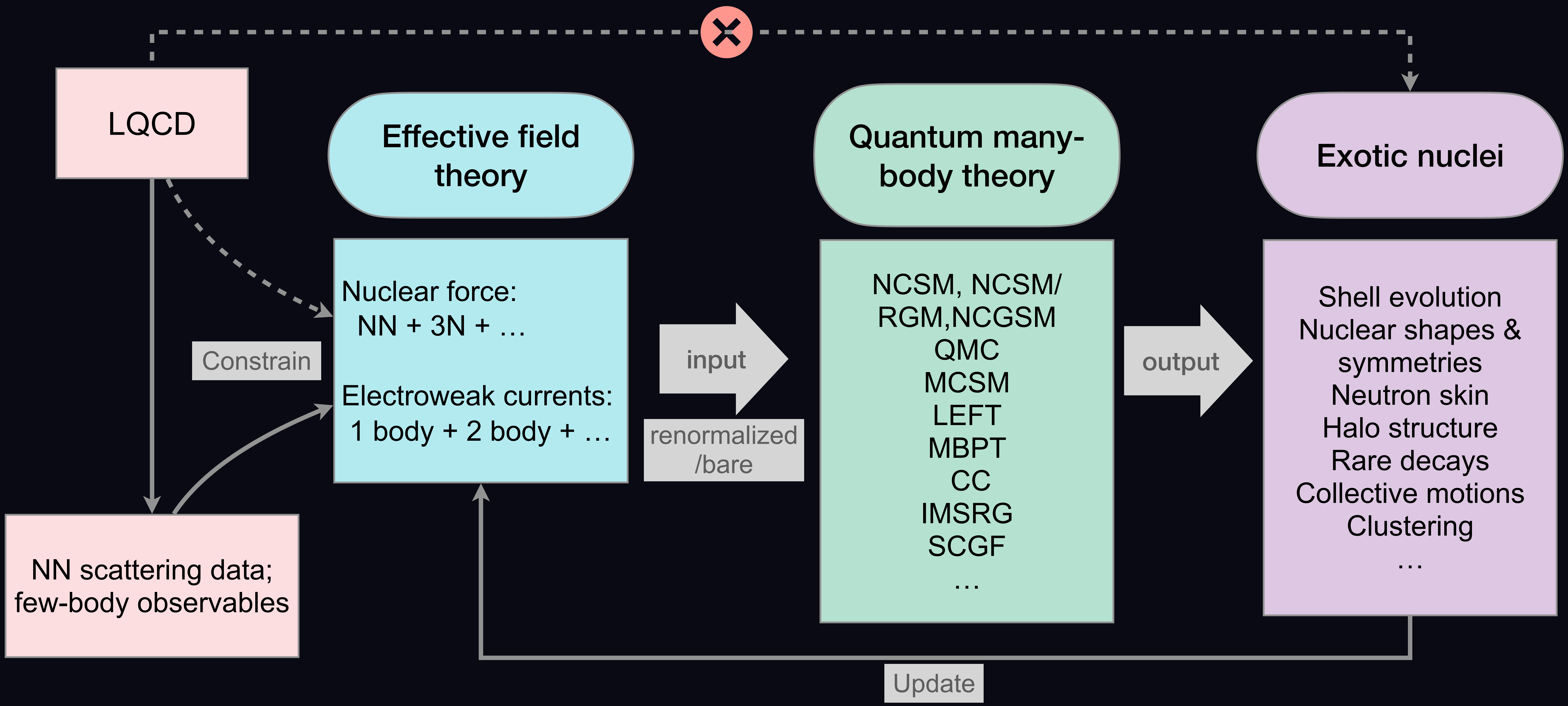
Elastic ν-nucleus scattering

Inelastic charged and neutral current ν-nucleus scattering

Summary

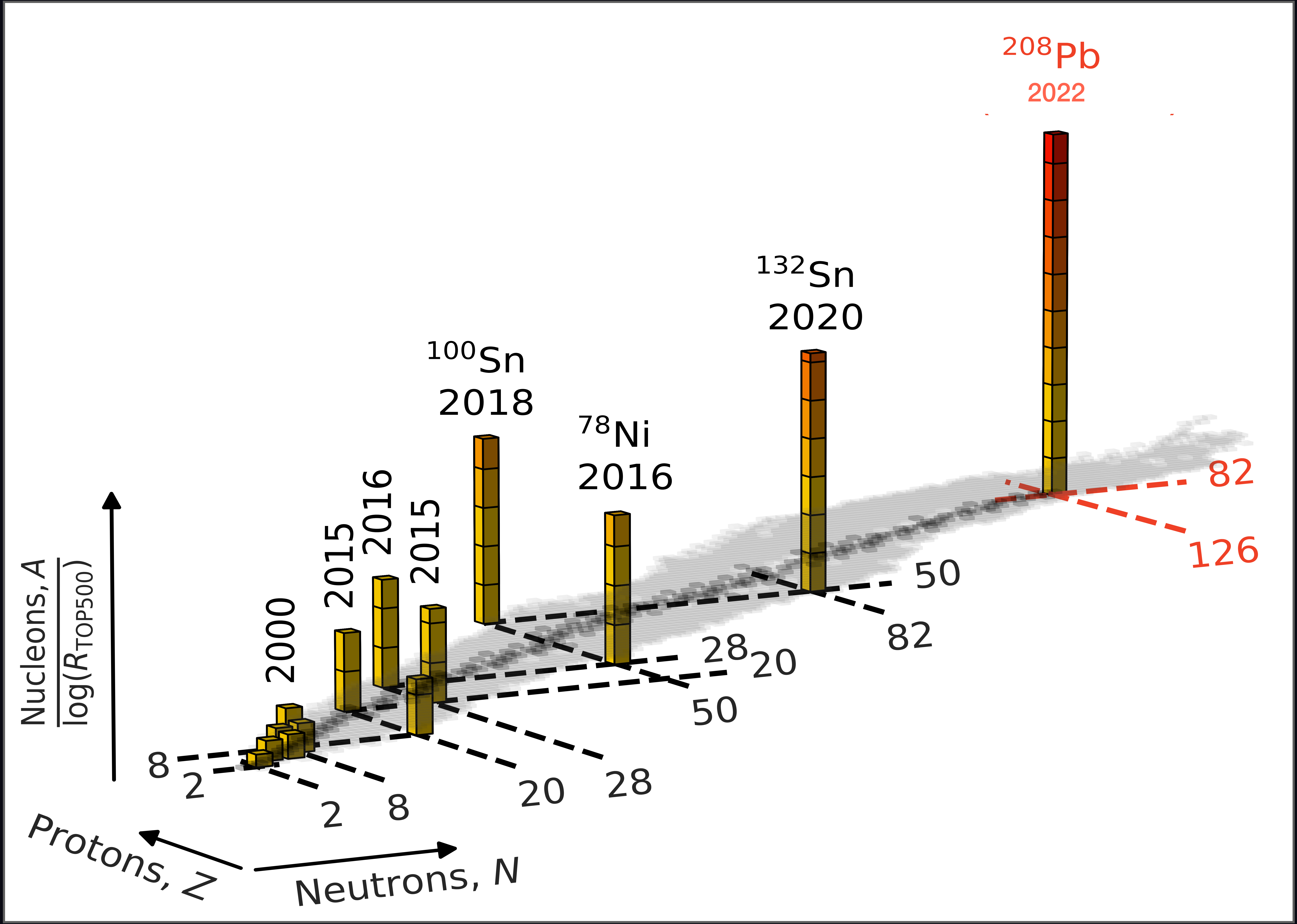
I. *Ab initio* nuclear theory for neutrino-nucleus scattering

Workflow of *ab initio* nuclear calculation

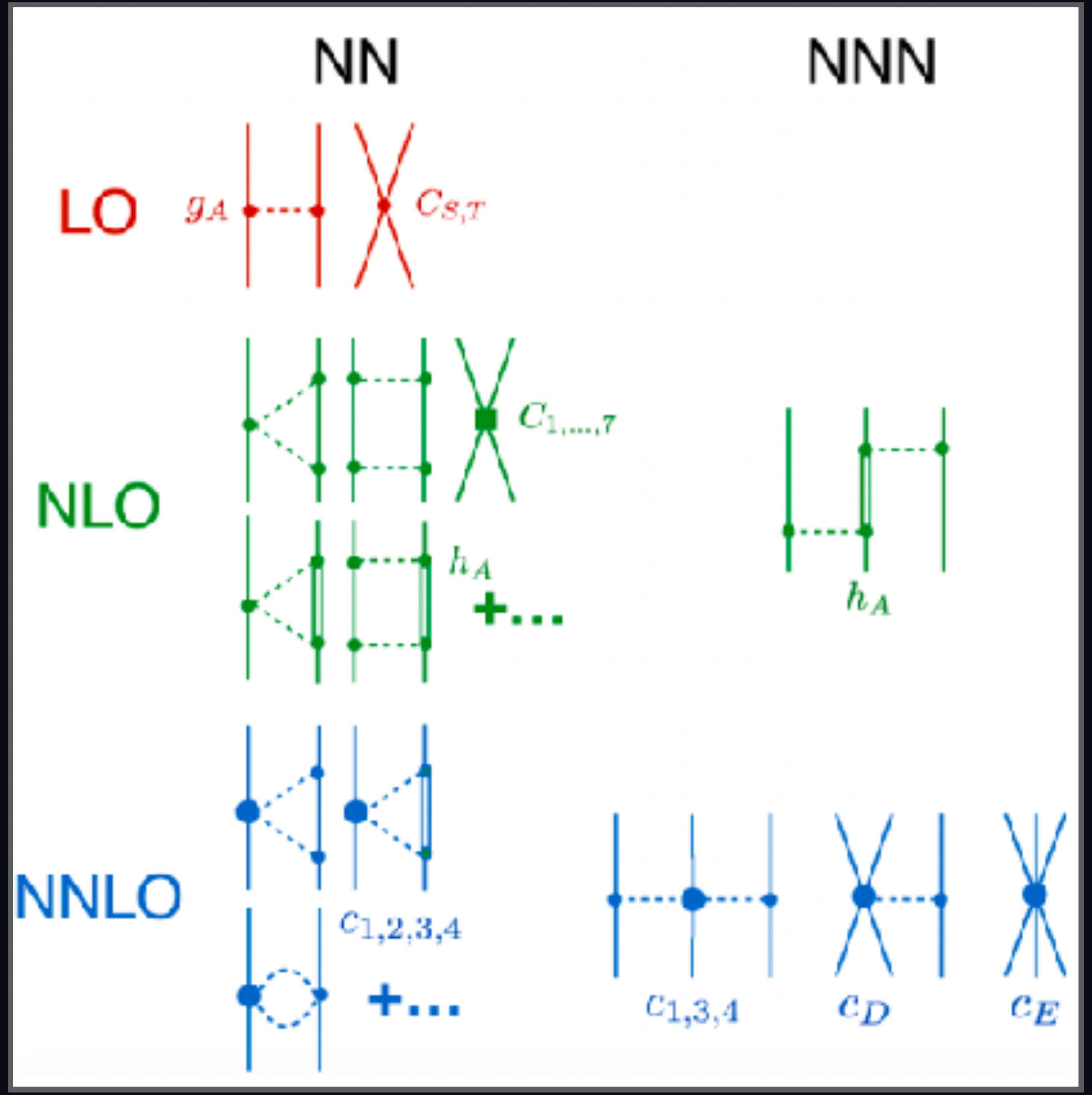


Y L Ye, X F Yang, H Sakurai and BSHu. Invited review article, Nature Reviews Physics (2024)

Ab initio calculation of ^{208}Pb

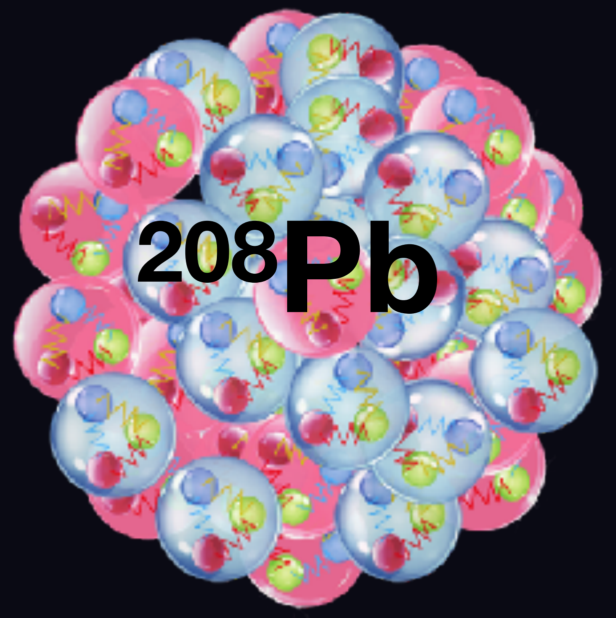


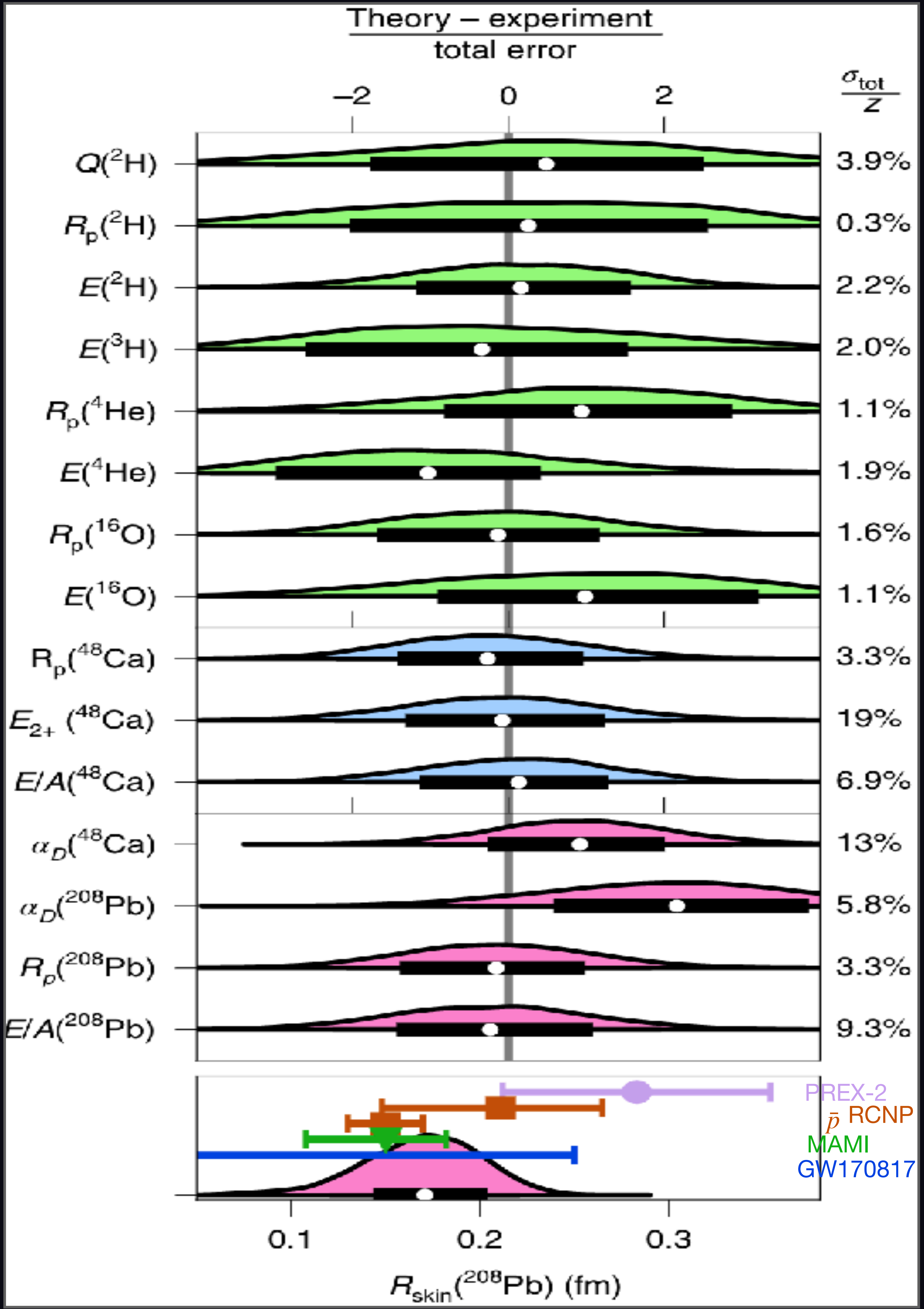
BSHu, W G Jiang, T Miyagi, Z H Sun, et al., Nat Phys 18, 1196 (2022)



History matching
Emulator technology
Bayesian statistics

IMSRG, CC

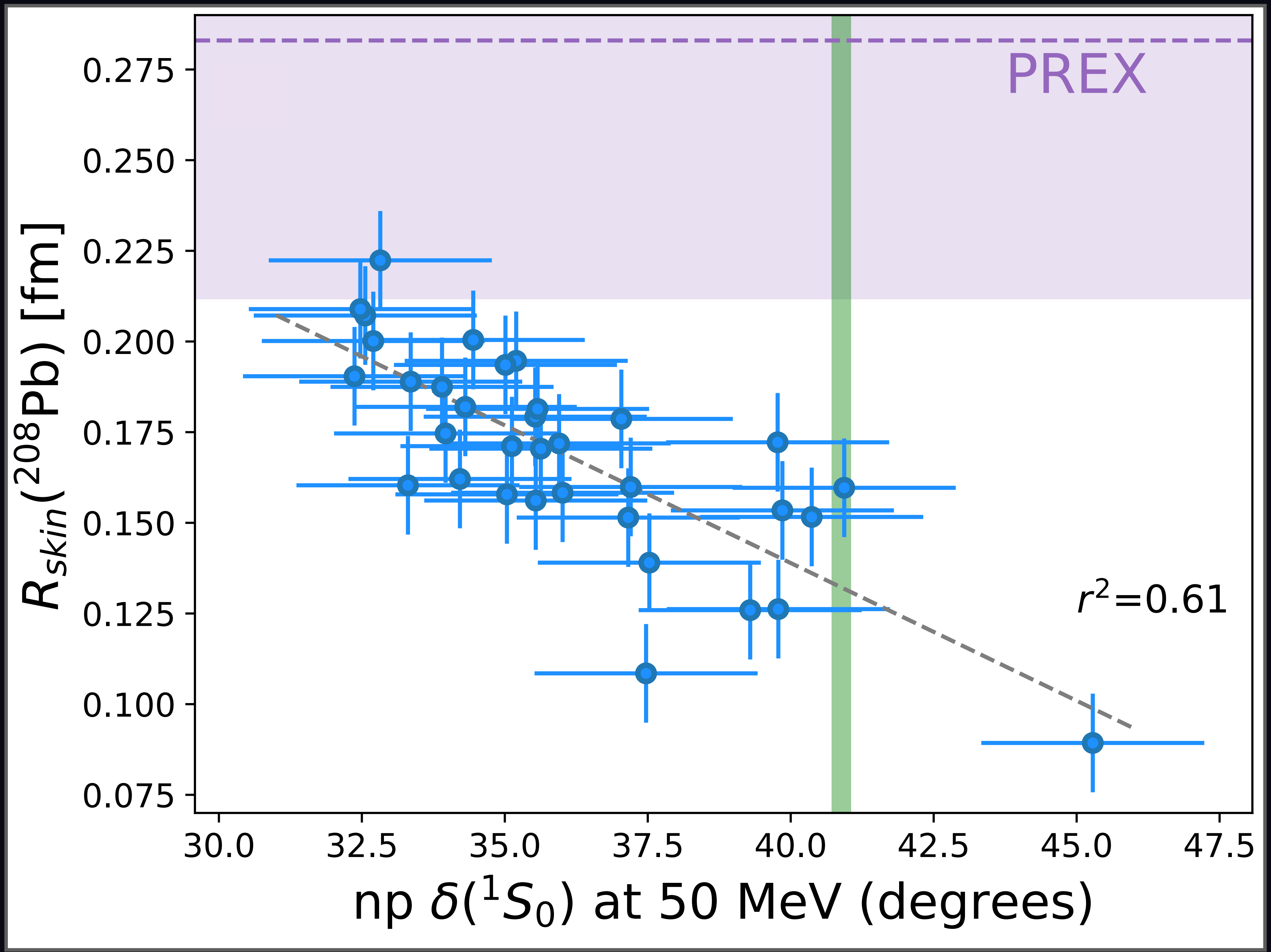




History matching identifies samples of non-implausible interaction at NNLO (34 out of 10^9 parameterizations)

Likelihood calibration yields probability distribution

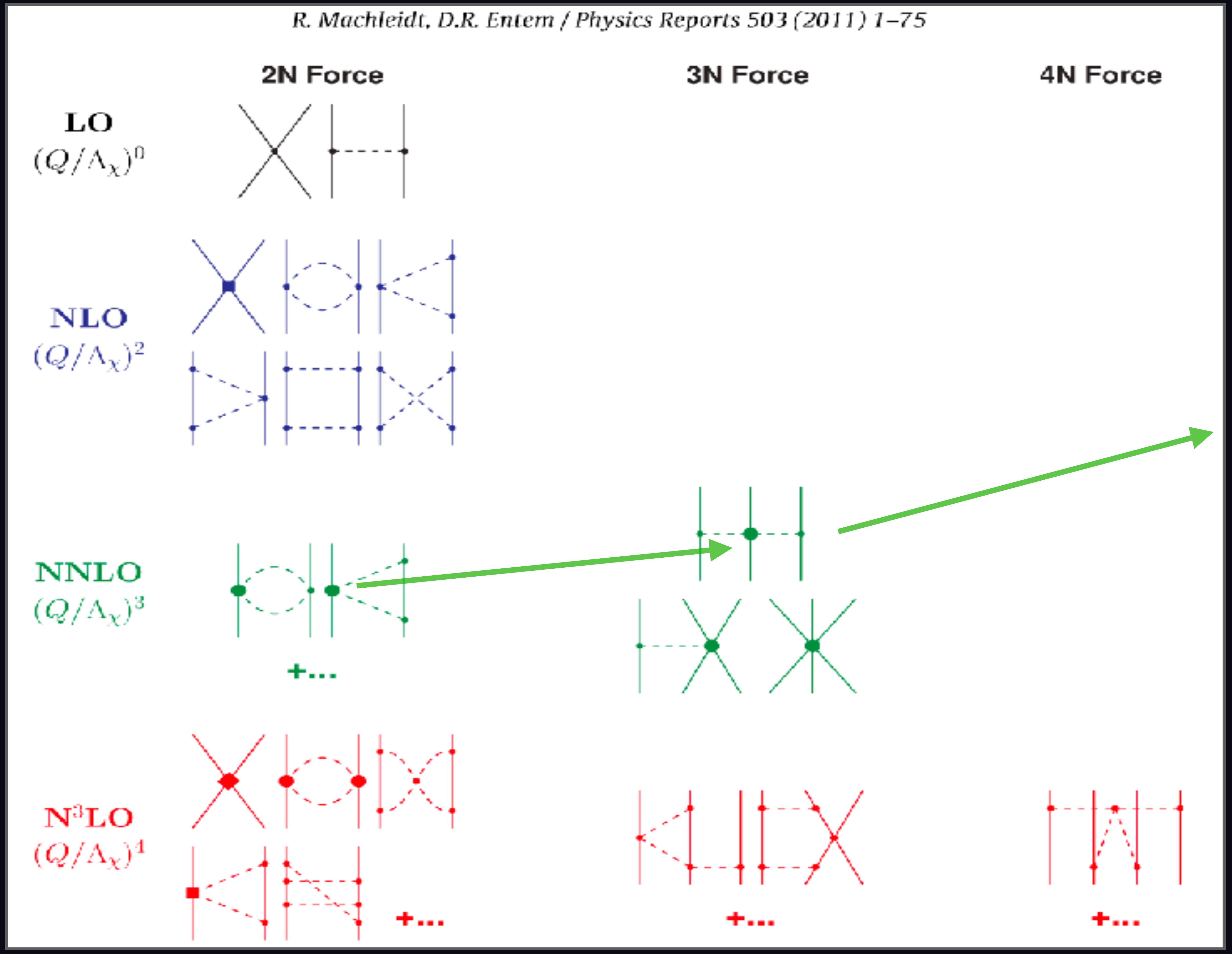
Pure predictions for observables in ^{208}Pb

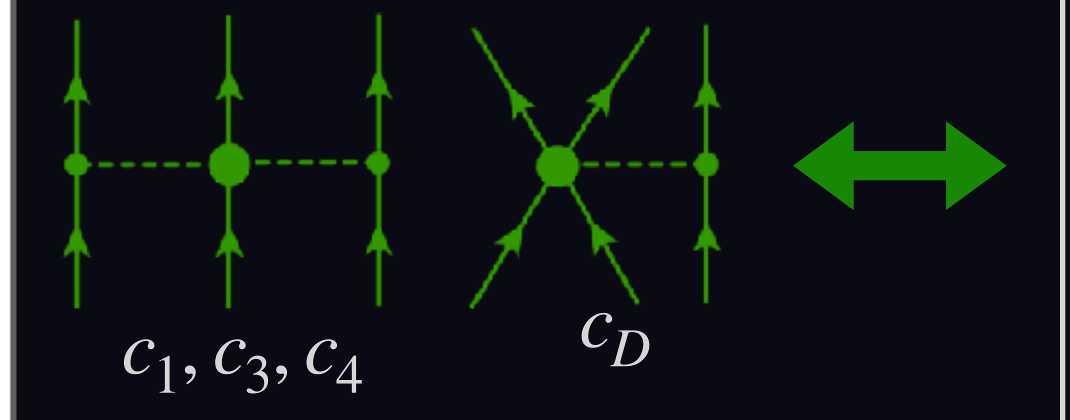


- Agreement with *NN* scattering data in 1S0 channel precludes large neutron skin
- CEvNS mainly probes neutron distribution, neutron skin is important for CEvNS

BSHu, et al., Nat Phys 18, 1196 (2022)

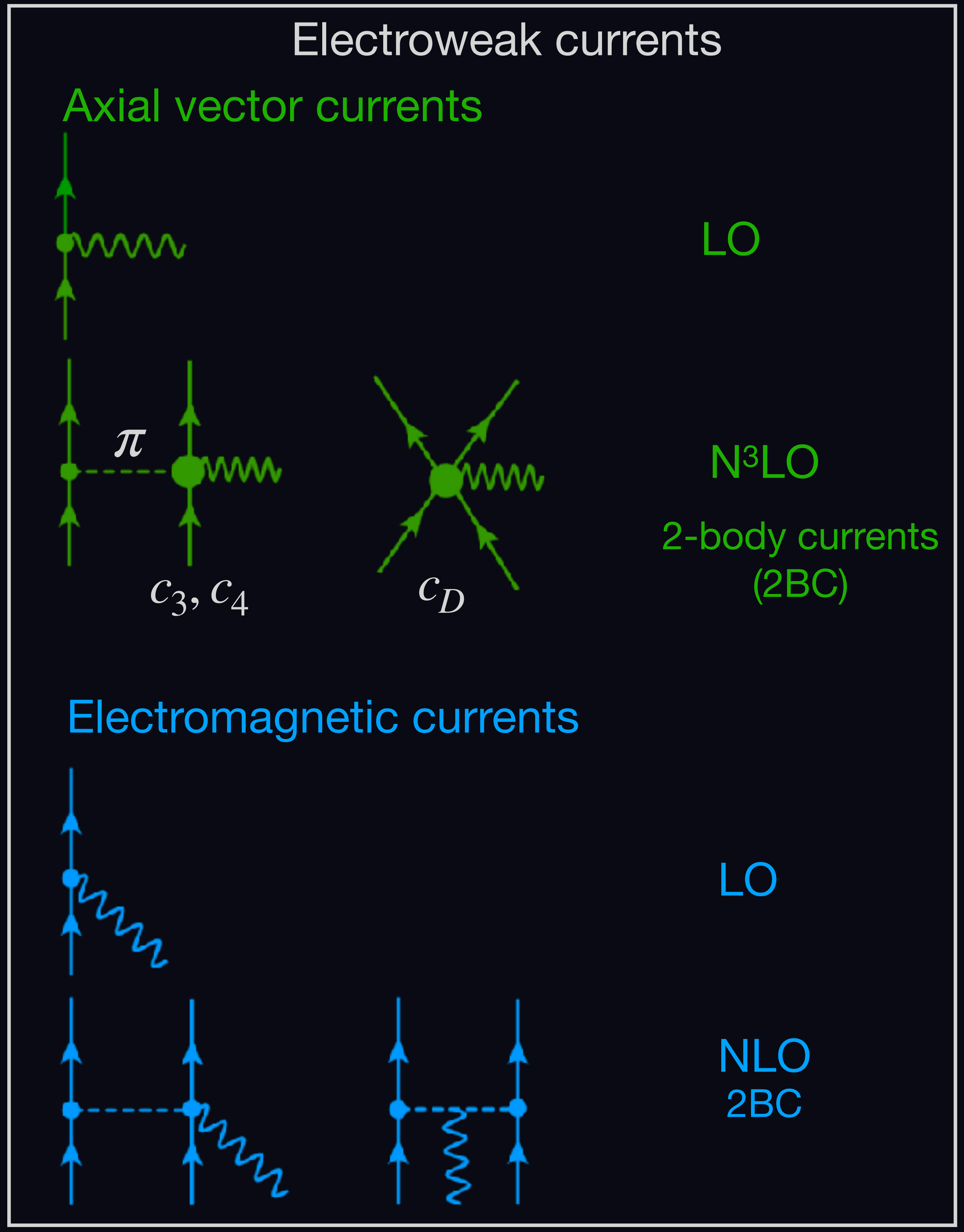
Electroweak two-body current (2BC) is important





Chiral EFT provides a systematic scheme for constructing consistent interactions & currents

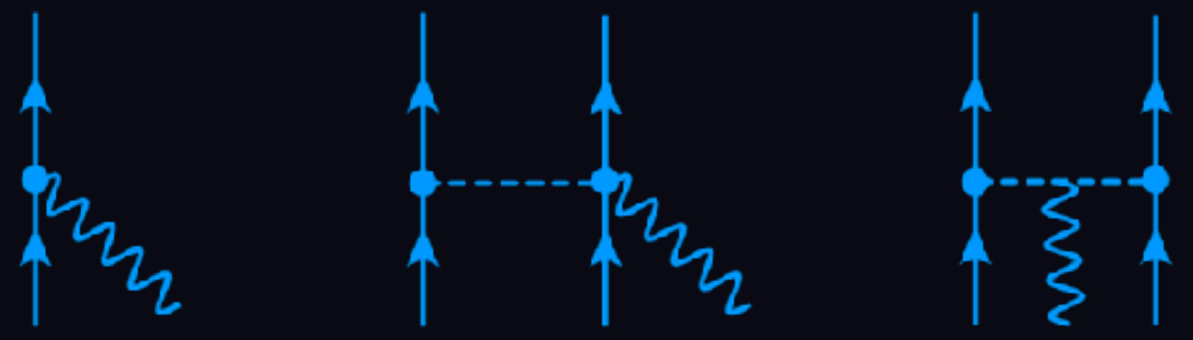
Quantifiable uncertainties

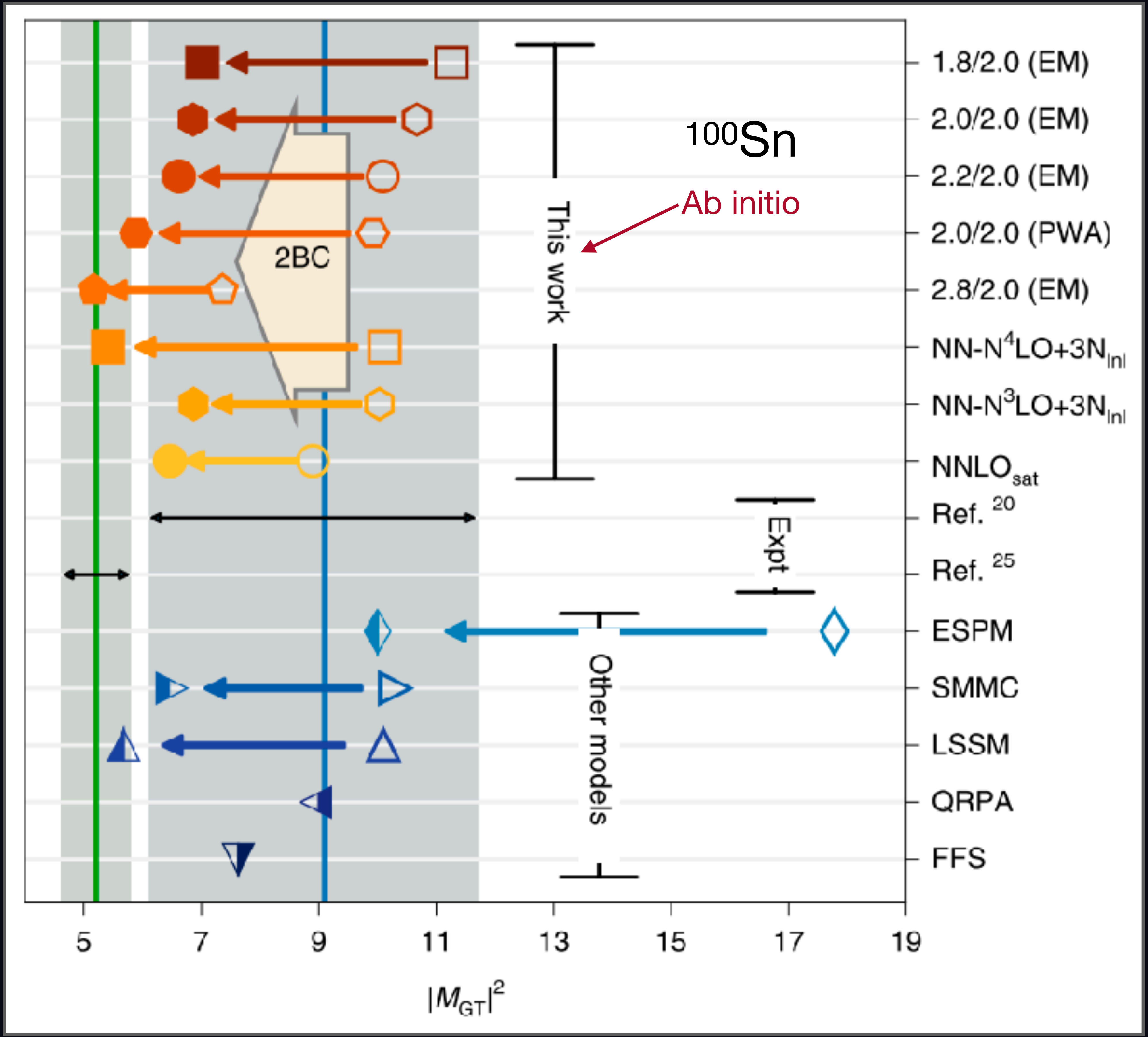


2BC is important

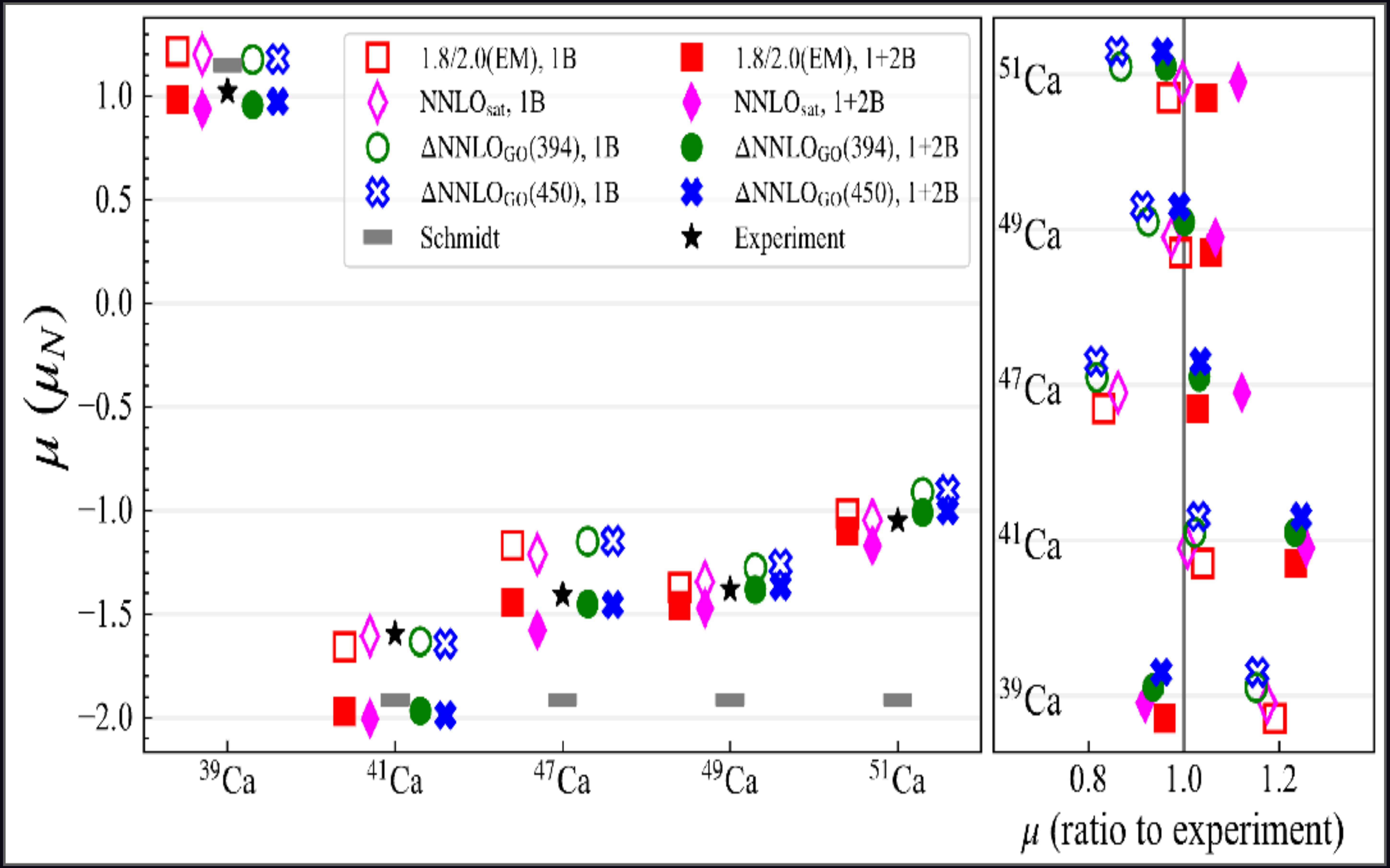
Gamow-Teller strength

magnetic moments
magnetic dipole transition moments





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



B Acharya, BSHu, et al., arXiv:2311.11438 (2023)
Accepted by Phys Rev Lett (2024)

II. *Ab initio* nuclear theory for CEvNS

Coherent Elastic Neutrino-Nucleus Scattering (CEνNS)

A neutrino interacts a nucleus via exchange of a Z, and the nucleus recoils as a whole

- 1960s: “theory of the unified weak and electromagnetic interaction, and prediction of the weak neutral current”
  Sheldon Glashow, Abdus Salam, and Steven Weinberg

1979

- 1973: discovery of a weak neutral current in a neutrino experiment at CERN
  F.J. Hasert *et al.*, Phys Lett B 46, 138 (1973)

- 1974: CE*ν*NS suggested by Daniel Freedman
  D.Z. Freedman, Phys Rew D 9, 1389 (1974)

- 2017: Observation of CE*ν*NS by COHERENT collaboration
  D. Akimov et al. (COHERENT). Science 357, 1123 (2017)

CEvNS differential cross section

$$\frac{d\sigma_A}{dT}(E_\nu, T) = \frac{G_F^2 M_A}{4\pi}\left(1 - \frac{M_A T}{2E_\nu^2} - \frac{T}{E_\nu}\right) Q_w^2 \left|F_w(\mathbf{q}^2)\right|^2 + \frac{G_F^2 M_A}{4\pi}\left(1 + \frac{M_A T}{2E_\nu^2} - \frac{T}{E_\nu}\right) F_A(\mathbf{q}^2)$$

- Weak charge

  $Q_w = ZQ_w^p + NQ_w^n$

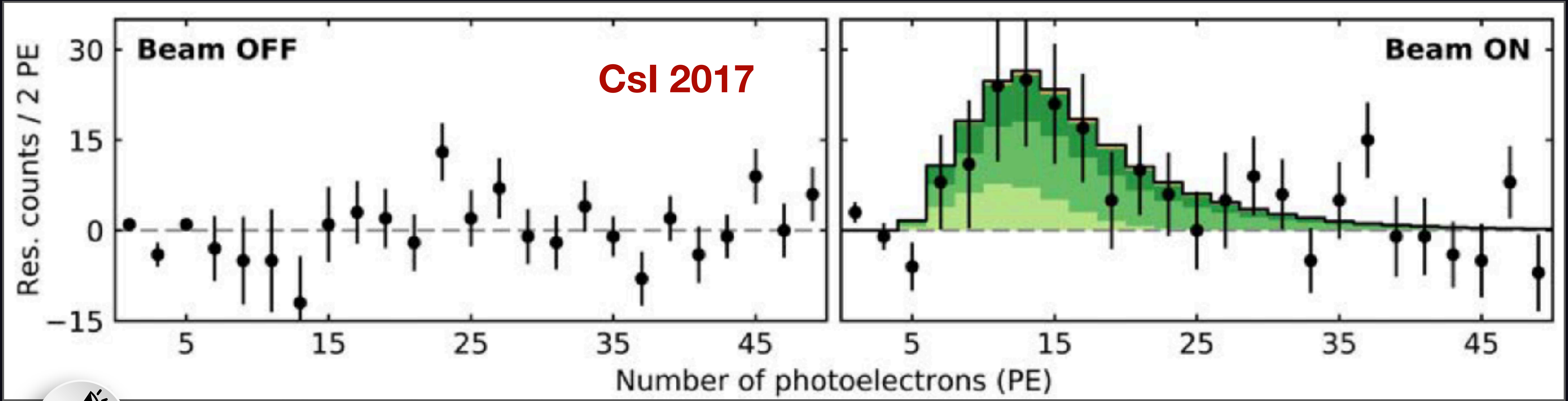
  $Q_w^p = 0.0714,\ Q_w^n = -0.9900$?

  Radiative corrections ?

  CEvNS mainly probes neutron distribution

- Nuclear weak form factor F_W
- Axial-vector form factor F_A

  Negligible ?



5% level non-negligible uncertainty from weak form factor F_W

D Akimov et al. (COHERENT). Science 357, 1123 (2017)

Chiral EFT: Systematic expansion of nuclear forces and electroweak currents

$$
\begin{aligned}
F_{\mathrm{w}}\left(\mathbf{q}^2\right) = \;& \frac{1}{Q_{\mathrm{w}}}\left\{\left[Q_{\mathrm{w}}^p\left(1-\frac{\langle r_E^2\rangle^p}{6}q^2-\frac{1}{8m_{\mathcal{N}}^2}q^2\right)-Q_{\mathrm{w}}^n\frac{\langle r_E^2\rangle^n+\langle r_{E,s}^2\rangle^N}{6}q^2\right]\mathcal{F}_p^M\left(\mathbf{q}^2\right)\right.\\
&+\left[Q_{\mathrm{w}}^n\left(1-\frac{\langle r_E^2\rangle^p+\langle r_{E,s}^2\rangle^N}{6}q^2-\frac{1}{8m_{\mathcal{N}}^2}q^2\right)-Q_{\mathrm{w}}^p\frac{\langle r_E^2\rangle^n}{6}q^2\right]\mathcal{F}_n^M\left(\mathbf{q}^2\right)\\
&+\frac{Q_{\mathrm{w}}^p\left(1+2\kappa^p\right)+2Q_{\mathrm{w}}^n\left(\kappa^n+\kappa_s^N\right)}{4m_{\mathcal{N}}^2}q^2\mathcal{F}_p^{\Phi''}\left(\mathbf{q}^2\right)\\
&\left.+\frac{Q_{\mathrm{w}}^n\left(1+2\kappa^p+2\kappa_s^N\right)+2Q_{\mathrm{w}}^p\kappa^n}{4m_{\mathcal{N}}^2}q^2\mathcal{F}_n^{\Phi''}\left(\mathbf{q}^2\right)\right\}.
\end{aligned}
$$

$$
F_A\left(\mathbf{q}^2\right) = \frac{8\pi}{2J+1}\left[\left(g_A^{s,N}\right)^2S_{00}^{\mathcal{T}}\left(\mathbf{q}^2\right)-g_Ag_A^{s,N}S_{01}^{\mathcal{T}}\left(\mathbf{q}^2\right)+\left(g_A\right)^2S_{11}^{\mathcal{T}}\left(\mathbf{q}^2\right)\right]
$$

$$
S_{00}^{\mathcal{T}} = \sum_L\left[\mathcal{F}_+^{\Sigma_L'}\left(\mathbf{q}^2\right)\right]^2,
$$

$$
S_{11}^{\mathcal{T}} = \sum_L\left[\left[1+\delta'\left(\mathbf{q}^2\right)\right]\mathcal{F}_-^{\Sigma_L'}\left(\mathbf{q}^2\right)\right]^2,
$$

$$
S_{01}^{\mathcal{T}} = \sum_L 2\left[1+\delta'\left(\mathbf{q}^2\right)\right]\mathcal{F}_+^{\Sigma_L'}\left(\mathbf{q}^2\right)\mathcal{F}_-^{\Sigma_L'}\left(\mathbf{q}^2\right).
$$

Details:
M. Hoferichter et al., PRD 102 (2020) 074018
L.A. Ruso et al., arXiv:2203.09030 (2022)

Nuclear response functions

- $\mathcal{F}_\tau^M$: mainly from neutron distribution
- $\mathcal{F}_\tau^{\Phi''}$: spin-orbit correction
- $\mathcal{F}_\tau^{\Sigma'}$: axial-vector contribution; two-body currents important

Leading order contribution in elastic ν-Nucleus scattering

- nuclear density M_{00}

$$\mathcal{F}^M(q^2) = \int e^{i\vec{q}\cdot\vec{r}}\rho(r)d^3\vec{r}$$

CEvNS mainly probes neutron distribution;
This dominant nuclear response is usually assumed to be equal for proton and neutron. But this is clearly not the case.

- nuclear spin current

$$\Sigma'_{LM;\tau}(q) \qquad \Sigma'_{1M;\tau}(q) \xrightarrow{q\to 0} \frac{1}{\sqrt{6\pi}}\sum_{i=1}^{A}\sigma_{1M}$$

$$\Sigma''_{LM;\tau}(q) \qquad \Sigma''_{1M;\tau}(q) \xrightarrow{q\to 0} \frac{1}{\sqrt{12\pi}}\sum_{i=1}^{A}\sigma_{1M}$$

spin expectation values

- phenomenological Helm form factor

ρ(*r*) is assumed to be a uniform density with radius R_0 and a Gaussian profile with a folding width *s*

$$\mathcal{F}^{\text{Helm}}(q^2) = \frac{3j_1\left(qR_0\right)}{qR_0}\mathrm{e}^{-q^2s^2/2}$$

$$R_0^2 = c^2 + \frac{7}{3}\pi^2a^2 - 5s^2$$

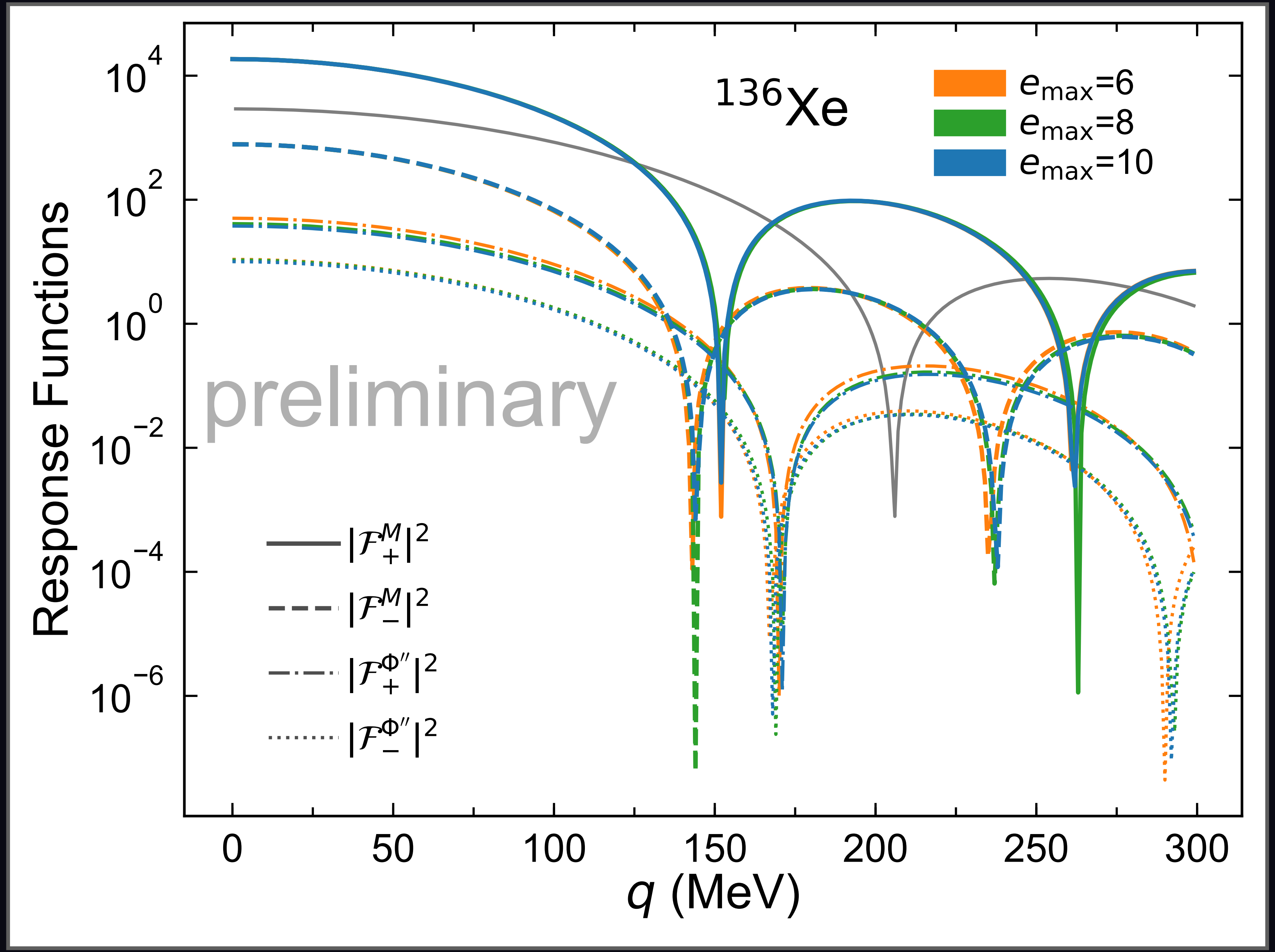
$$c = (1.23A^{1/3} - 0.60),\ a = 0.52,\ s = 0.9\ \text{fm}$$

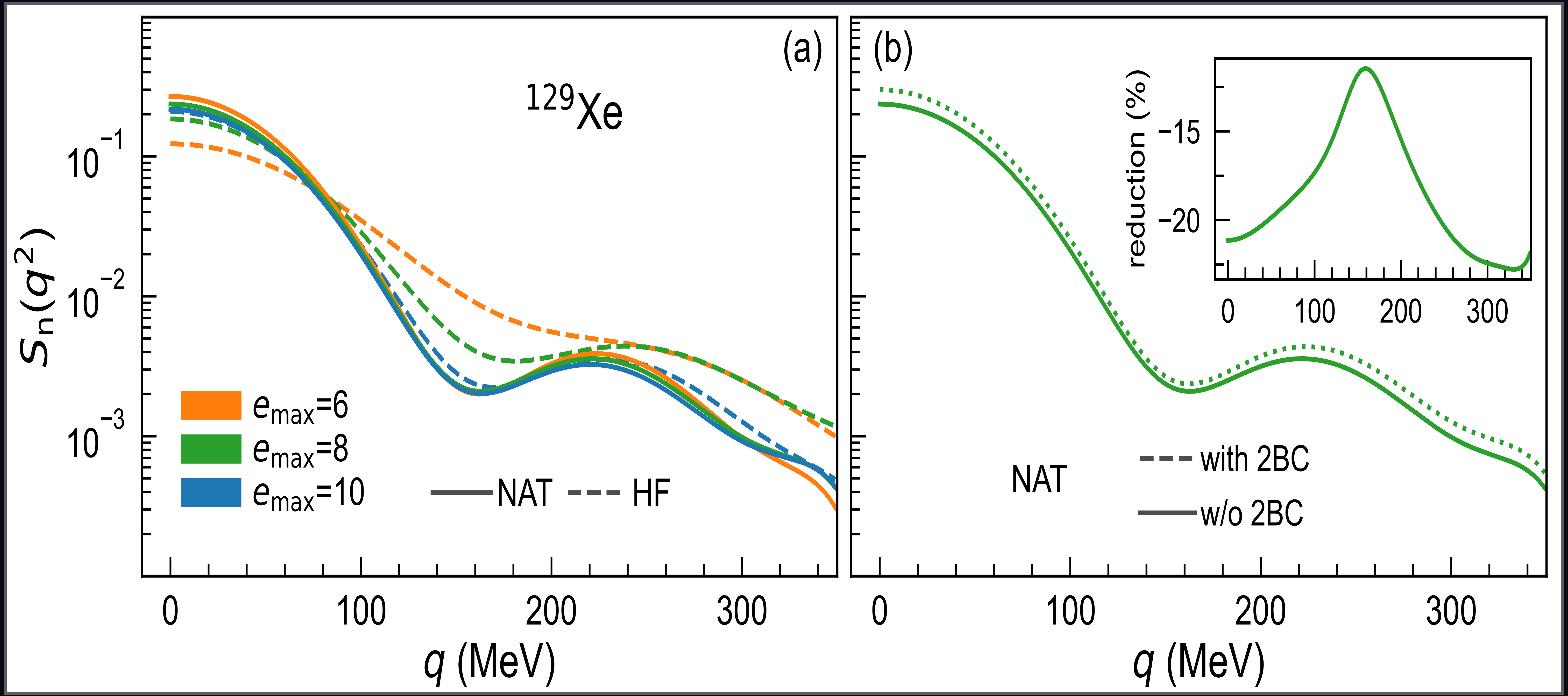
Heavy nuclei is challenging current *ab-initio* approaches

- Tensor operators are very heavy tasks
- Many q points (operators) need to calculate

$\underbrace{\mathcal{F}_\tau^{M},\ \mathcal{F}_\tau^{\Phi''}}$

$\underbrace{\mathcal{F}_\tau^{\Sigma'},\ \mathcal{F}_\tau^{\Sigma''}}$





BSHu, et al, Phys Rev Lett 128, 072502 (2022)

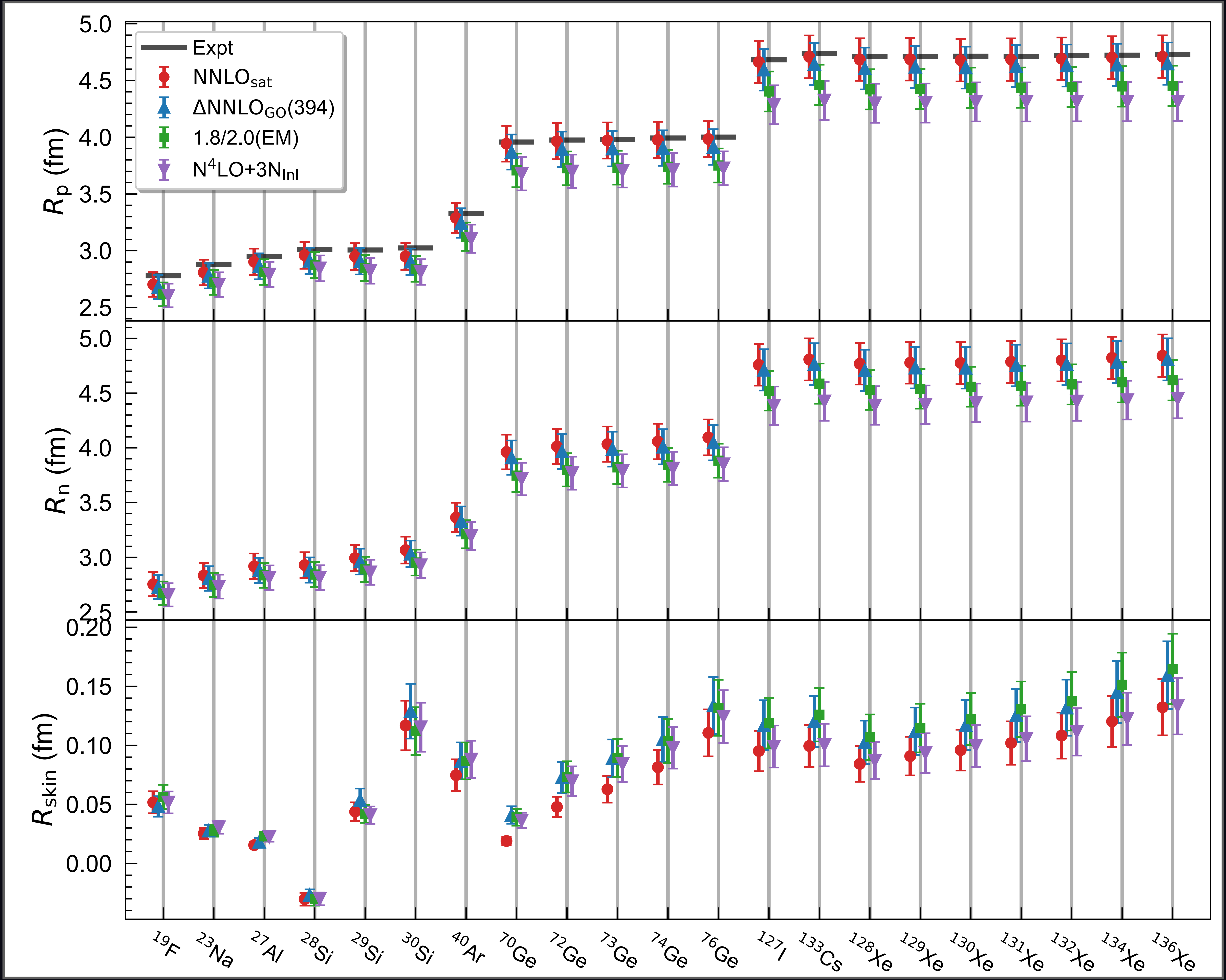
Natural orbitals (NAT)
allows heavy nuclei

A. Tichai, et al., Phys Rew C 99, 034321 (2019)

$$\rho_{pq} = \left\langle \Psi \left| c_p^\dagger c_q \right| \Psi \right\rangle$$

MBPT ⇨ $|\Psi\rangle \approx \left|\Psi^{(0)}\right\rangle + \left|\Psi^{(1)}\right\rangle + \left|\Psi^{(2)}\right\rangle$

Ab initio results of nuclear radii

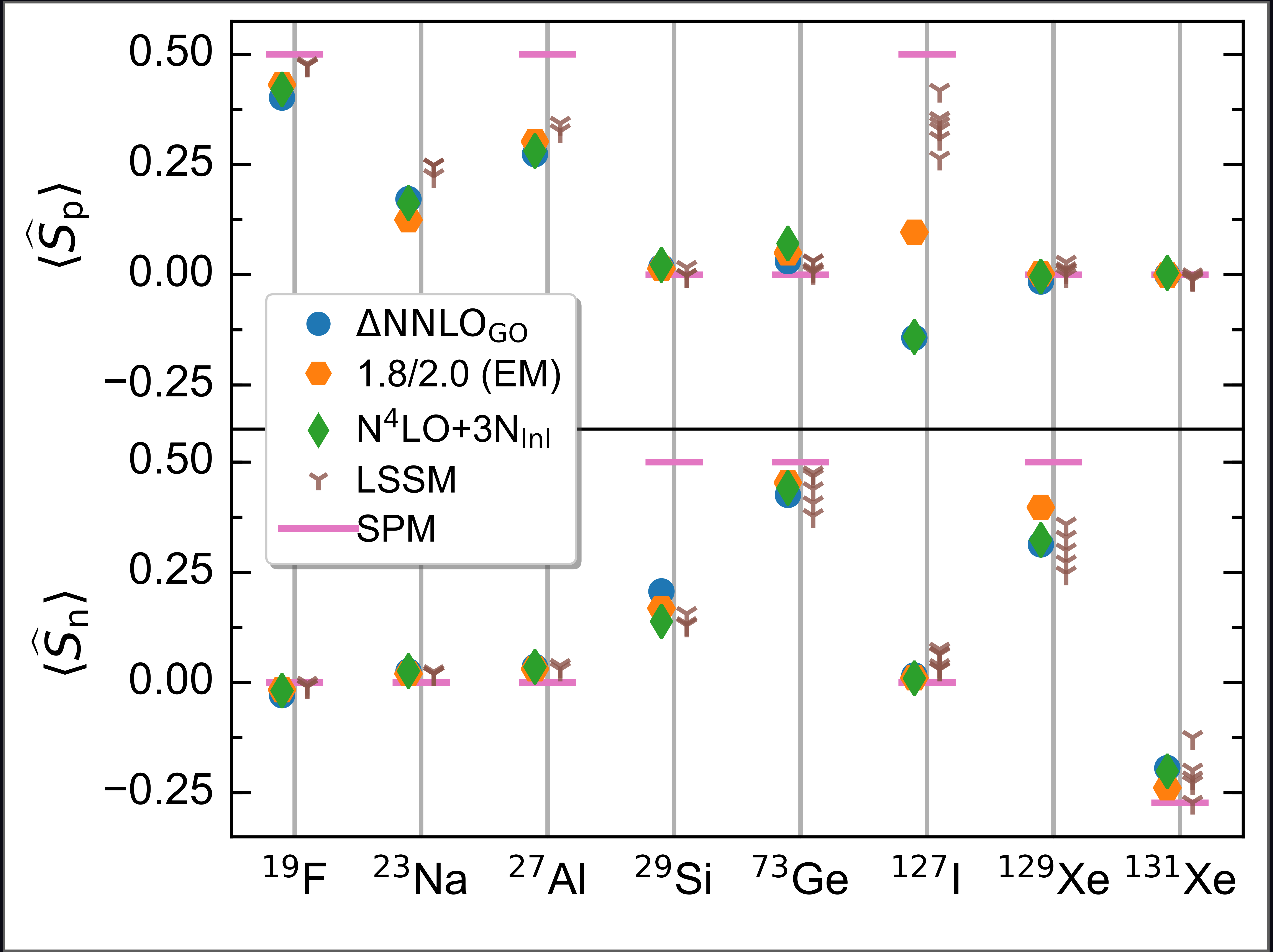


BSHu, et al., In preparation (2024)

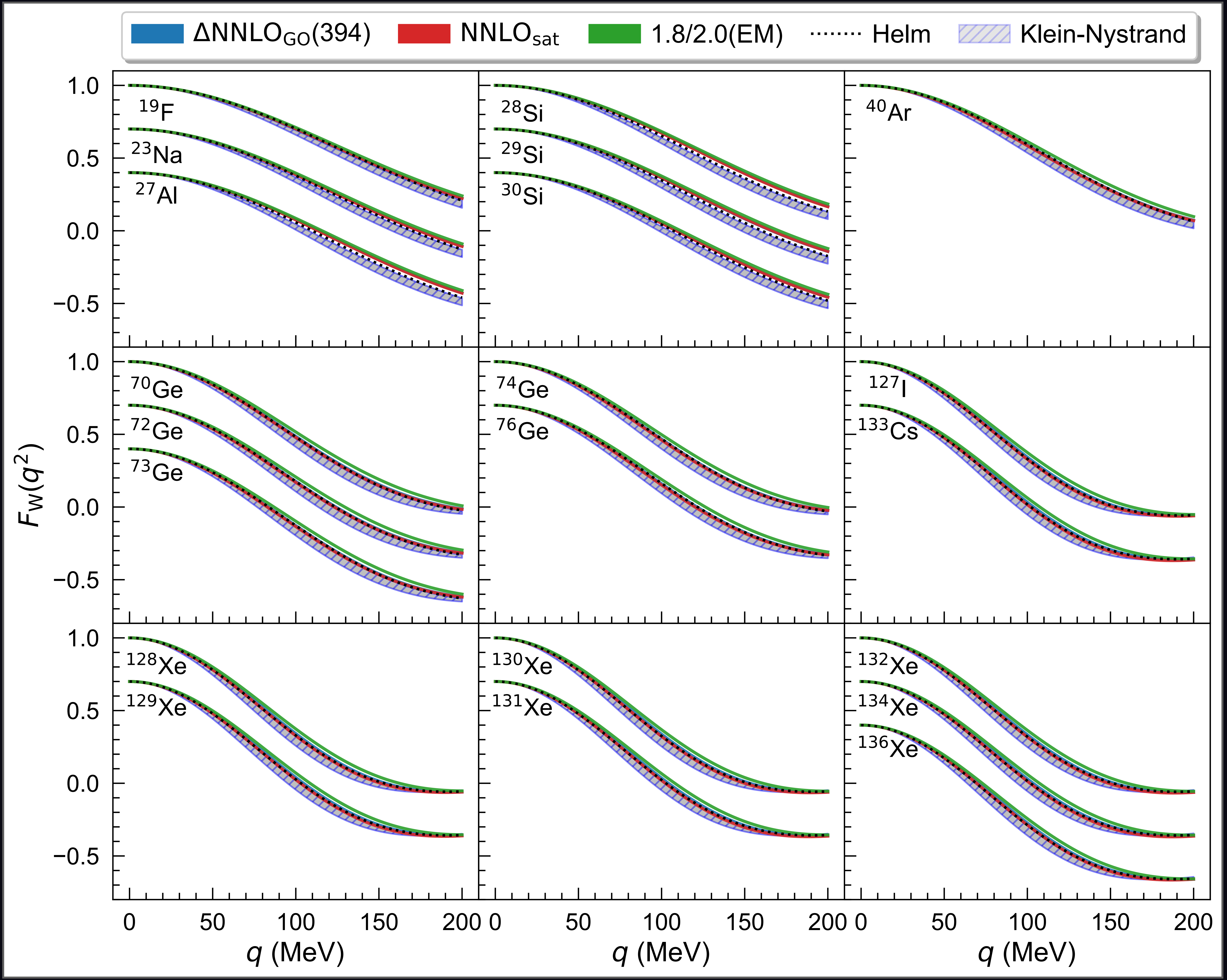
Using these ab initio analysis, we present a refined Helm form factor

Spin expectation values from first principles

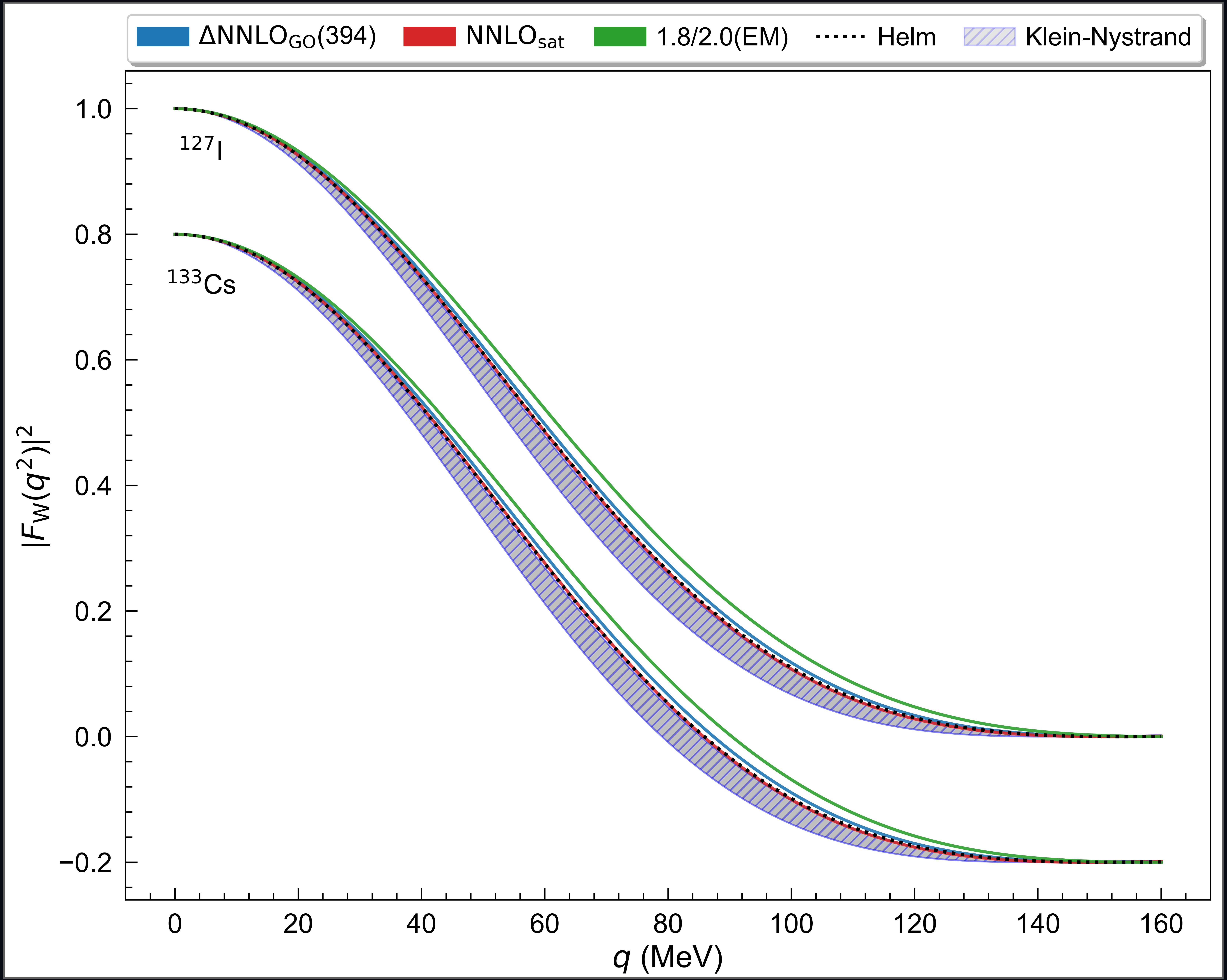
$$S_A(0) = \frac{(2J+1)(J+1)}{4\pi J} \left| (a_+ + a'_-) \left\langle \hat{S}_p \right\rangle + (a_+ - a'_-) \left\langle \hat{S}_n \right\rangle \right|^2 \qquad q \to 0$$



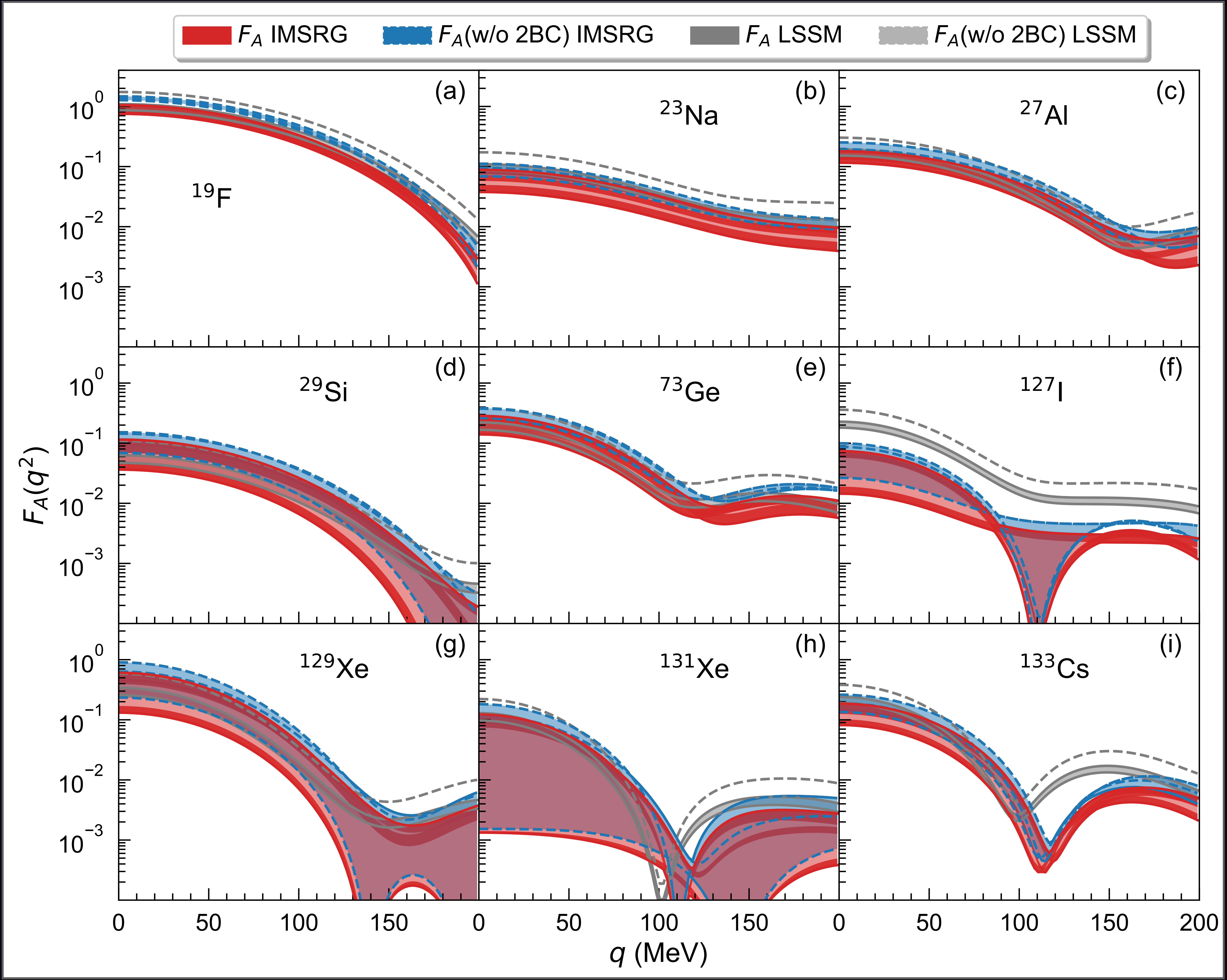
BSHu, et al, Phys Rev Lett 128, 072502 (2022)



BSHu, et al., In preparation (2024)

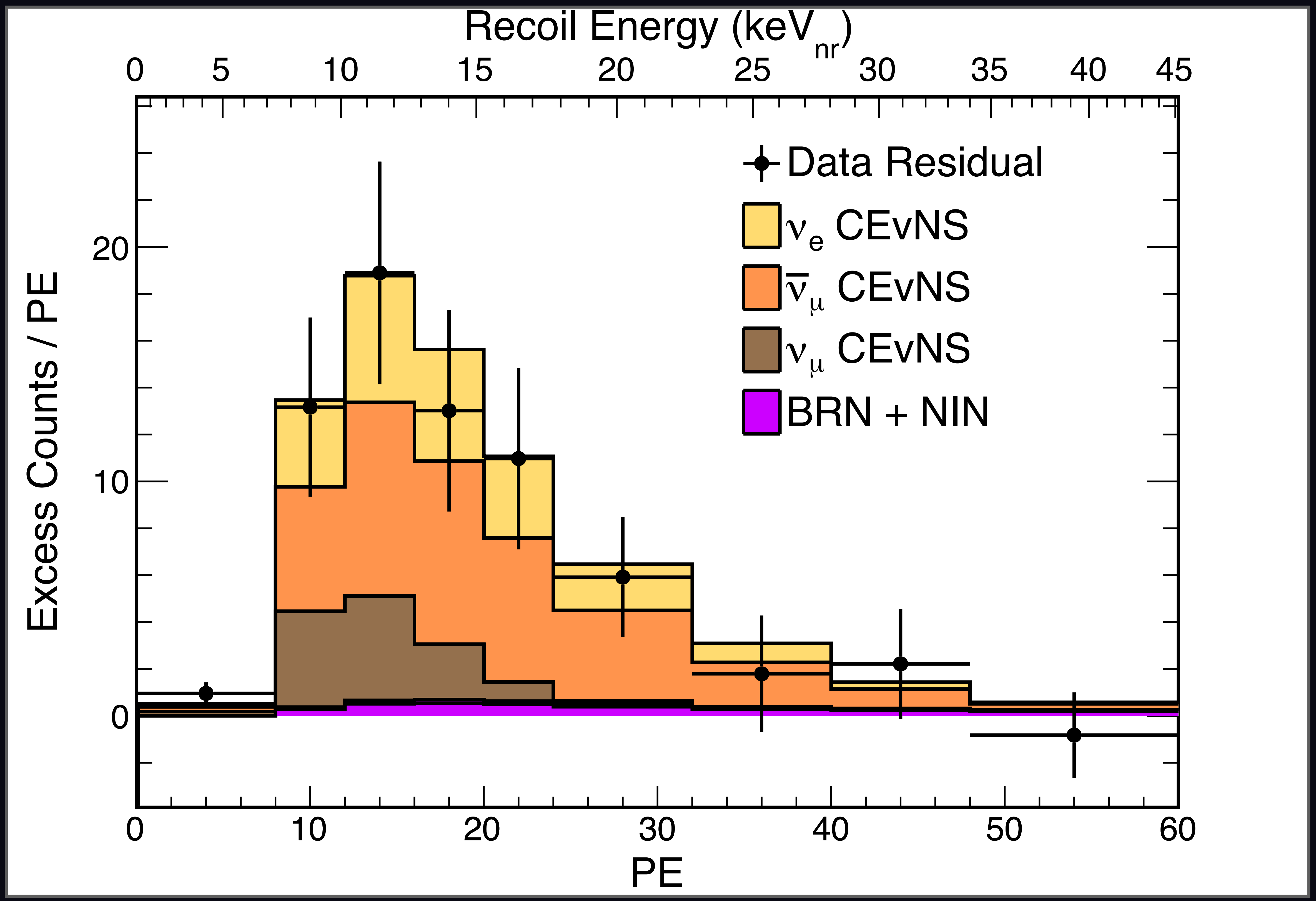


ΔNNLO_GO(394)
NNLO_sat
1.8/2.0(EM)
Helm
Klein-Nystrand
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
|F_W(q^2)|^2
127I
133Cs
0
20
40
60
80
100
120
140
160
q (MeV)

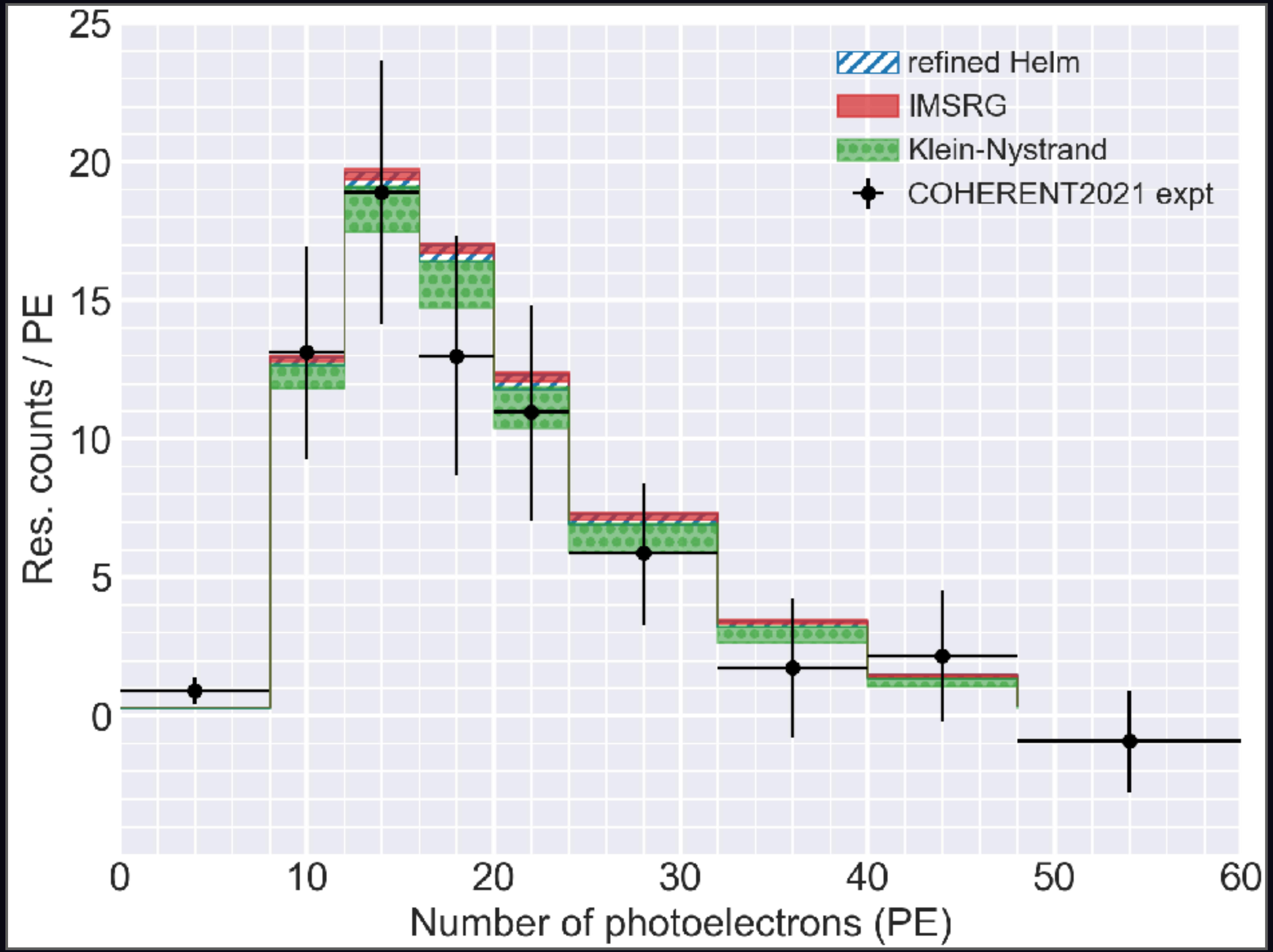


BSHu, et al., In preparation (2024)

$$\frac{dR}{dT} = \sum_i \left[N_{\text{target}} X_i \mathcal{N}_\nu \int_{E_\nu^{\min}}^{E_\nu^{\max}} \phi\left(E_\nu\right) \frac{d\sigma_i}{dT} dE_\nu \right]$$

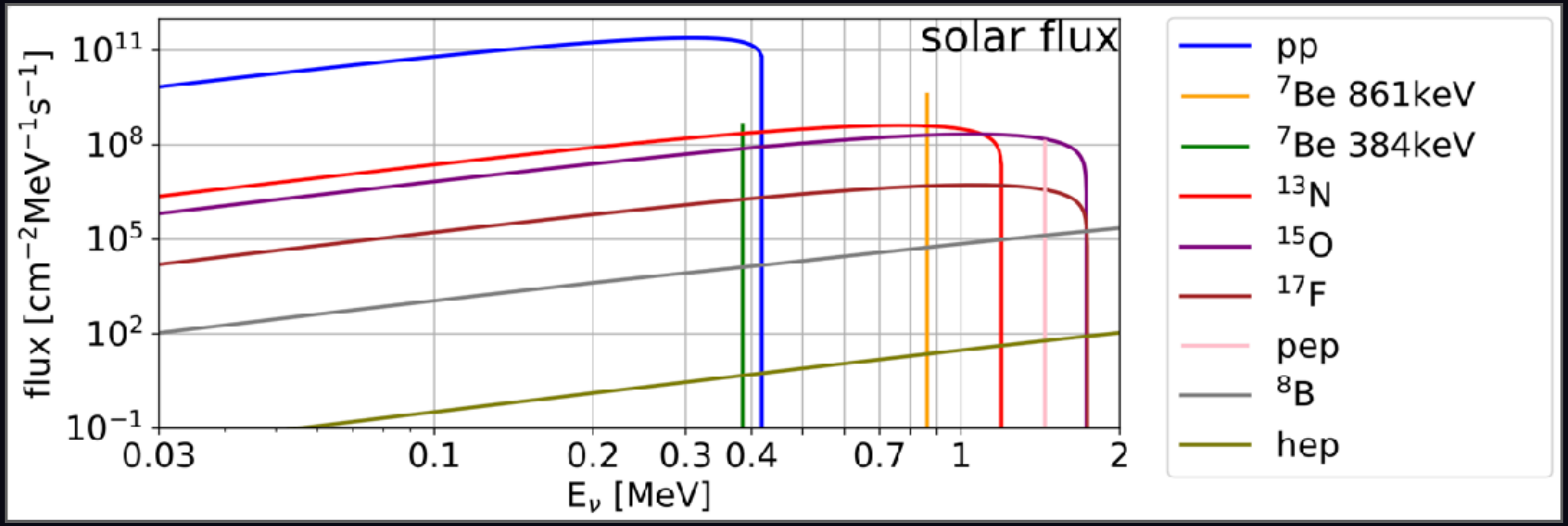


D. Akimov et al. (COHERENT). Phys. Rev. Lett. 129, 081801 (2022)



BSHu, et al., In preparation (2024)

III. Inelastic charged and neutral current *ν*-nucleus scattering



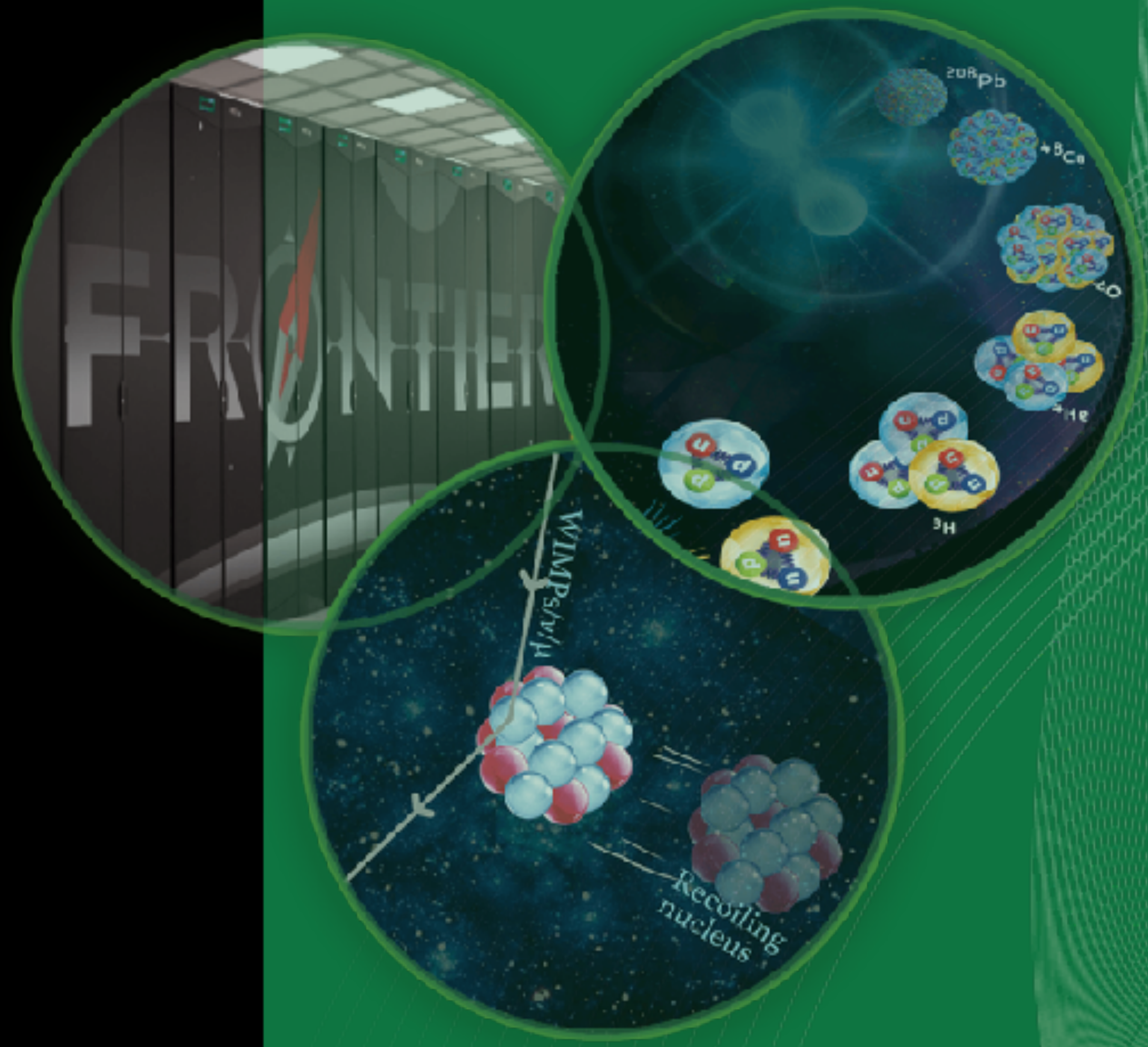
B. Dutta, W. C. Huang, BSHu, L. Strigari, Y. Zhuang, In preparation (2024)

Summary

Ab initio form factors/nuclear responses
for ^{19}F, ^{23}Na, ^{27}Al, Si, ^{40}Ar, Ge, ^{127}I, ^{133}Cs, Xe

VS-IMSRG: from light to heavy nuclei;
Chiral EFT 1b + 2b currents

Inelastic charged and neutral current neutrino-nucleus scattering;
BSM constrains



This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

Thank you !

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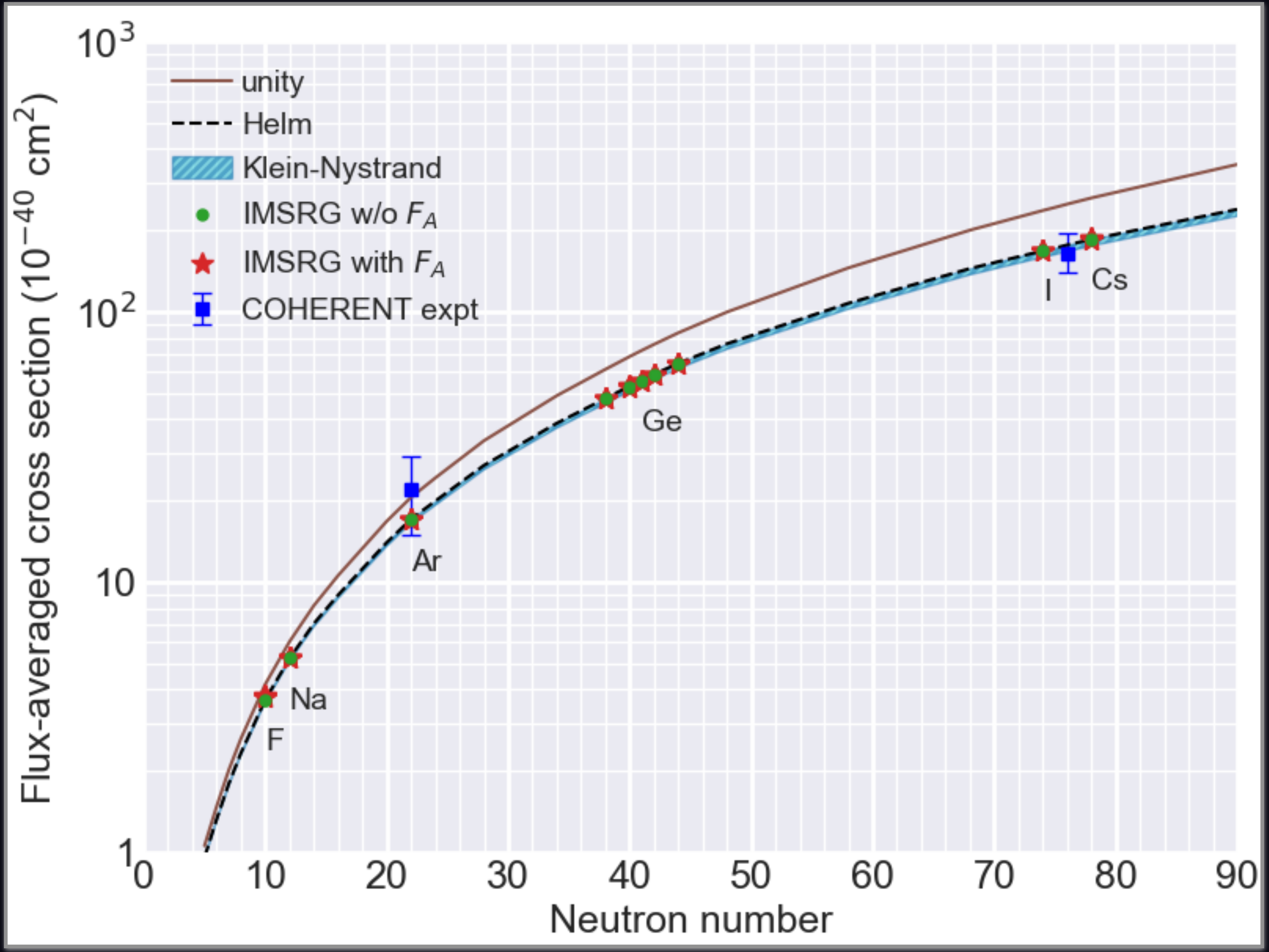
Backup



BSH, et al., In preparation (2024)

- **Helm form factor reproduces ab initio results within NNLOsat well:**

  less than 0.3% in heavy nuclei,
  about 1% in light nuclei

$$F_{\text{Helm}}(q^2) = \frac{3j_1(qR)}{qR} e^{-q^2 s^2/2}$$

$$R^2 = c^2 + \frac{7}{3}\pi^2 a^2 - 5s^2$$

$$c = (1.23A^{1/3} - 0.60)\ \text{fm}$$

$$a = 0.52\ \text{fm},\ s = 0.9\ \text{fm}$$

- **Weak charges:** 1.5% level

$$Q^p_{\text{w}} = 0.0714,\ Q^n_{\text{w}} = -0.9900$$

$$Q^n_{\text{w}} = -1,\ Q^p_{\text{w}} = 1 - 4\sin^2\theta_W \quad \sin^2\theta_W = 0.23122 \pm 0.00003$$

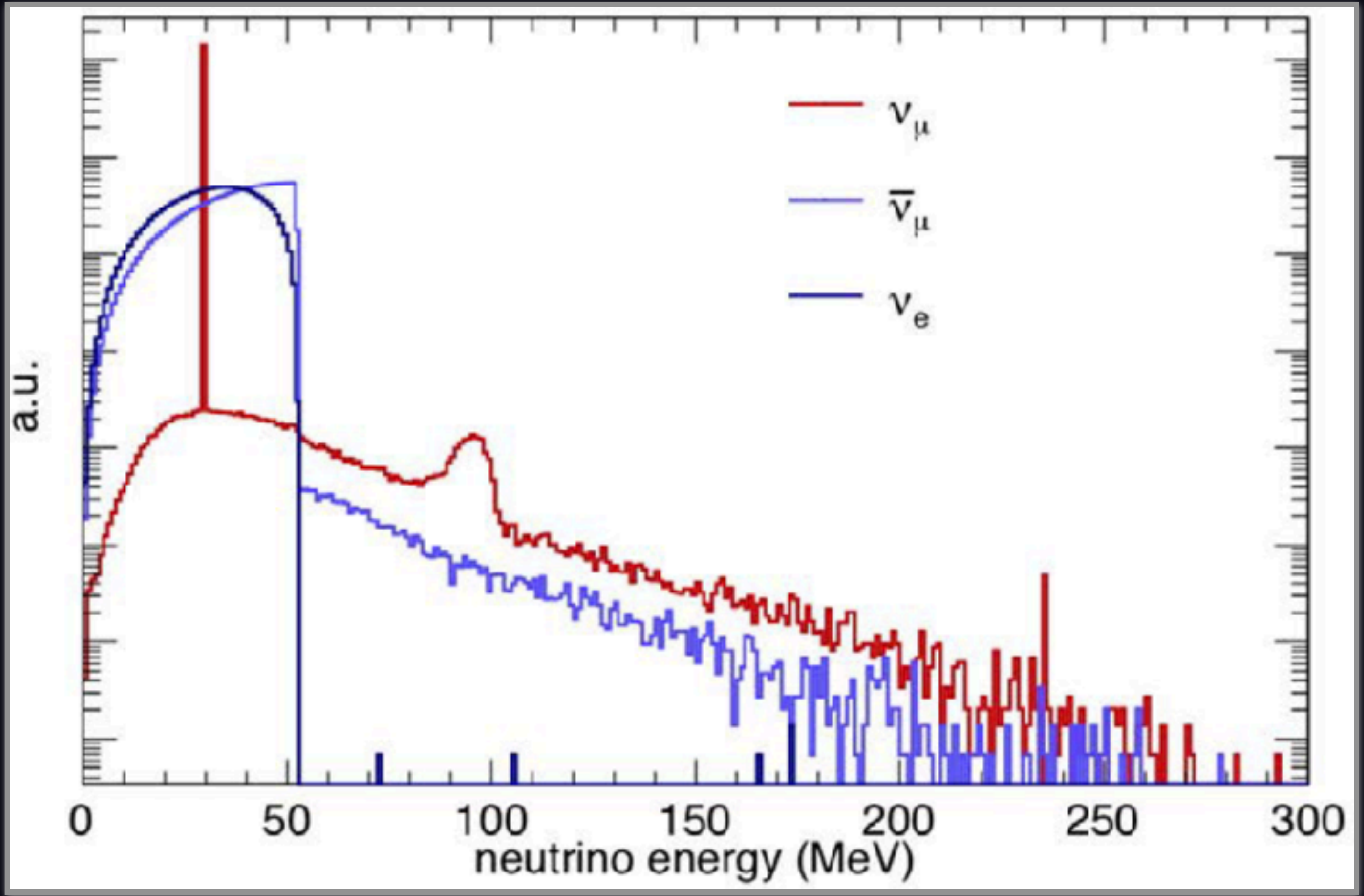
- **Spin-orbit current $\mathcal{F}^{\Phi''}_{\tau}$:**

  less than 10^(-6)%

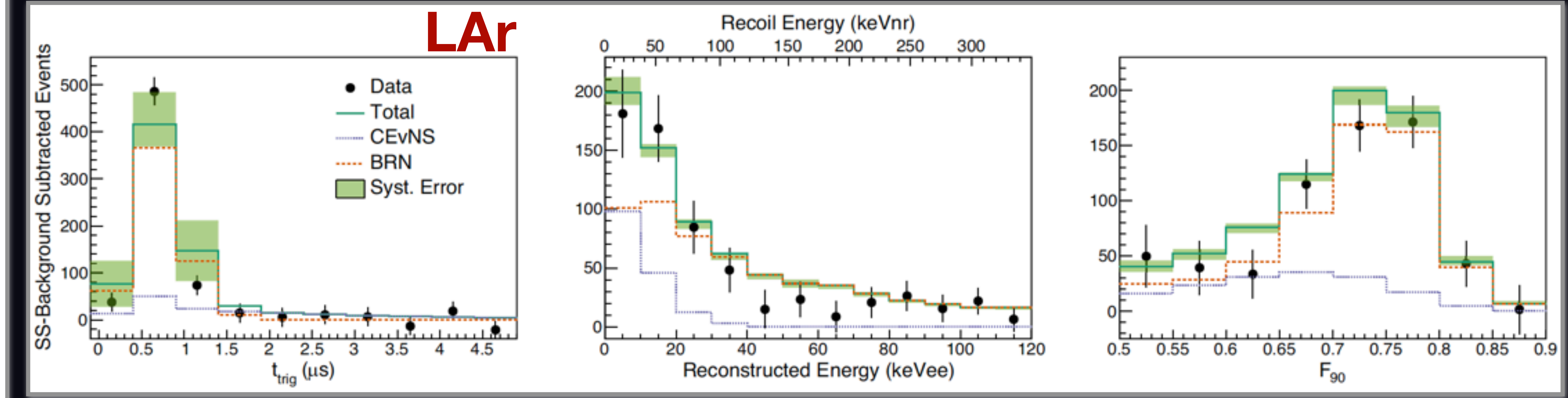
- **Axial-vector form factor F_A:**

  3%(^{19}F), 0.1%(^{23}Na), 0.03%(^{73}Ge),
  less than 0.007%(^{127}I and ^{133}Cs)

COHERENT experiment



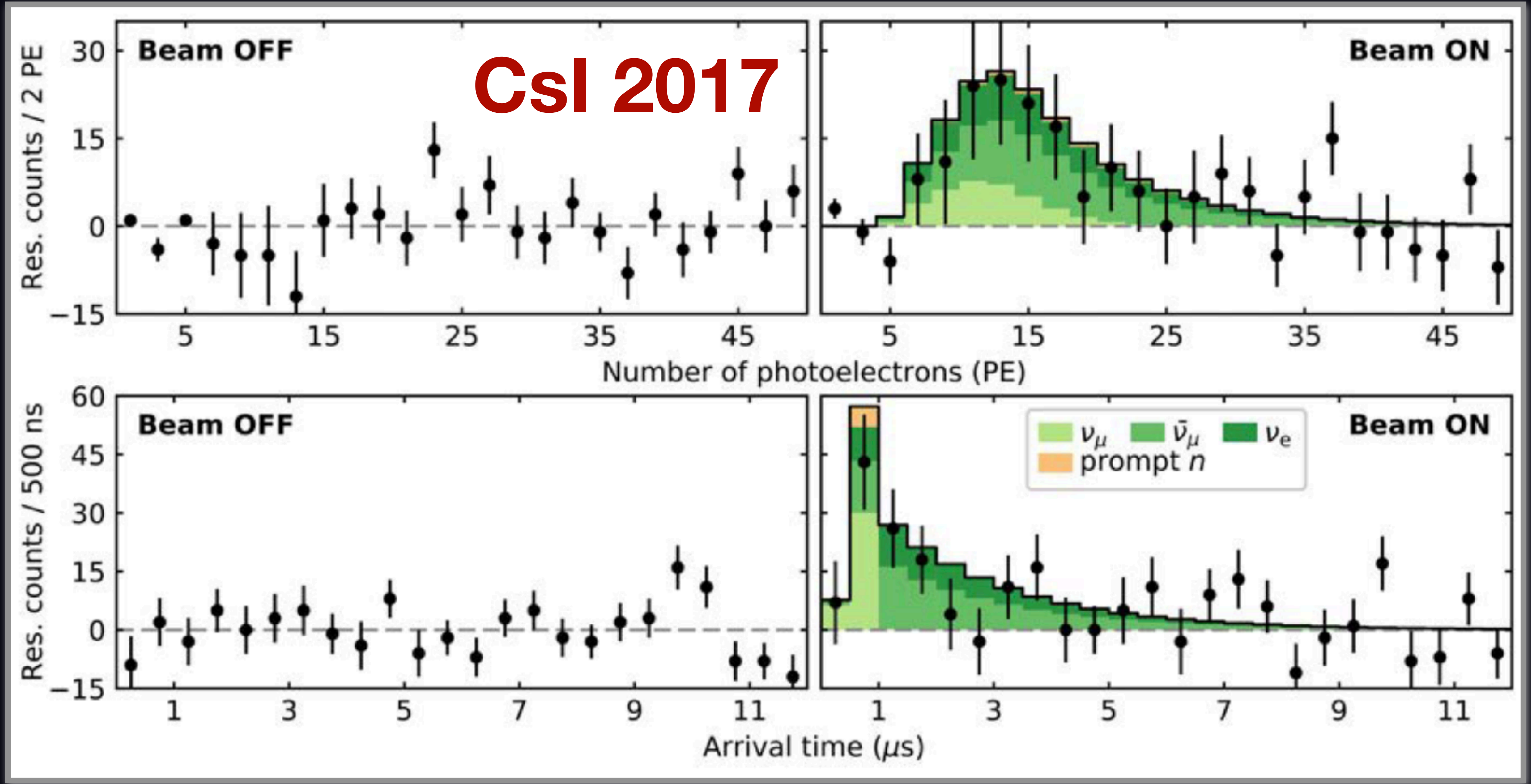
D. Akimov et al. (COHERENT). Science 357 (2017) 1123

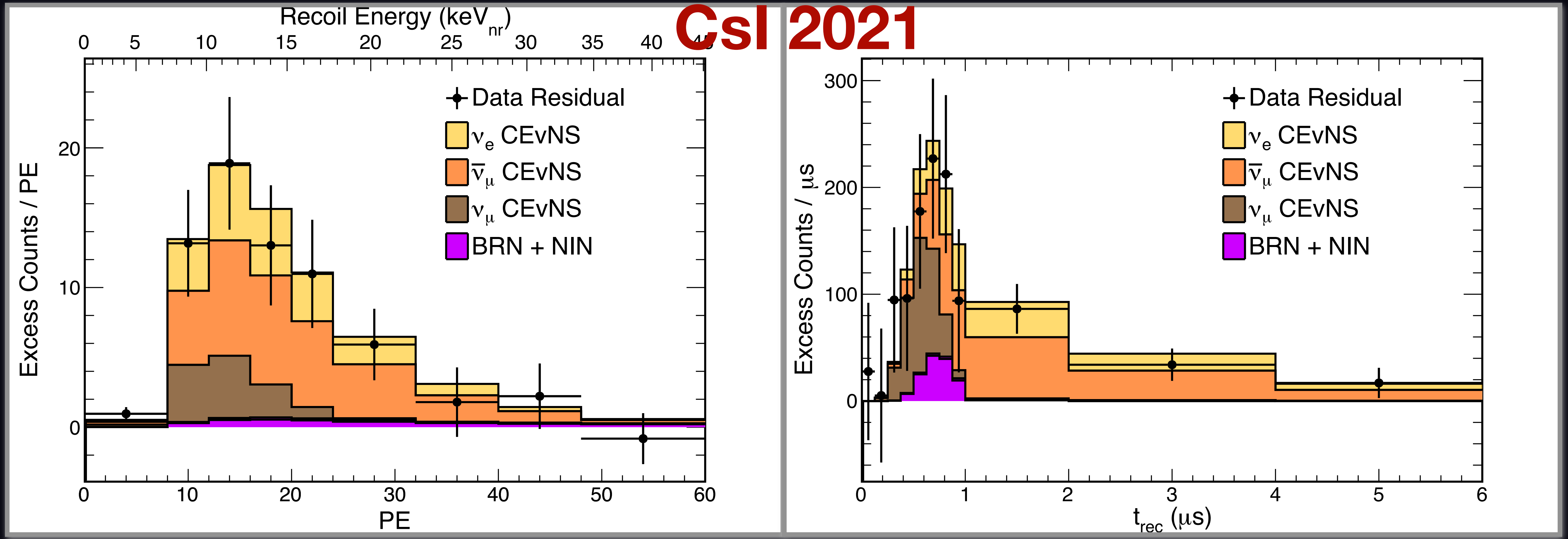


D. Akimov et al. (COHERENT). Phys. Rev. Lett. 126 (2021) 012002

SNS as a neutrino source

$$\pi^+ \to \mu^+ + \nu_\mu$$
$$\downarrow$$
$$\mu^+ \to e^+ + \bar{\nu}_\mu + \nu_e$$

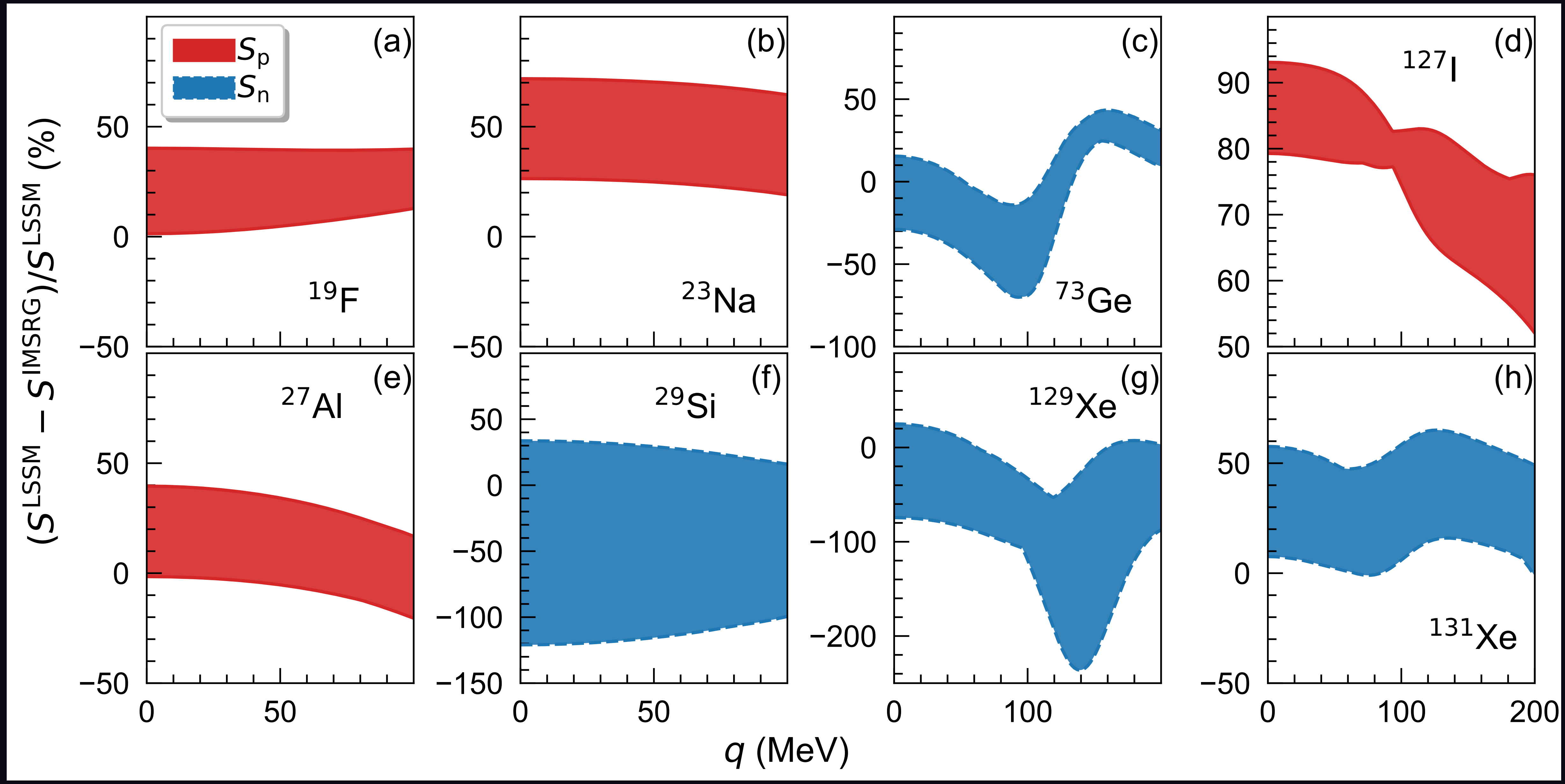




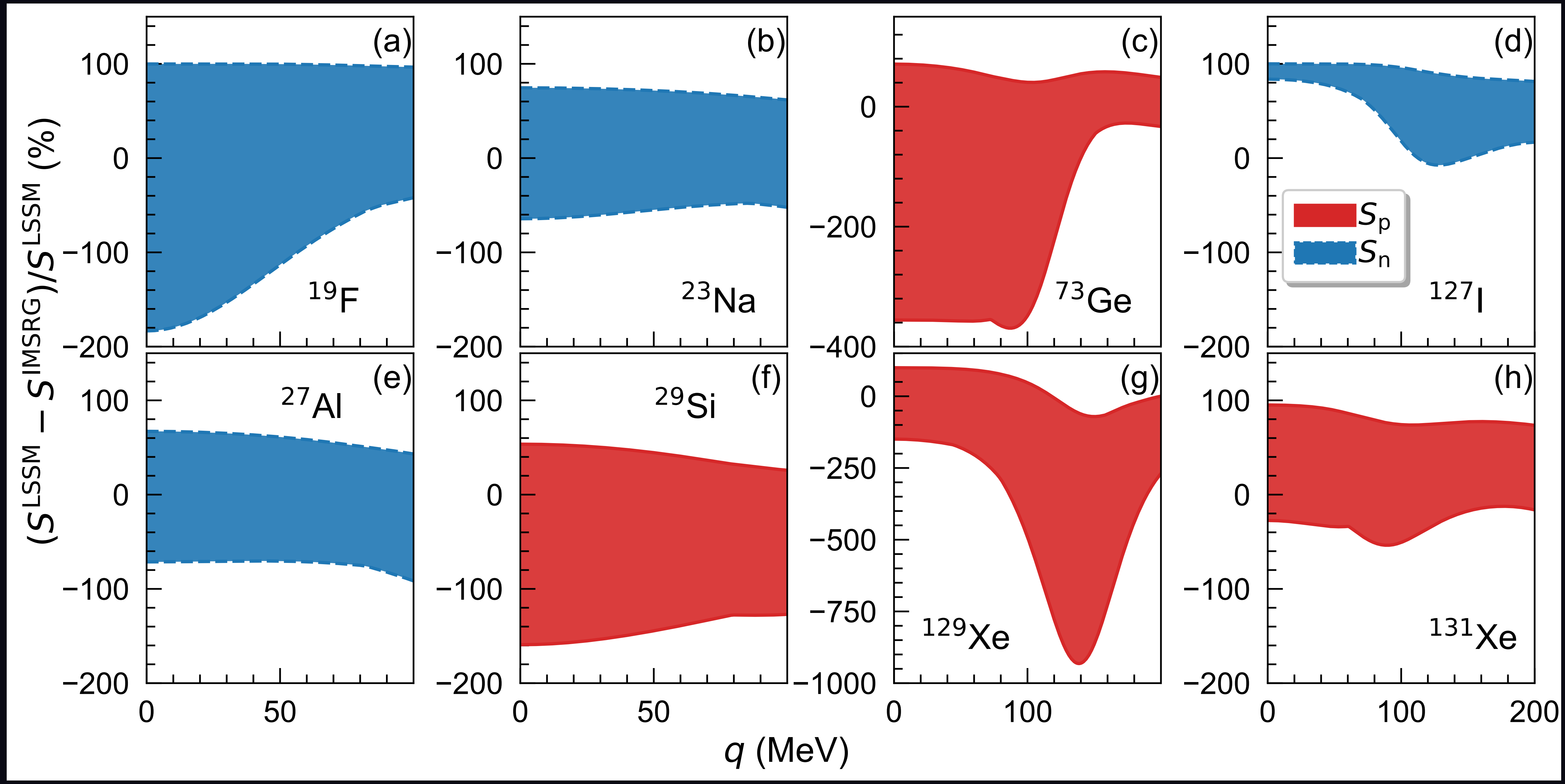
D. Akimov et al. (COHERENT). arXiv:2110.07730 (2021)

Discrepancy between LSSM and IMSRG

Dominant structure factor

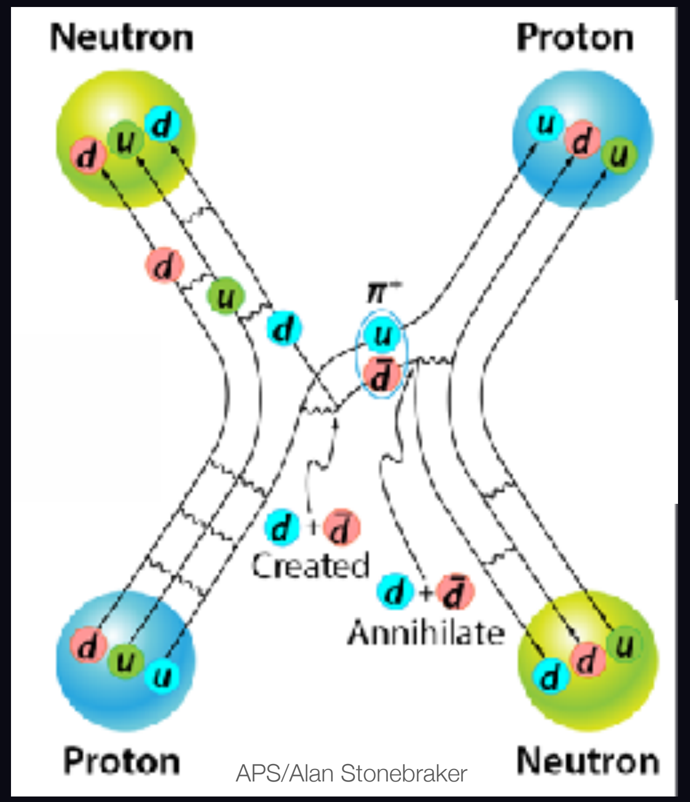


Non-dominant structure factor



Challenge of ab initio nuclear theory

To compute the properties of complex nuclei from first principles, there are two significant issues:



- **Nuclear force**

  $H = T + V$

  Quantum Chromodynamics (QCD) becomes highly non-perturbative at the low energy scale relevant to nuclear physics

- **Many-body problem**

  Solve many-body Schrödinger equation ranging from 2 to 208, even up to an infinite number of strongly interacting particles

Challenge of ab initio nuclear theory

Many-body problem $$H = \sum_{i=1}^{A} T_i + \sum_{i<j} V_{ij}^{NN} + \sum_{i<j<k} V_{ijk}^{3N} + \cdots$$

Solve many-body Schrödinger equation

$$H|\psi_n^A\rangle == E_n|\psi_n^A\rangle$$

$$|\psi^A\rangle = \sum_{i=1}^{n_{\mathrm{dim}}} C_i|\phi_i^A >$$

$$H_{ij} = \langle\phi_i^A|H|\phi_j^A\rangle$$

$$\begin{pmatrix} H_{11} & \cdots & H_{1n_{\mathrm{dim}}} \\ \vdots & \ddots & \vdots \\ H_{n_{\mathrm{dim}}1} & \cdots & H_{n_{\mathrm{dim}}n_{\mathrm{dim}}} \end{pmatrix} \begin{pmatrix} C_1 \\ \vdots \\ C_{n_{\mathrm{dim}}} \end{pmatrix} = E^A \begin{pmatrix} C_1 \\ \vdots \\ C_{n_{\mathrm{dim}}} \end{pmatrix}$$

Ex: 300 orbits to study ^{12}C

The total number of Slater determinants is:

$$n_{\mathrm{dim}} = \binom{300}{6} \times \binom{300}{6} \approx 10^{24}$$

Numerical budgets:

1) $2 < \mathrm{dim} < 10^5$ ⇨ exact diagonalization
2) $10^5 < \mathrm{dim} < 10^{10}$ ⇨ few E_n (Lanczos)
3) $\mathrm{dim} > 10^{10}$ ⇨ intractable

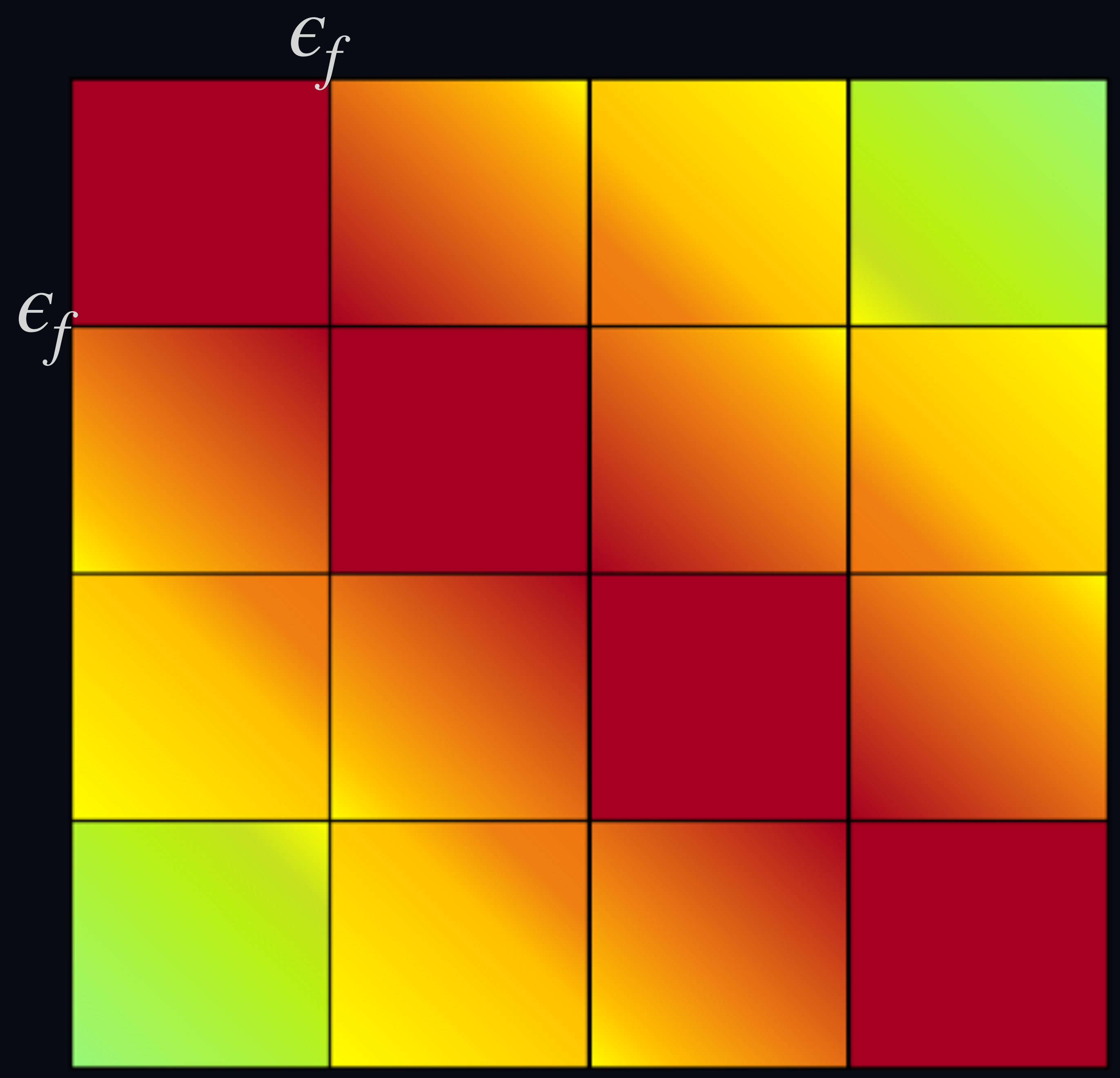
Scale exponentially with mass A

Polynomially scaling methods

In-Medium Similarity Renormalization Group (IMSRG); named driven SRG in quantum chemistry

drive the Hamiltonian towards a band- or block-diagonal form via continuous unitary transformation

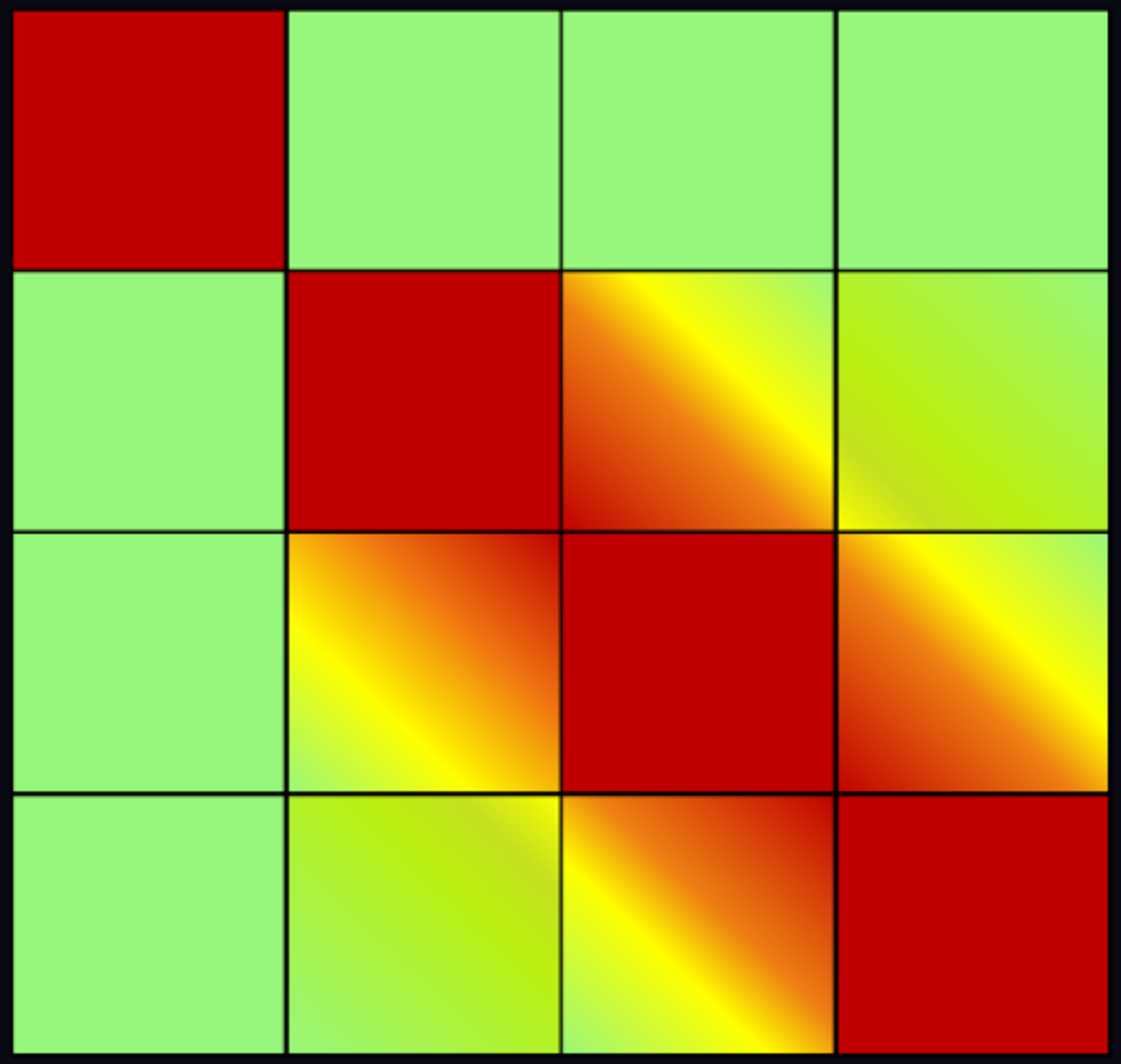
$$H|\psi^A\rangle = = E|\psi^A\rangle$$



$\langle i|H(s=0)|j\rangle$

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

$$e^{-\Omega(s)} e^{\Omega(s)} = 1$$



$\langle i|H(s\to\infty)|j\rangle$

Coupled cluster theory (CC)

$$|\psi^A\rangle = e^T|\phi^A\rangle$$

$$T = T_1 + T_2 + T_3 + \cdots$$

$$T_1 = \sum_{h<\epsilon_f,\ p><\epsilon_f} t_{ph} a_p^\dagger a_h$$

$$\tilde{H} = e^{-T} H e^T$$

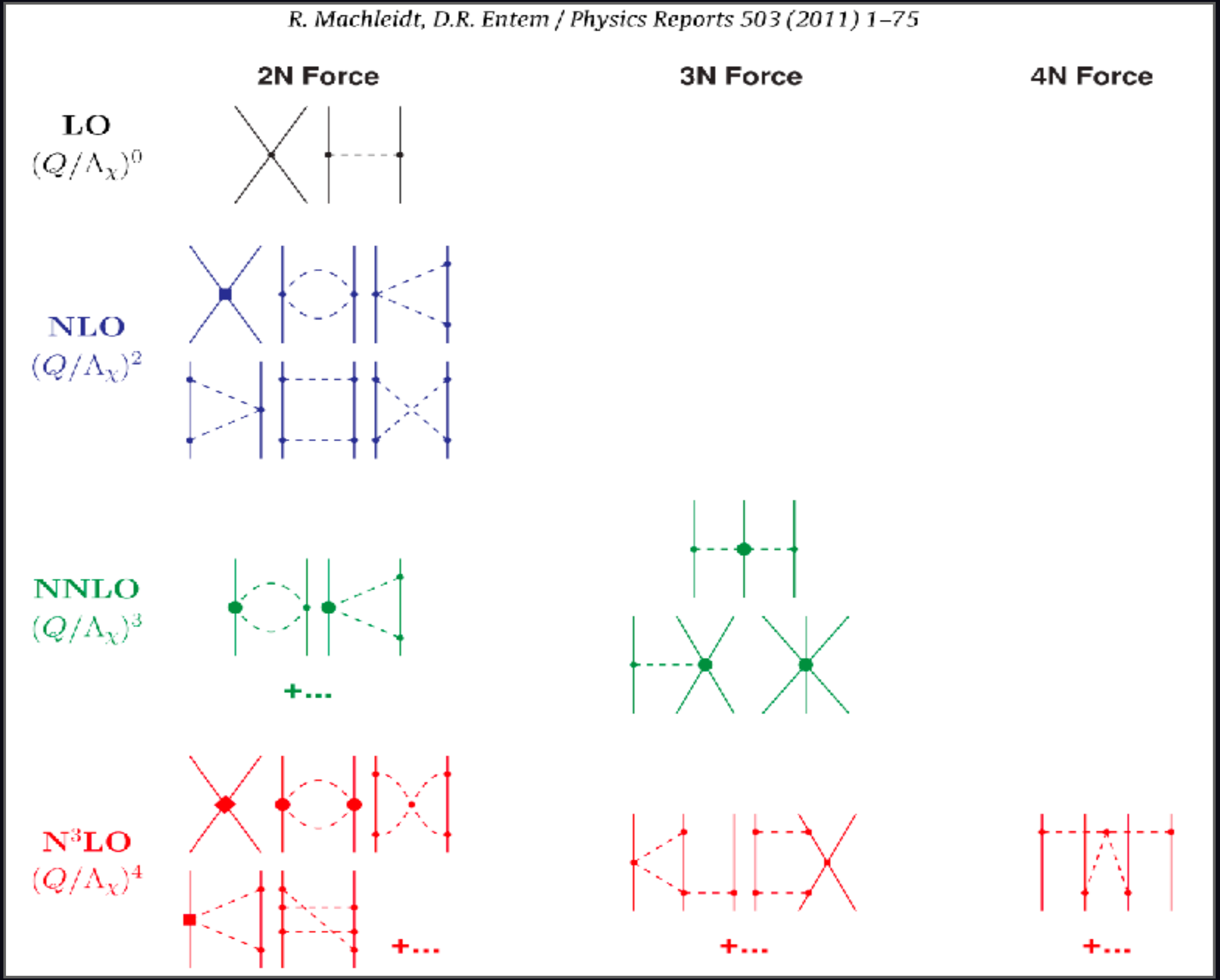
$$E = \langle \Phi|\bar{H}|\Phi\rangle$$

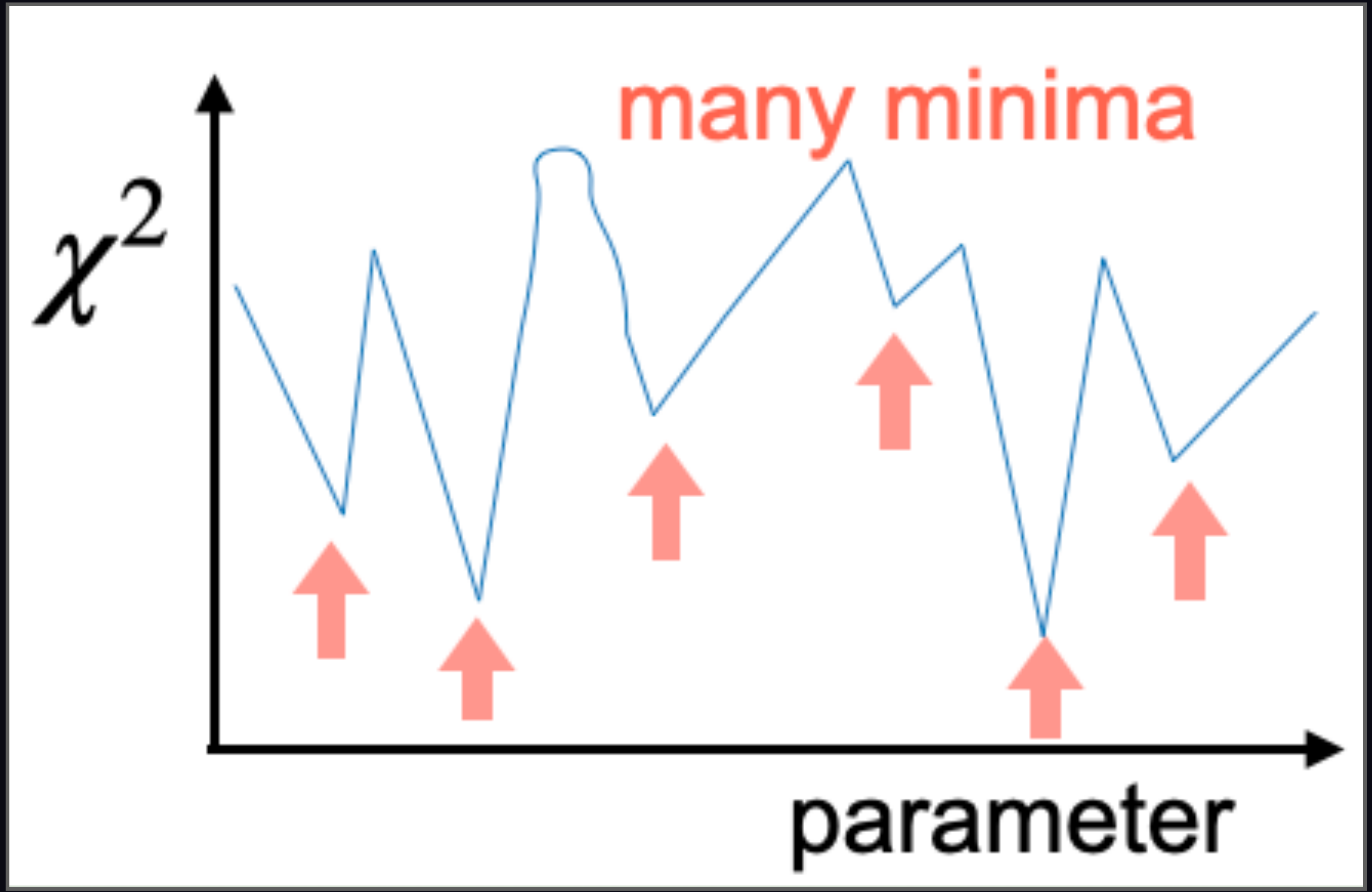
$$0 = \left\langle \Phi_{h_1 h_2 \cdots}^{p_1 p_2 \cdots} |\bar{H}|\Phi \right\rangle$$

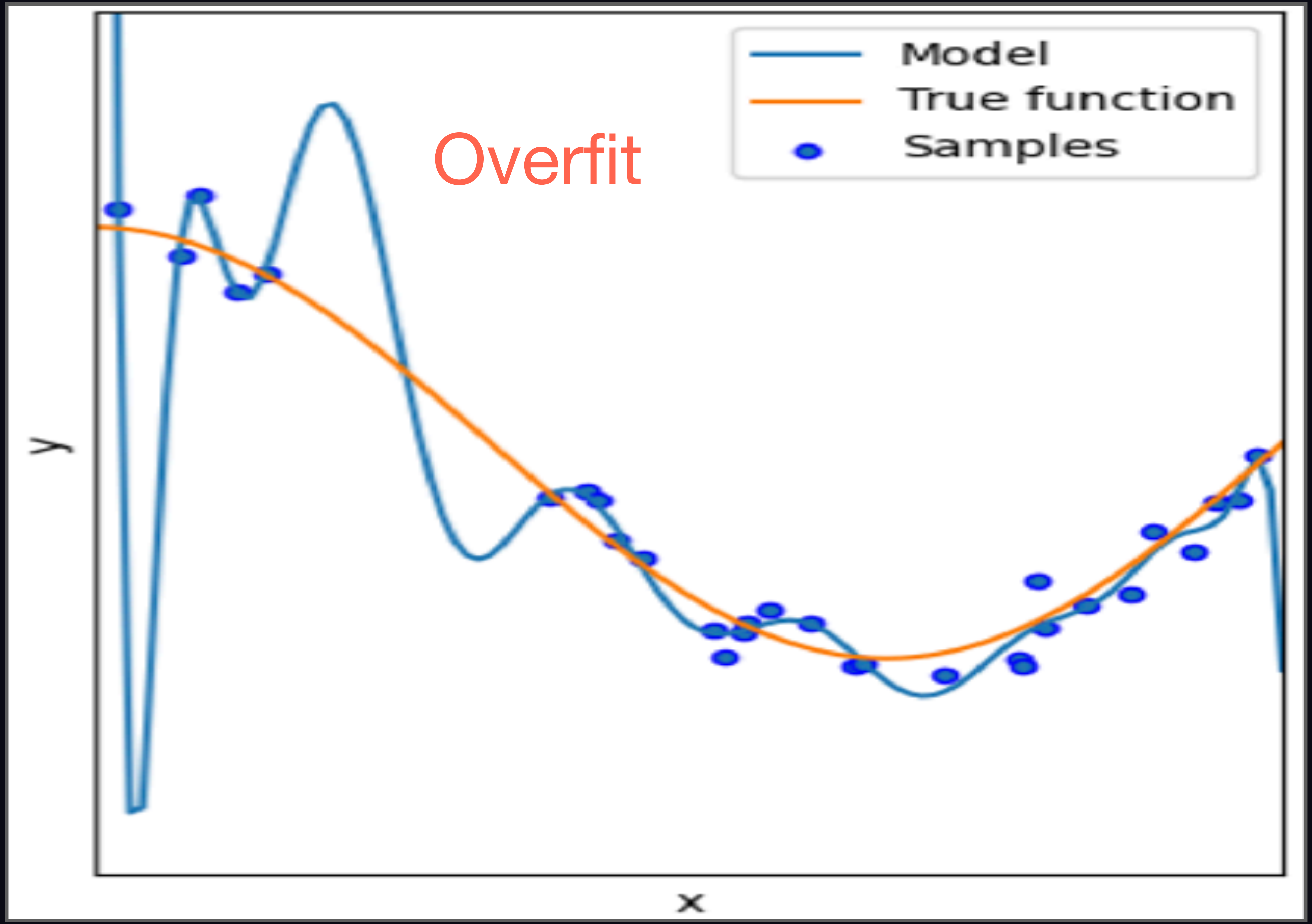
$$e^{-T} e^T \neq 1$$

Optimize chiral interaction

NN unknown LECs: 2 (LO) + 7 (NLO) + 15 (N^3LO)
3N unknown LECs: 2 (N^2LO)







Sampled chiral interactions: history matching

I. Vernon, et al, Statistical Science 29 (2014) 81; I. Vernon, et al, arXiv:1607.06358v1(2016)

$$z_{\rm exp} = z_{\rm th} + \delta z_{\rm th} + \delta z_{\rm exp}$$

$$z_{\rm exp} = z_{\rm th}(\theta) + \varepsilon_{\rm model} + \varepsilon_{\rm em} + \varepsilon_{\rm method} + \varepsilon_{\rm exp}$$

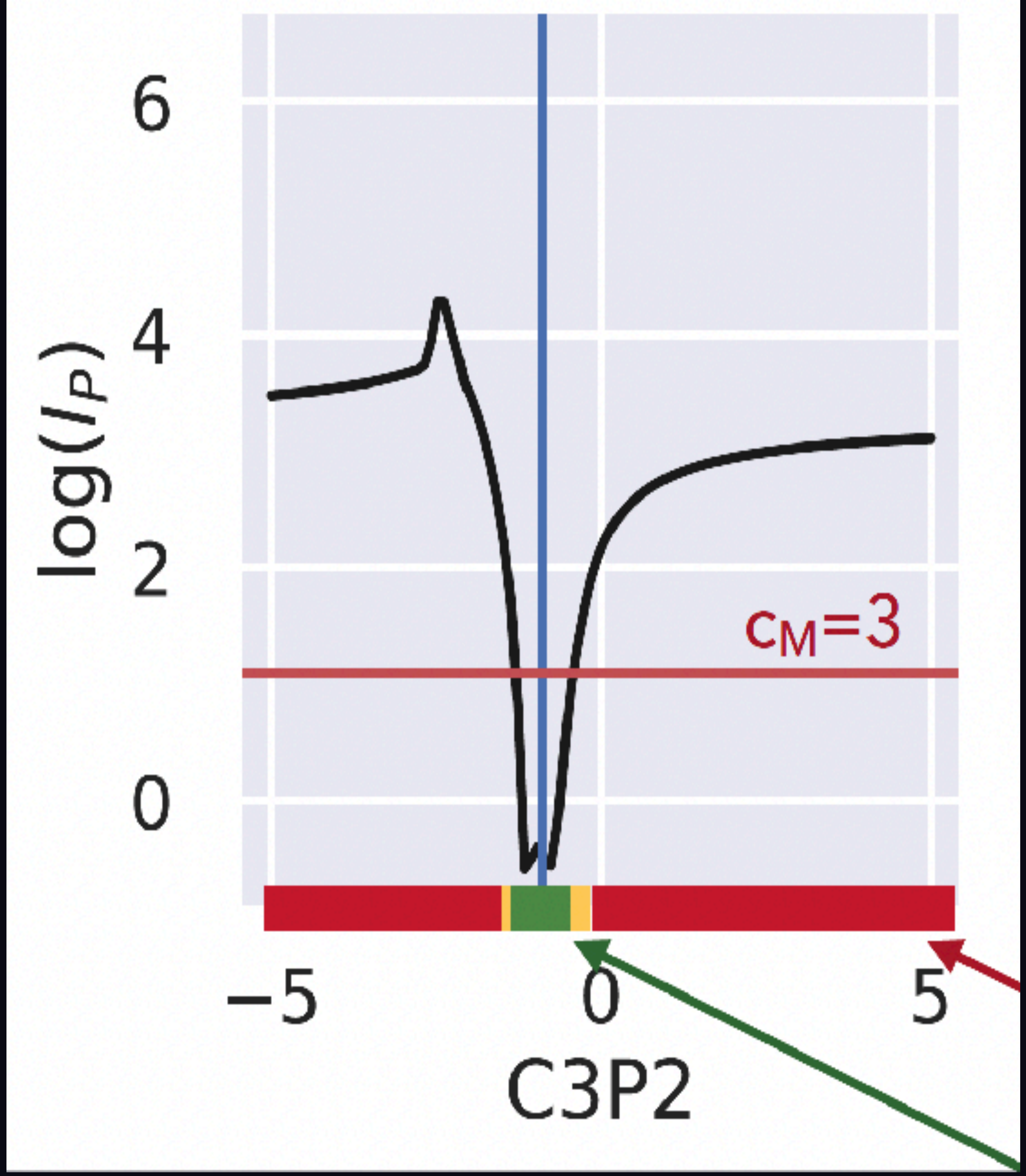
θ :

$\varepsilon_{\rm exp}$: experimental uncertainty

$\varepsilon_{\rm model}$: EFT truncation

$\varepsilon_{\rm method}$: model-space truncations, *ab initio* many-body solvers

$\varepsilon_{\rm em}$: emulator precision/sharing



Implausible!

Non-implausible!

Figure from Christian Forssén's talk @ abinitio.triumf.ca/2020

Implausibility measure:

$$I_i^2(\theta) = \frac{|z_i^{\rm th}(\theta) - z_i^{\rm exp}|^2}{\mathrm{Var}\left(z_i^{\rm th}(\theta) - z_i^{\rm exp}\right)}$$

$$I_M(\theta) \equiv \max_{z_i \in \mathcal{Z}} I_i(\theta) > c_M$$

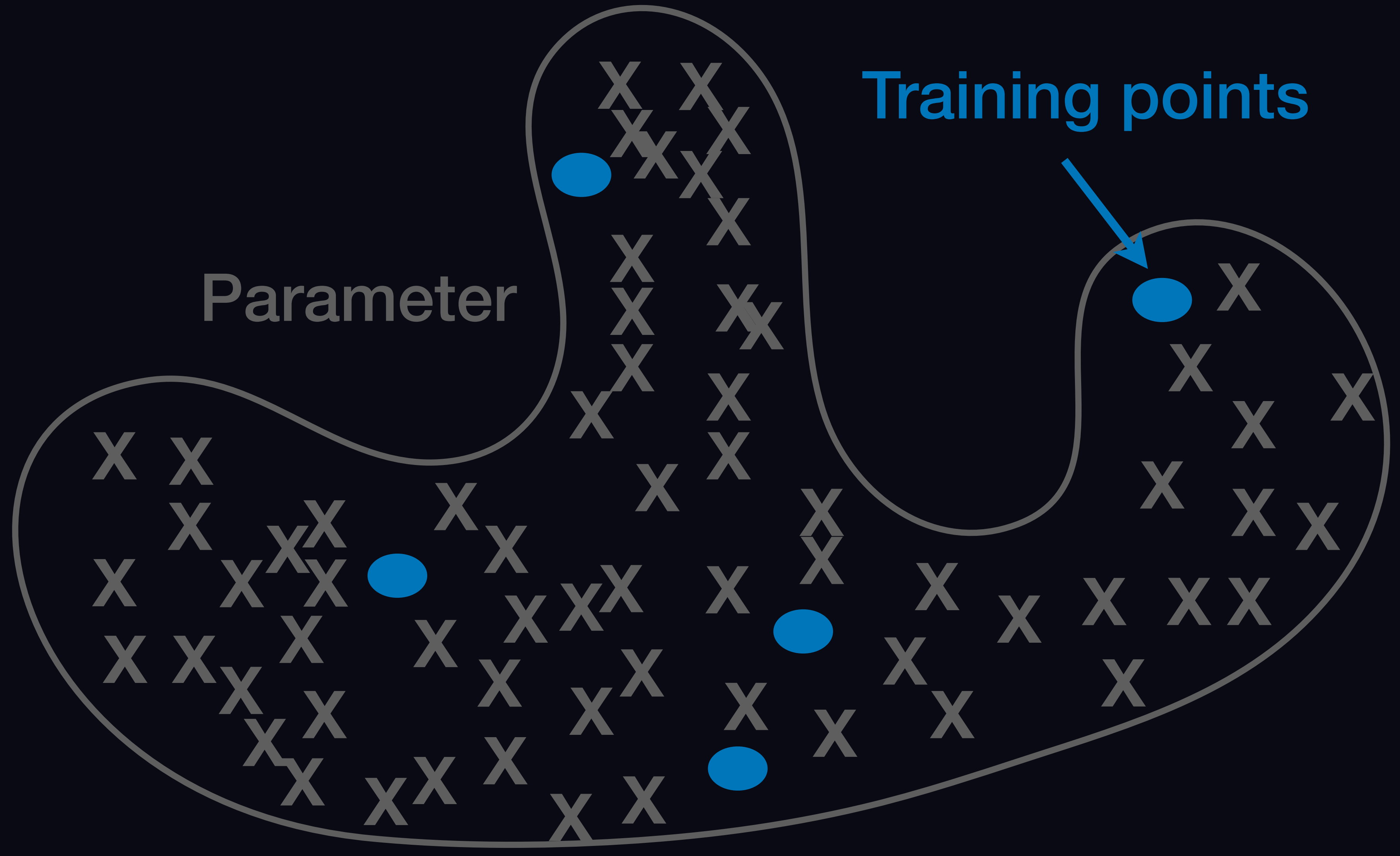
c_M=3, Pukelheim's three-sigma rule

Model order reduction emulator: eigenvector continuation

D. Frame, et al, PRL121 (2018) 032501

CCSD compute ^{16}O 10^9 times:

All 9000 nodes of ORNL's Frontier run 100 years vs laptop run 1 month



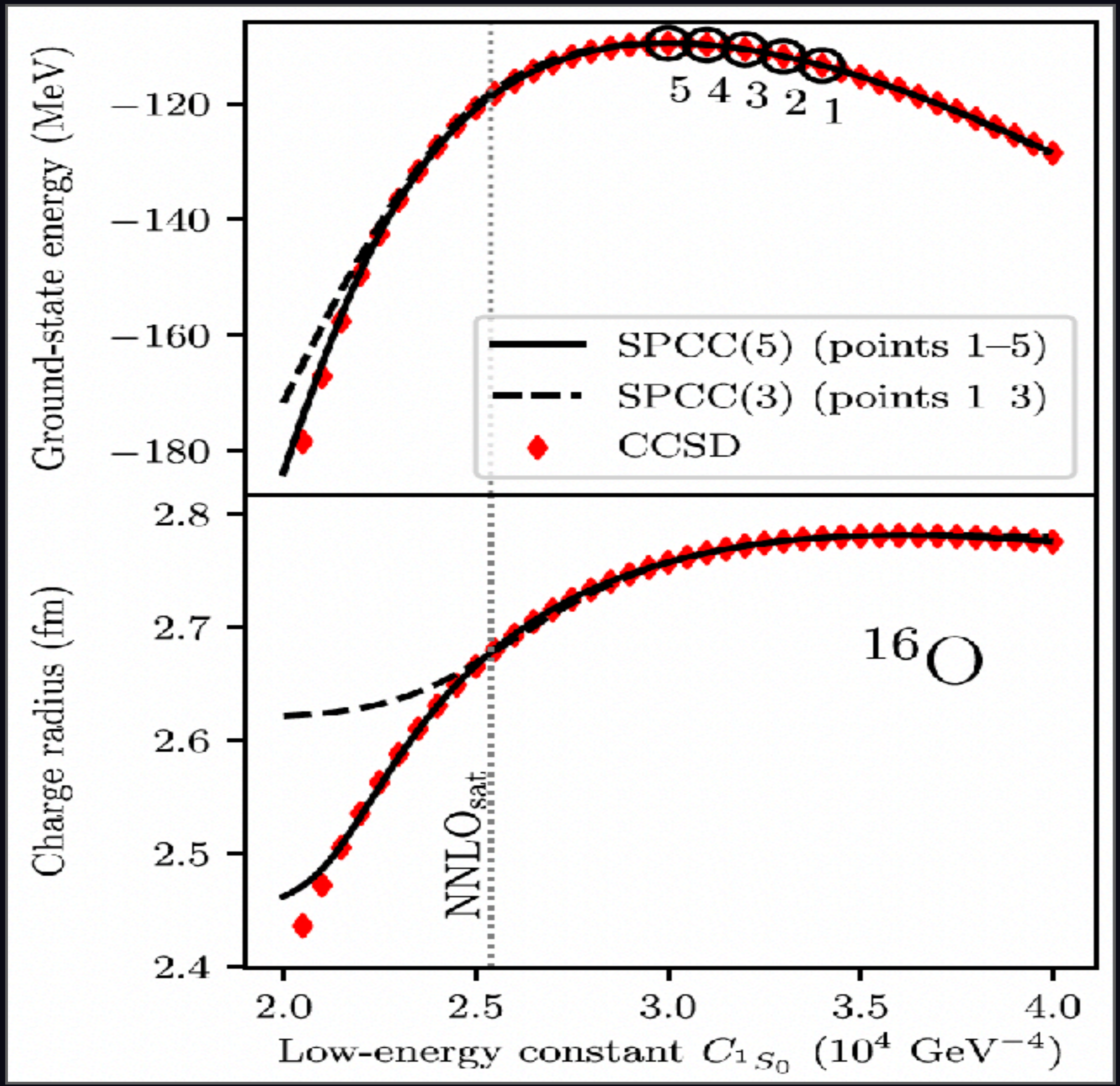
$$\hat{H}(\theta_i) = \hat{T} + \hat{V}(\theta_i) \quad \text{for } i = 1, \ldots N_{\text{EC}}$$

$$\hat{H}(\theta_i)\,|\psi(\theta_i)\rangle = E(\theta_i)\,|\psi(\theta_i)\rangle$$

$$|\psi(\theta_\odot)\rangle \simeq \sum_{i=1}^{N_{\text{EC}}} c_i\,|\psi(\theta_i)\rangle$$

$$\hat{H}(\theta_\odot)\,|\psi(\theta_\odot)\rangle = E(\theta_\odot) N\,|\psi(\theta_\odot)\rangle$$

$$H_{ij} = \langle\psi(\theta_i)\,|\,\hat{H}(\theta_\odot)\,|\,\psi(\theta_j)\rangle,\ N_{ij} = \langle\psi(\theta_i)\,|\,\psi(\theta_j)\rangle$$



A Ekström and G Hagen, Phys Rev Lett 123, 252501 (2019)