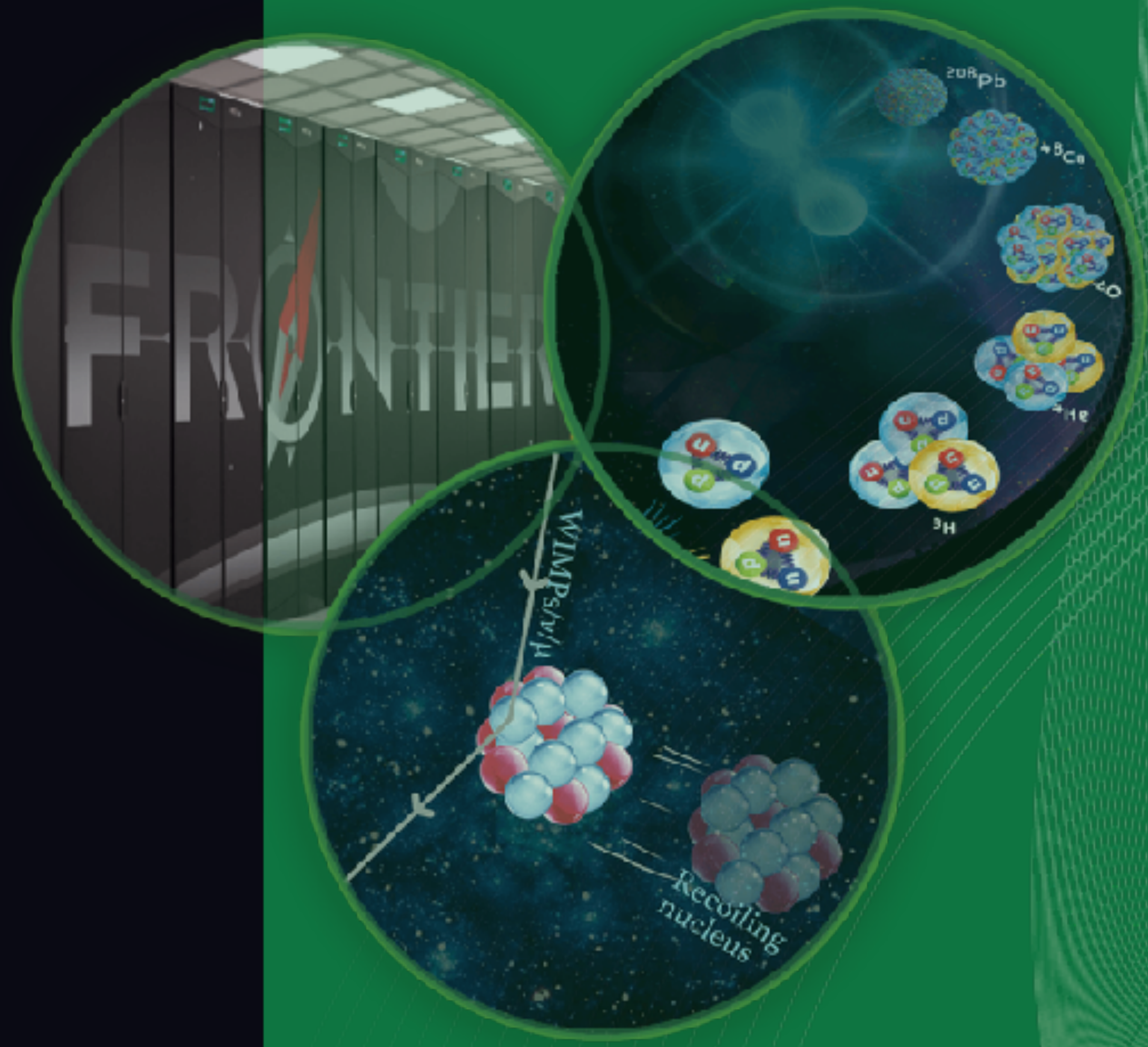
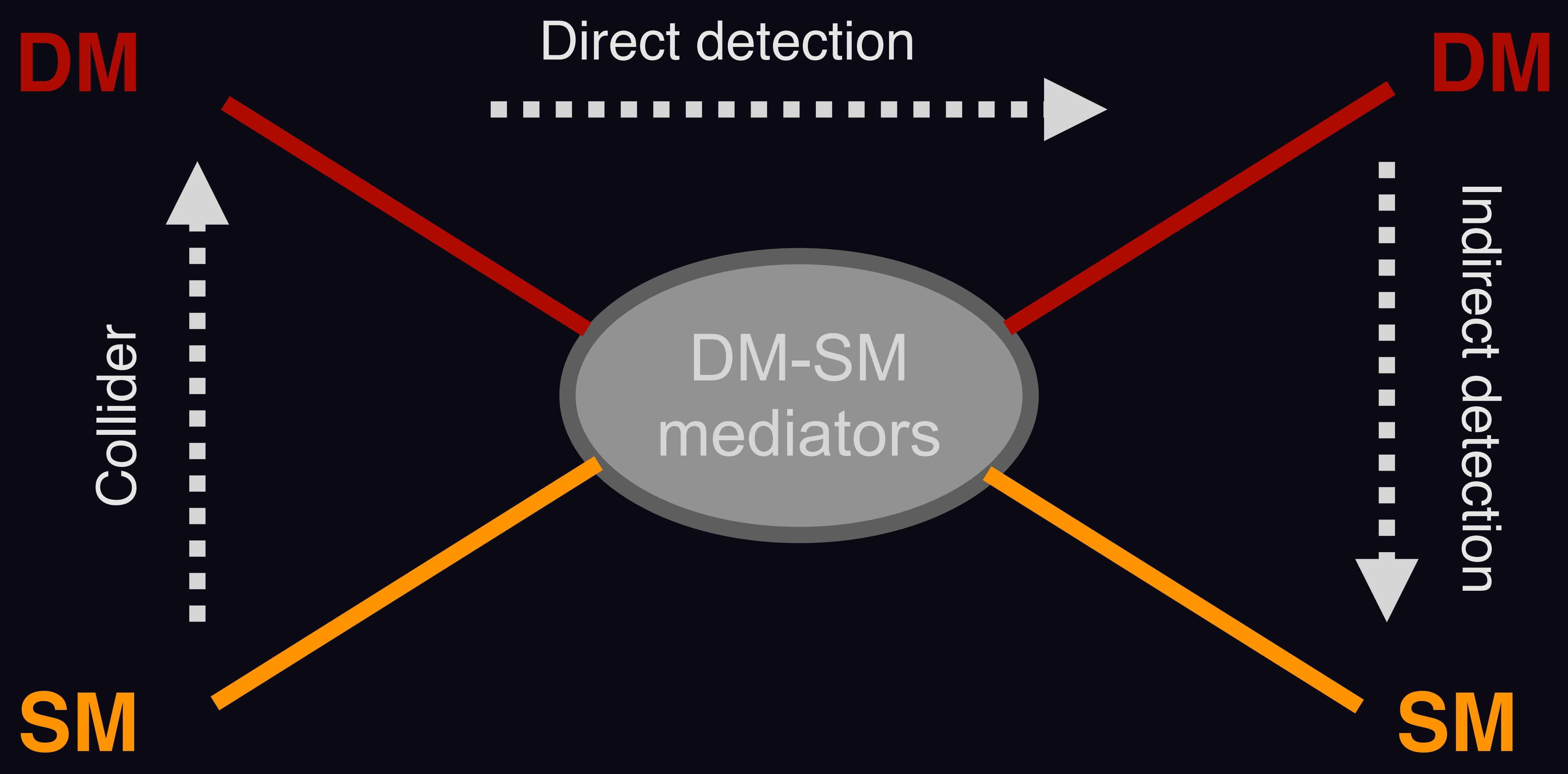
Mitchell Conference on Collider, Dark Matter, and Neutrino Physics 2024

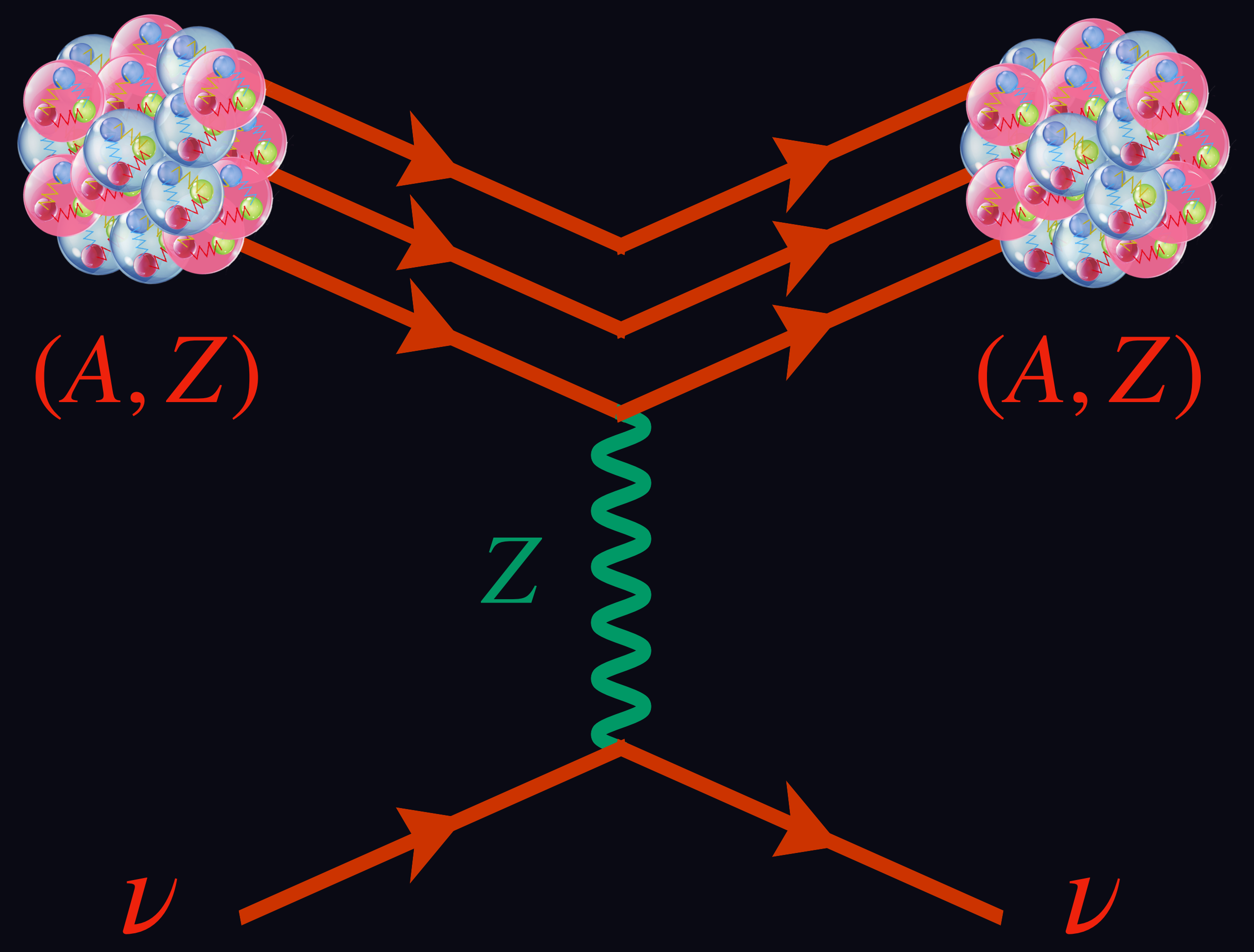


Ab initio Nuclear Calculations for Dark Matter Detection and CEvNS

Bai-Shan Hu (胡柏山)

May 24, 2024 @ College Station



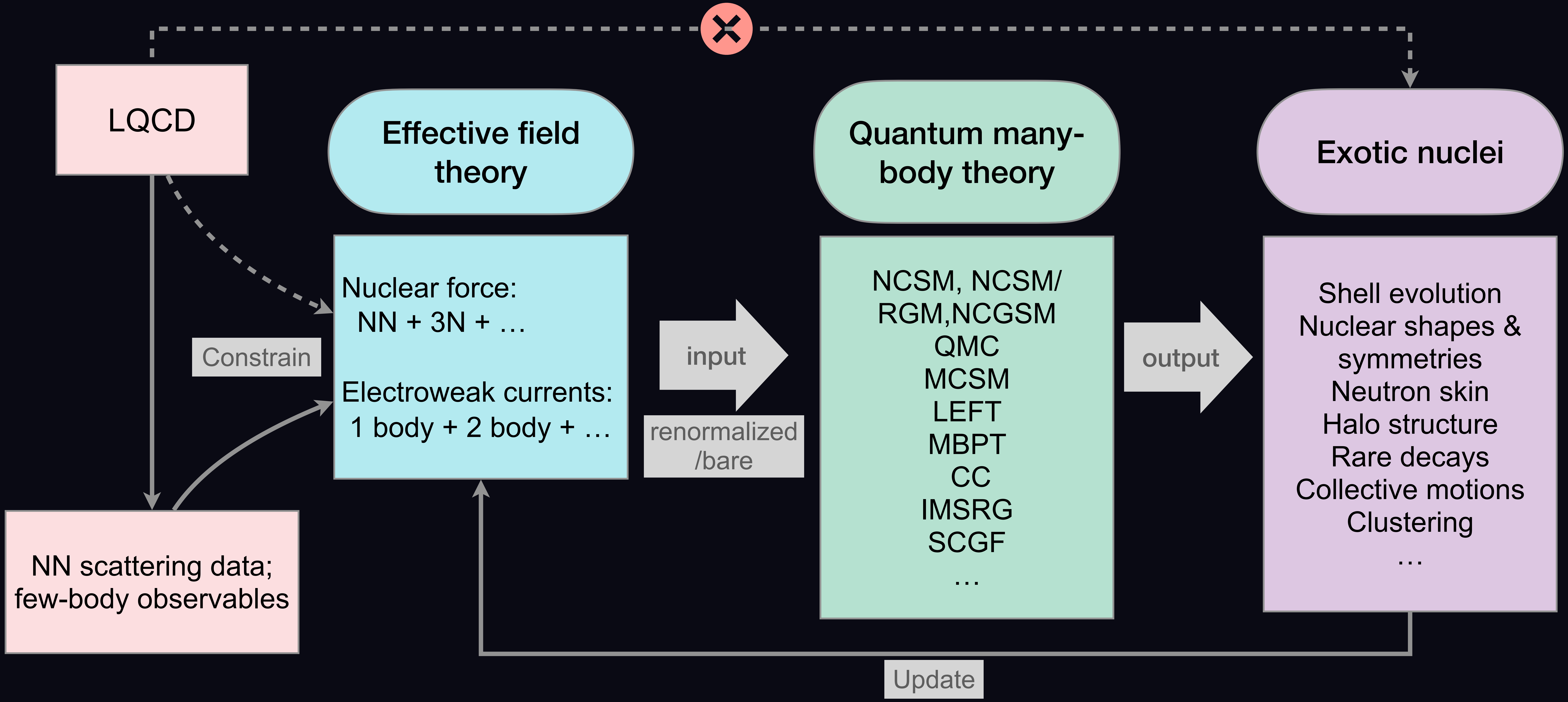


OAK RIDGE National Laboratory

Outline

- What is *ab initio* nuclear calculation?
- Elastic WIMP- and *ν*-nucleus scattering
- A novel investigation of the ATOMKI anomaly
- Summary

Workflow of *ab initio* nuclear calculation



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

WIMP(χ) scattering elastically off nucleus ($\mathcal{N}$)

Weakly interacting massive particles (WIMPs) are hypothetical particles
one of the proposed candidates for dark matter

$$\mathcal{N}(p) + \chi(k) \rightarrow \mathcal{N}(p') + \chi(k')$$

$$\mathscr{L}_\chi^{\mathrm{SD}} = -\frac{G_F}{\sqrt{2}} \int d^3\mathbf{r}\bar{\chi}\gamma\gamma_5\chi \cdot \sum_q C_q^{AA}\bar{q}\gamma\gamma_5 q, \qquad \mathscr{L}_\chi^{\mathrm{SI}}\ldots$$

EFT

particle physics

nuclear physics $\langle \mathcal{N} | H_{\chi A} | \mathcal{N} \rangle$

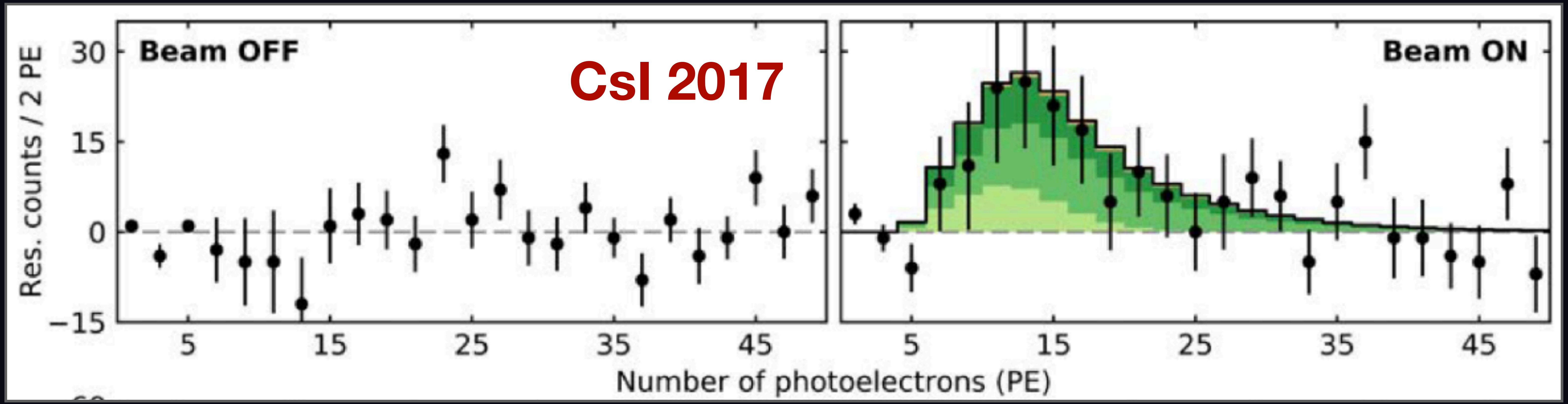
astrophysics

$$\frac{dR}{dE_\mathrm{r}} = \underbrace{\frac{\sigma_{\chi N}^{SD/SI}}{m_\chi \mu_N^2}}_{\text{particle physics}} \times \underbrace{\left| \mathscr{F}^{SD/SI}(\mathbf{q}^2) \right|^2}_{\text{nuclear physics}} \times \underbrace{M\rho_0 \int_{v_{\min}}^{v_{\mathrm{esc}}} \frac{f(v)}{v} d^3v}_{\text{astrophysics}}$$

Coherent Elastic Neutrino-Nucleus Scattering (CEνNS)

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

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



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

- Weak charge

  $Q_w = ZQ_w^p + NQ_w^n$

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

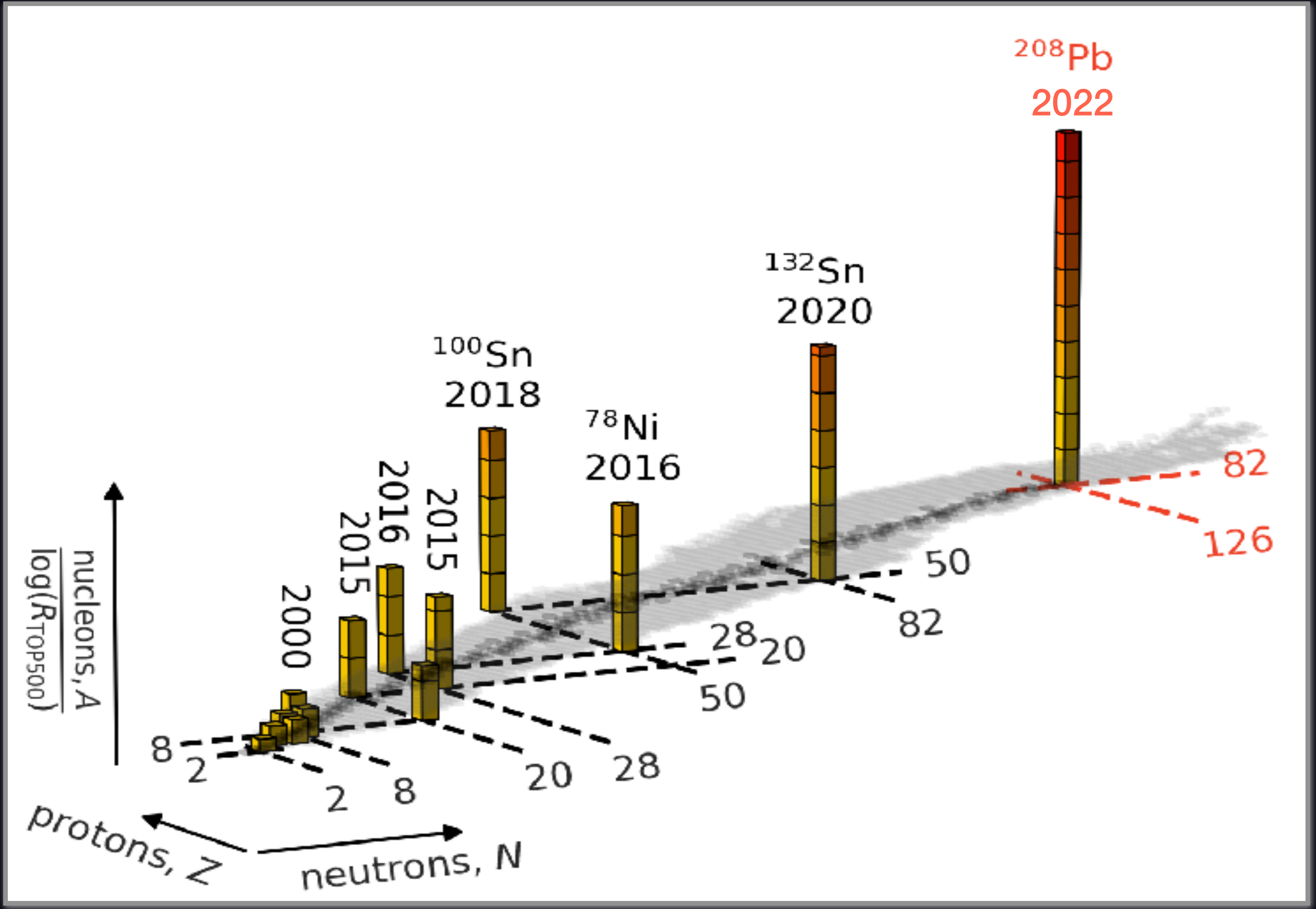
  CEvNS mainly probes neutron distribution

- Nuclear weak form factor F_W

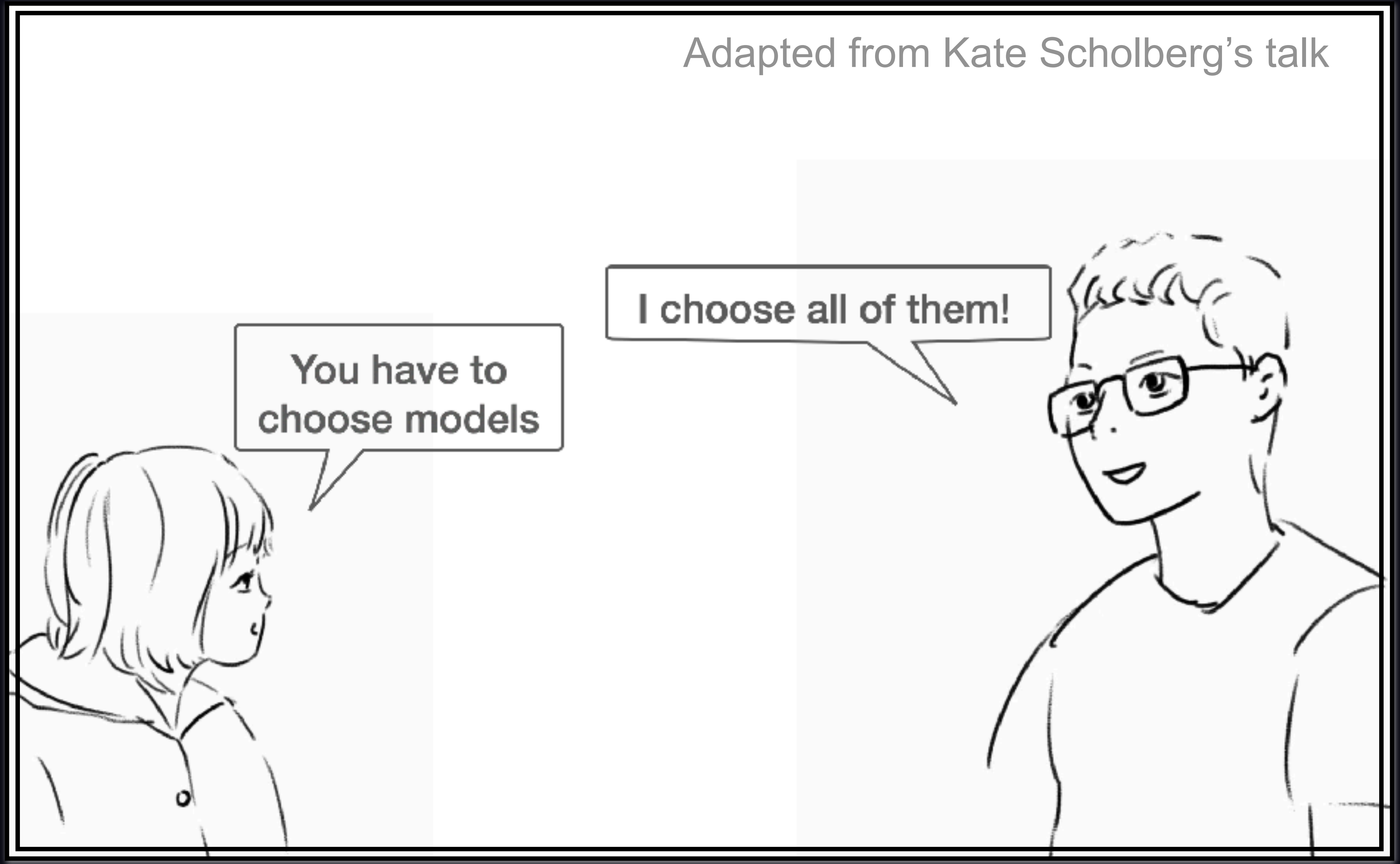
- Axial-vector form factor F_A

  Negligible ?

Spirit of *ab initio* nuclear calculation for weak progress



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



nuclear responses for all particle physics scenarios

$$\langle \mathcal{N} | H_{\chi A} | \mathcal{N} \rangle$$

$$M_{LM;\tau}(q), \quad \Sigma_{LM;\tau}(q), \quad \Delta'_{LM;\tau}(q), \quad \tilde{\Phi}'_{LM;\tau}(q), \quad \Phi''_{LM;\tau}(q)$$

$$\Sigma'_{LM;\tau}(q), \quad \Sigma''_{LM;\tau}(q), \quad \Delta_{LM;\tau}(q), \quad \Omega_{LM;\tau}(q)$$

Leading order contribution in elastic DM- and *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*

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

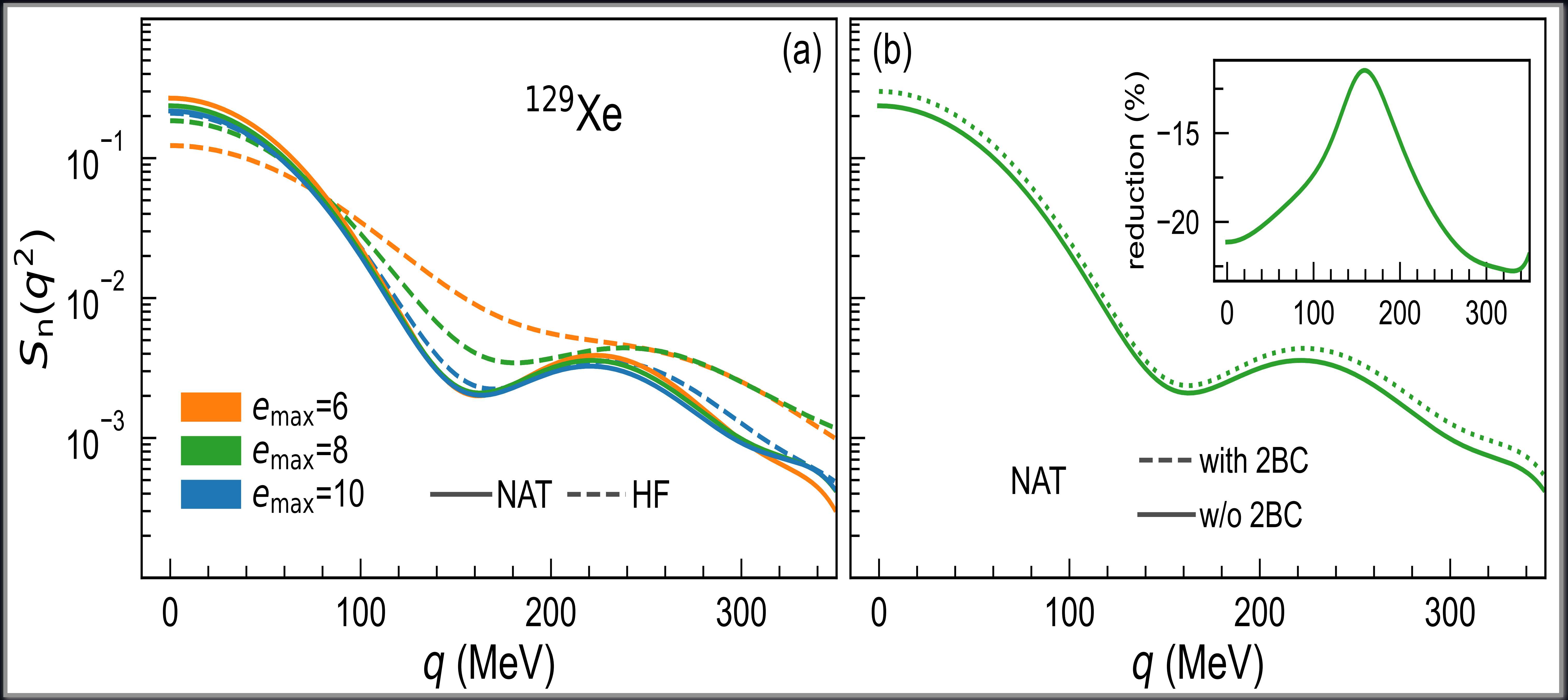
$$R_0^2 = c^2 + \frac{7}{3}\pi^2a^2 - 5s^2$$

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

Heavy nuclei is challenging current *ab-initio* approaches

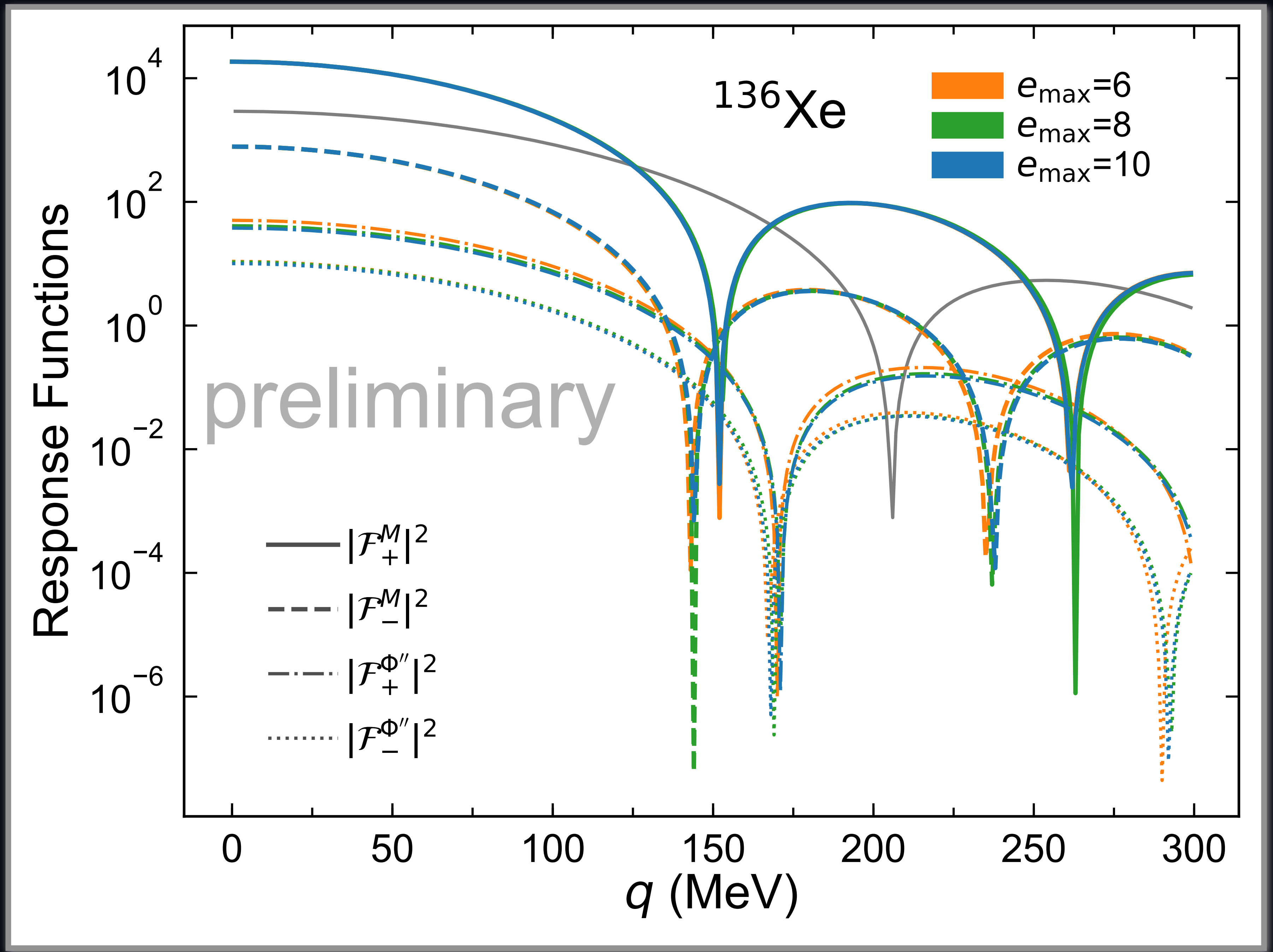
- Tensor operators are very heavy tasks
- Many q points (operators) need to calculate

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



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

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



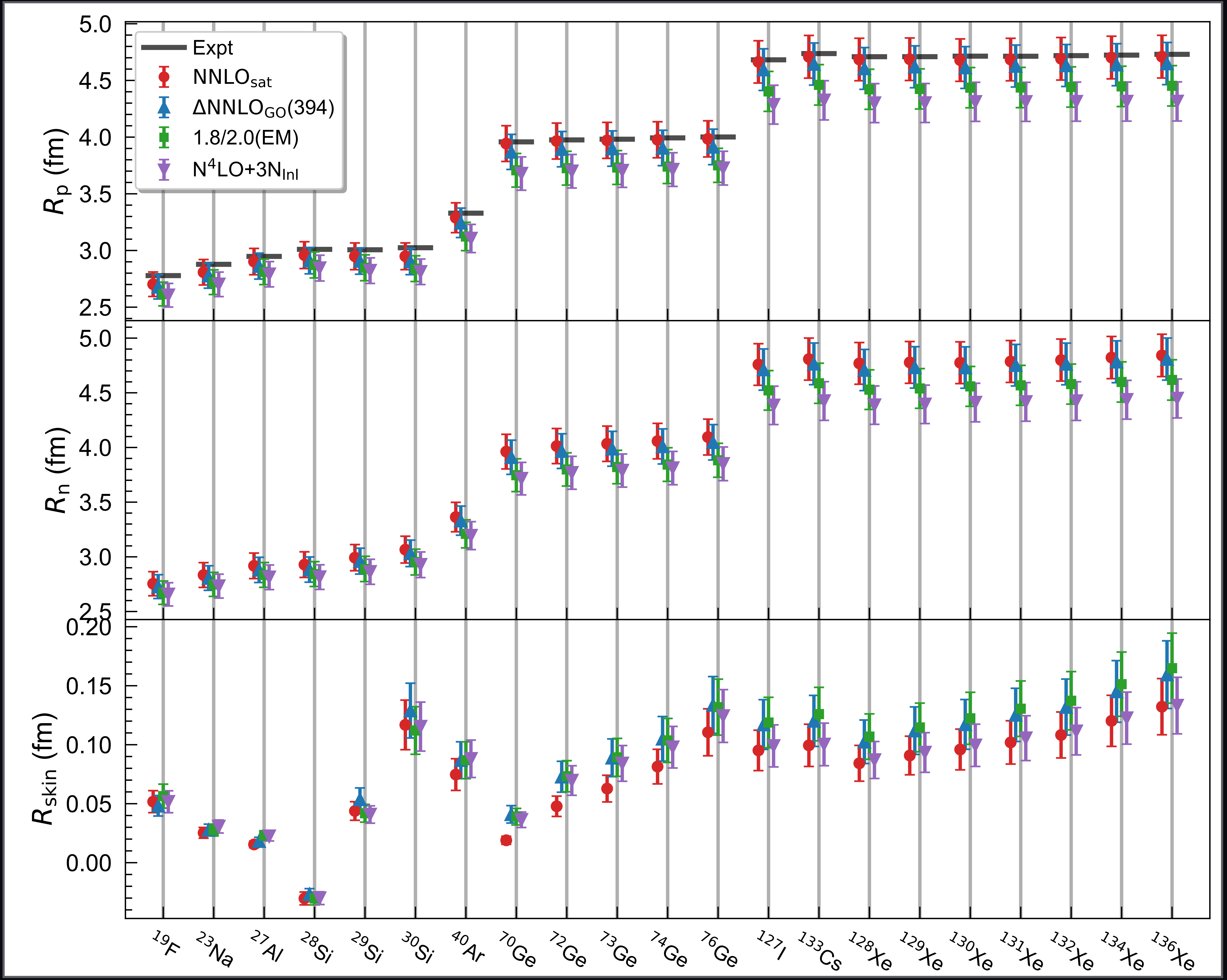
Natural orbitals (NAT) allows heavy nuclei

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

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

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

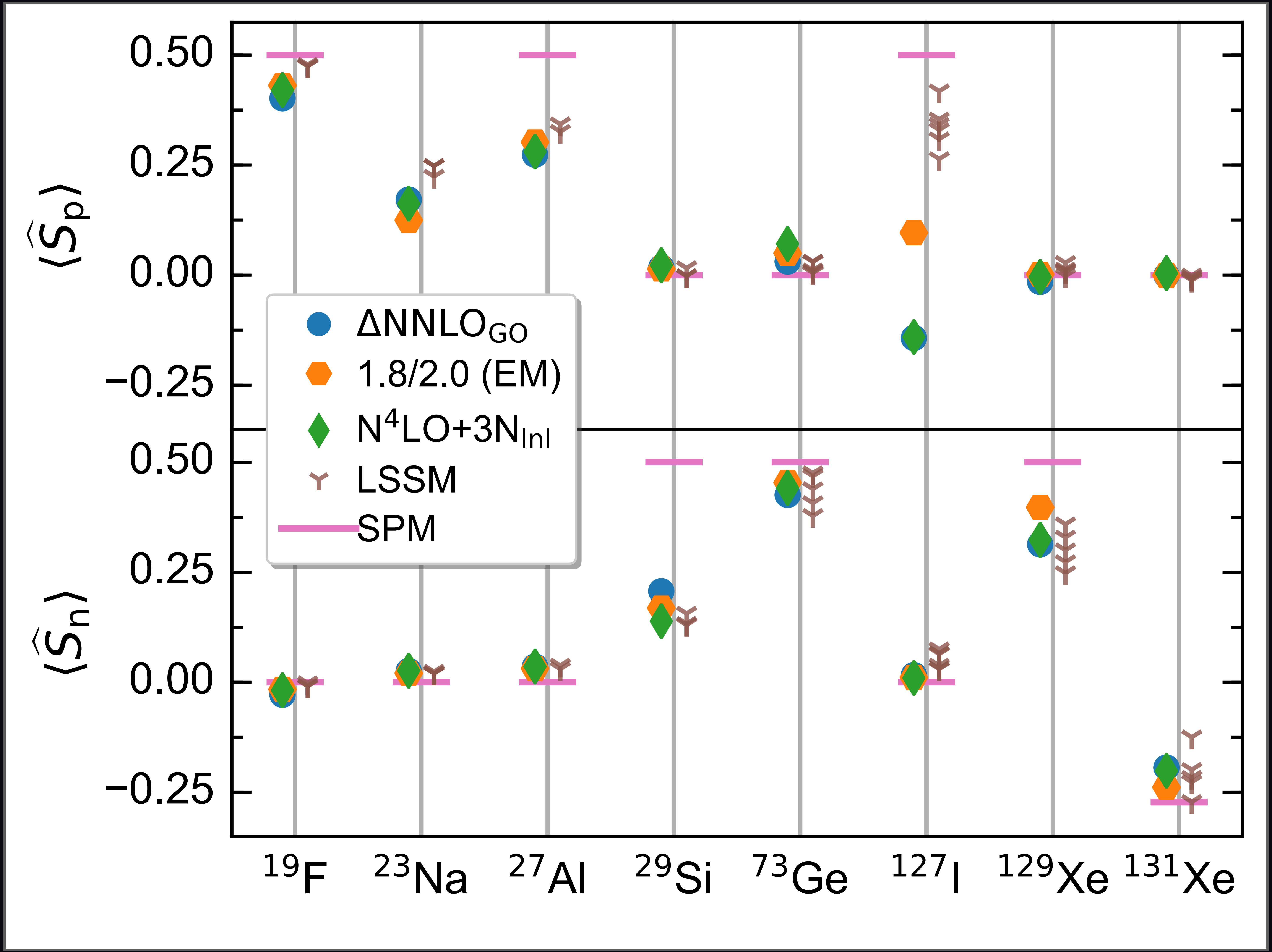


Using these ab initio analysis, we present a refined Helm form factor

BSHu, et al., In preparation (2024)

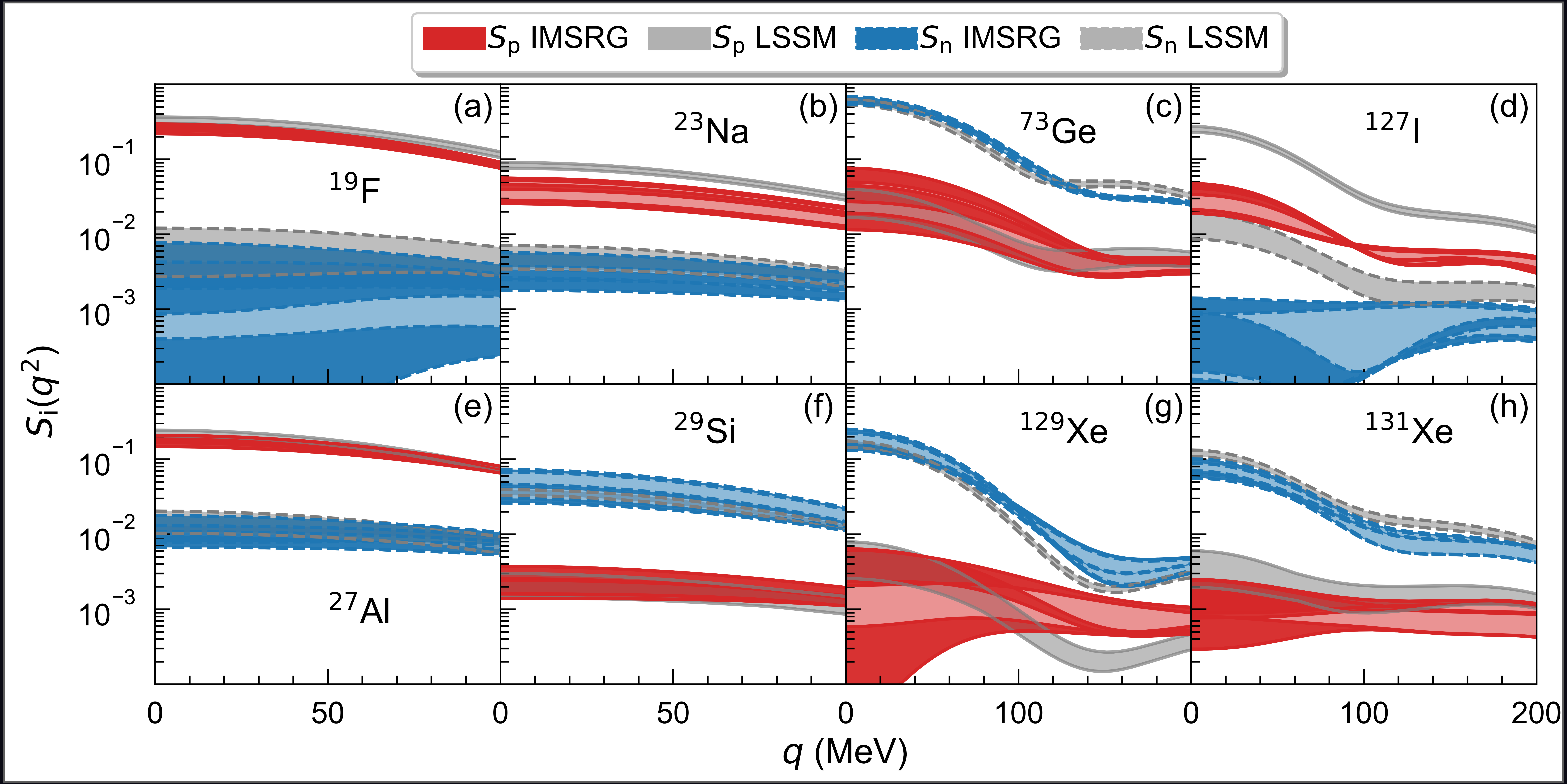
Spin expectation values from first principles

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



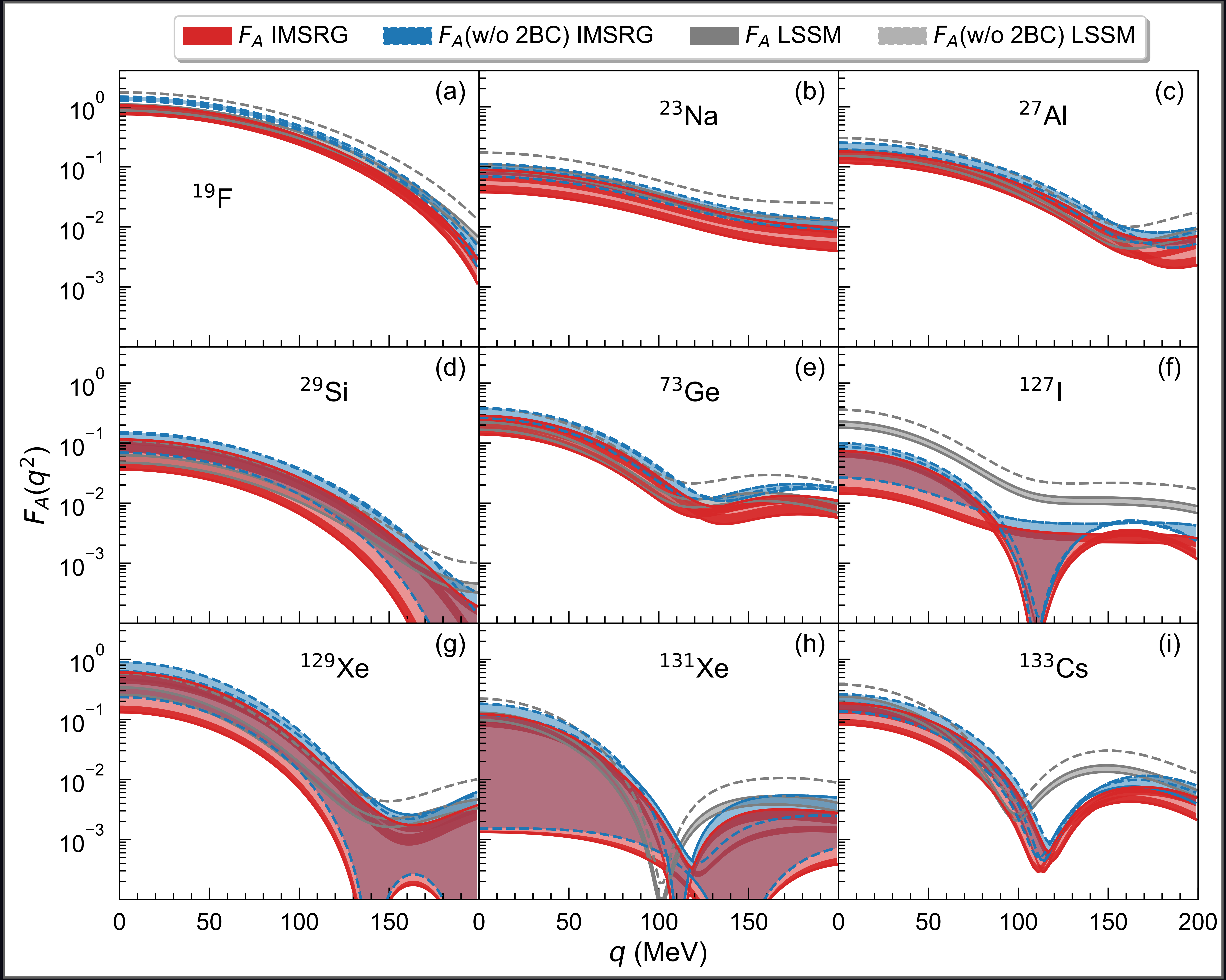
BSHu, et al, Phys Rev Lett 128, 072502 (2022)

Ab initio structure factors for spin-dependent WIMP-nucleus scattering

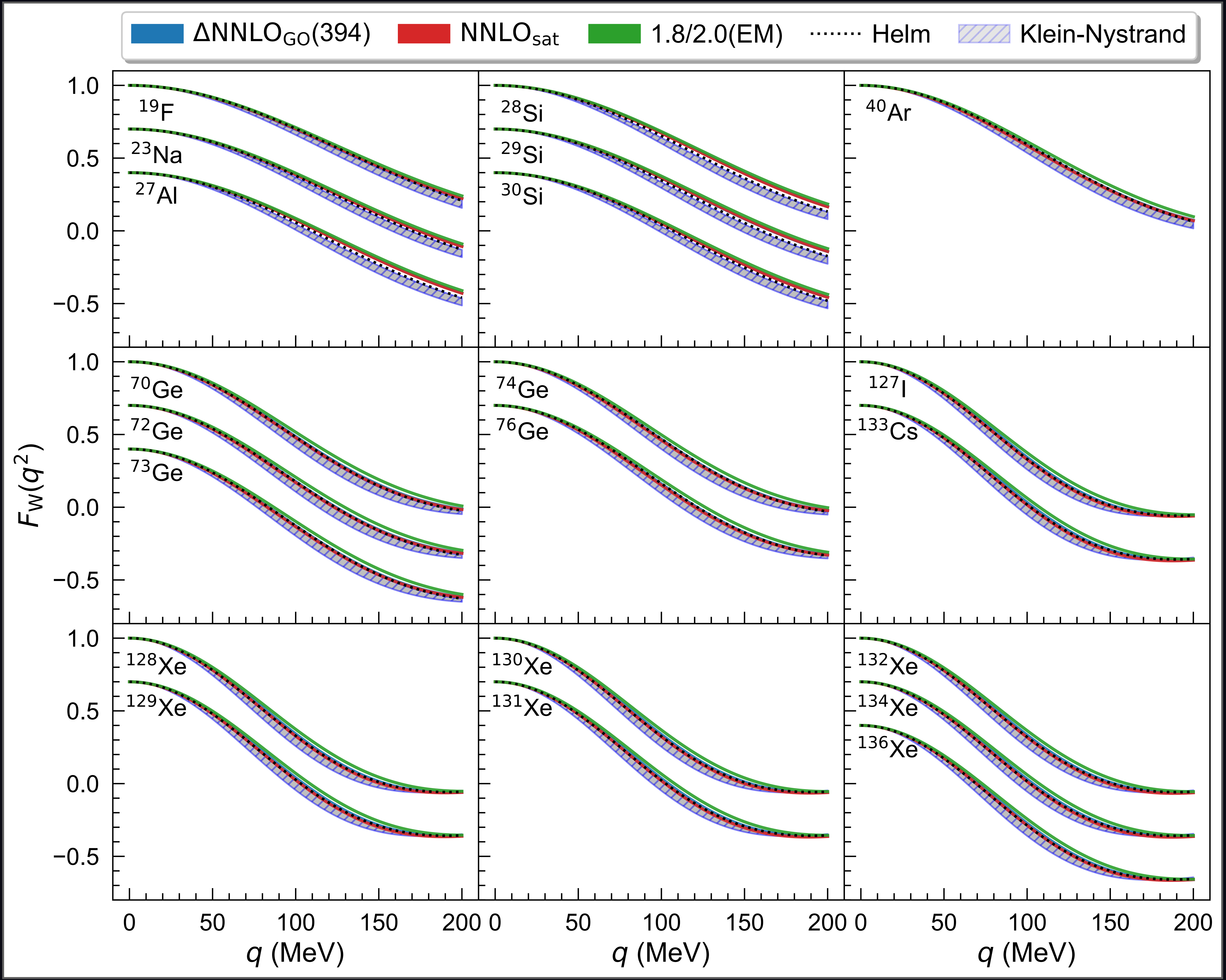


BSHu, et al, Phys Rev Lett 128, 072502 (2022); arXiv: 2109.00193

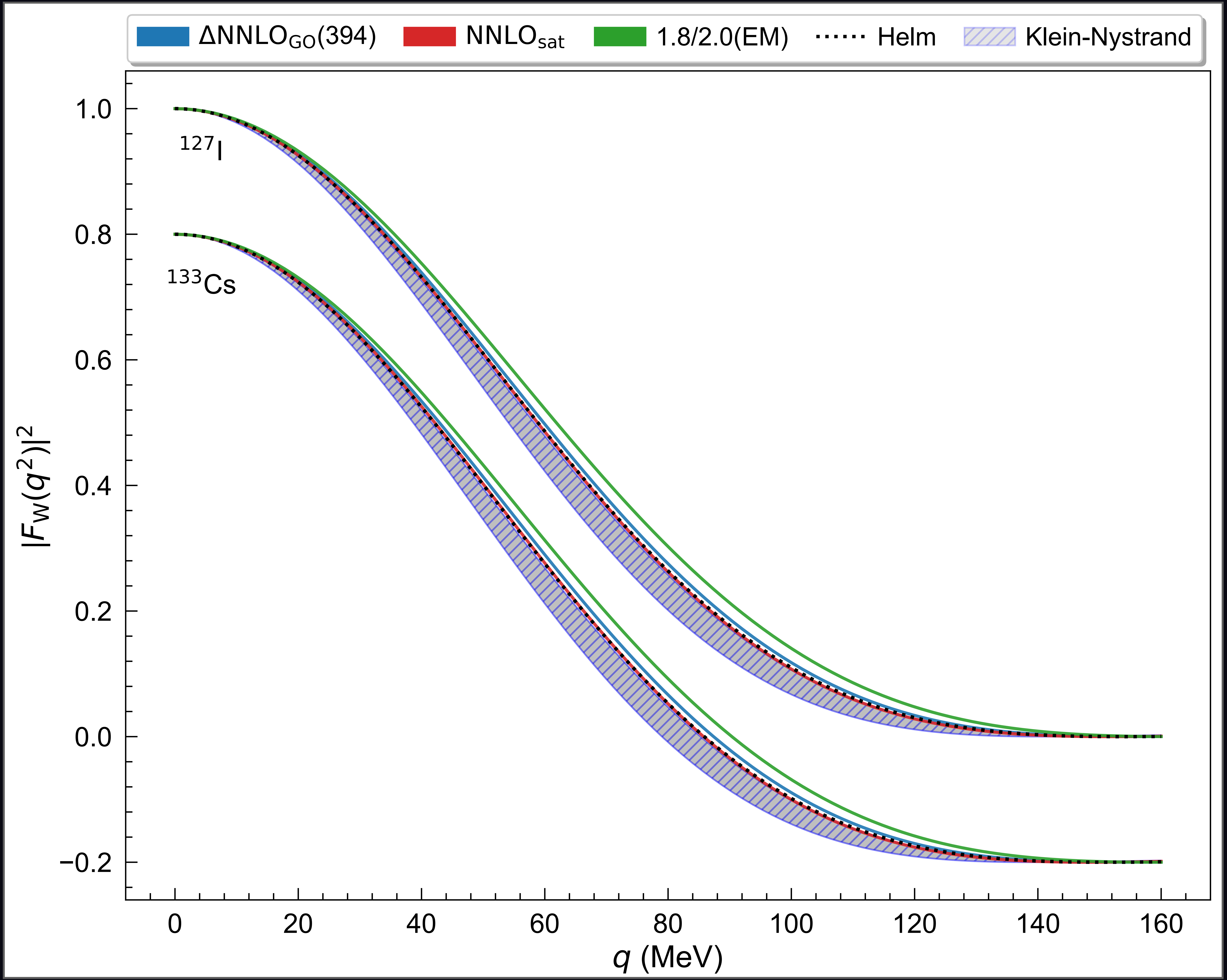
Axial-vector form factor for ν-nucleus scattering



BSHu, et al., In preparation (2024)

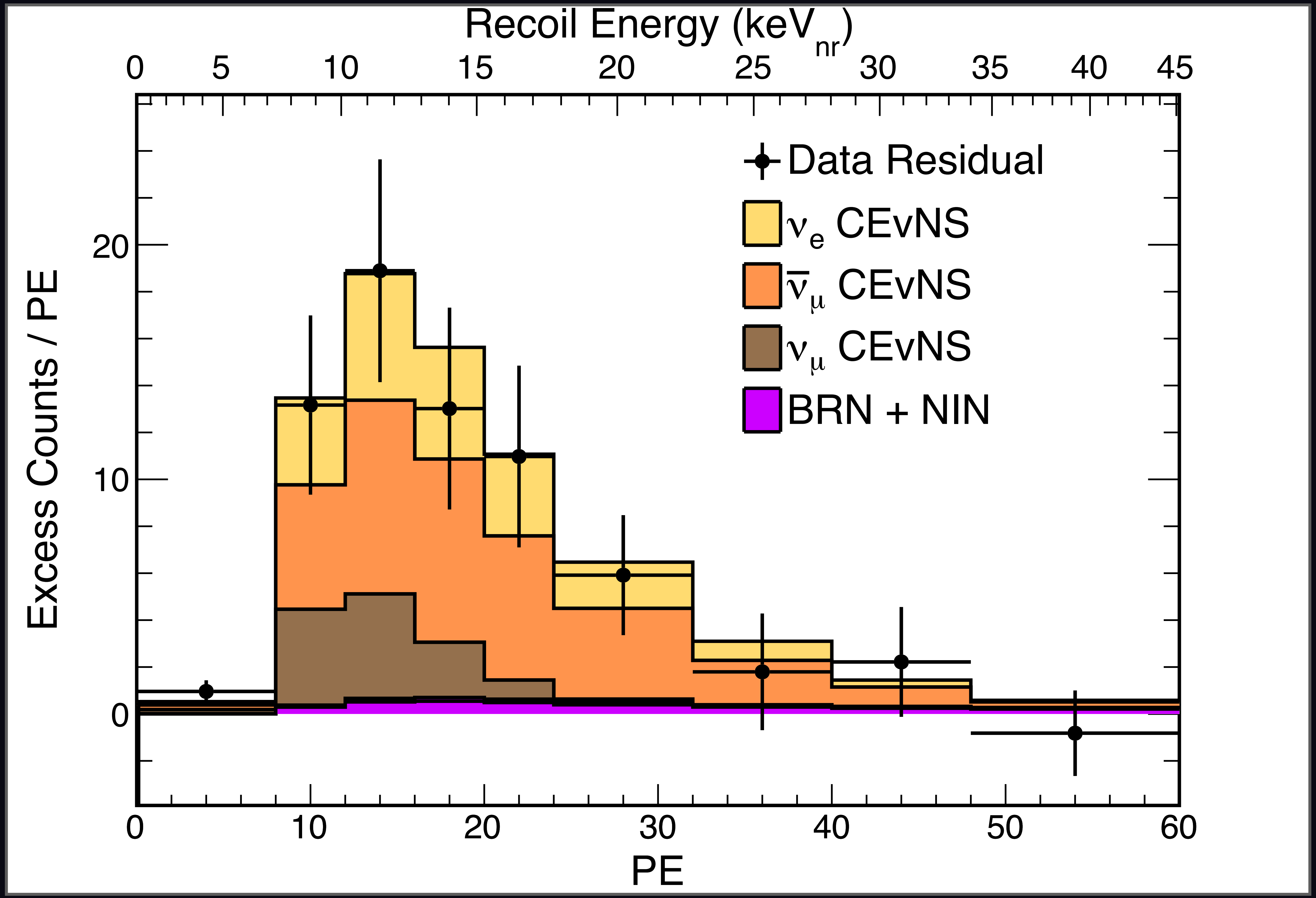


ΔNNLO_GO(394)
NNLO_sat
1.8/2.0(EM)
Helm
Klein-Nystrand
19F
23Na
27Al
28Si
29Si
30Si
40Ar
70Ge
72Ge
73Ge
74Ge
76Ge
127I
133Cs
128Xe
129Xe
130Xe
131Xe
132Xe
134Xe
136Xe
F_W(q^2)
1.0
0.5
0.0
−0.5
0
50
100
150
200
q (MeV)

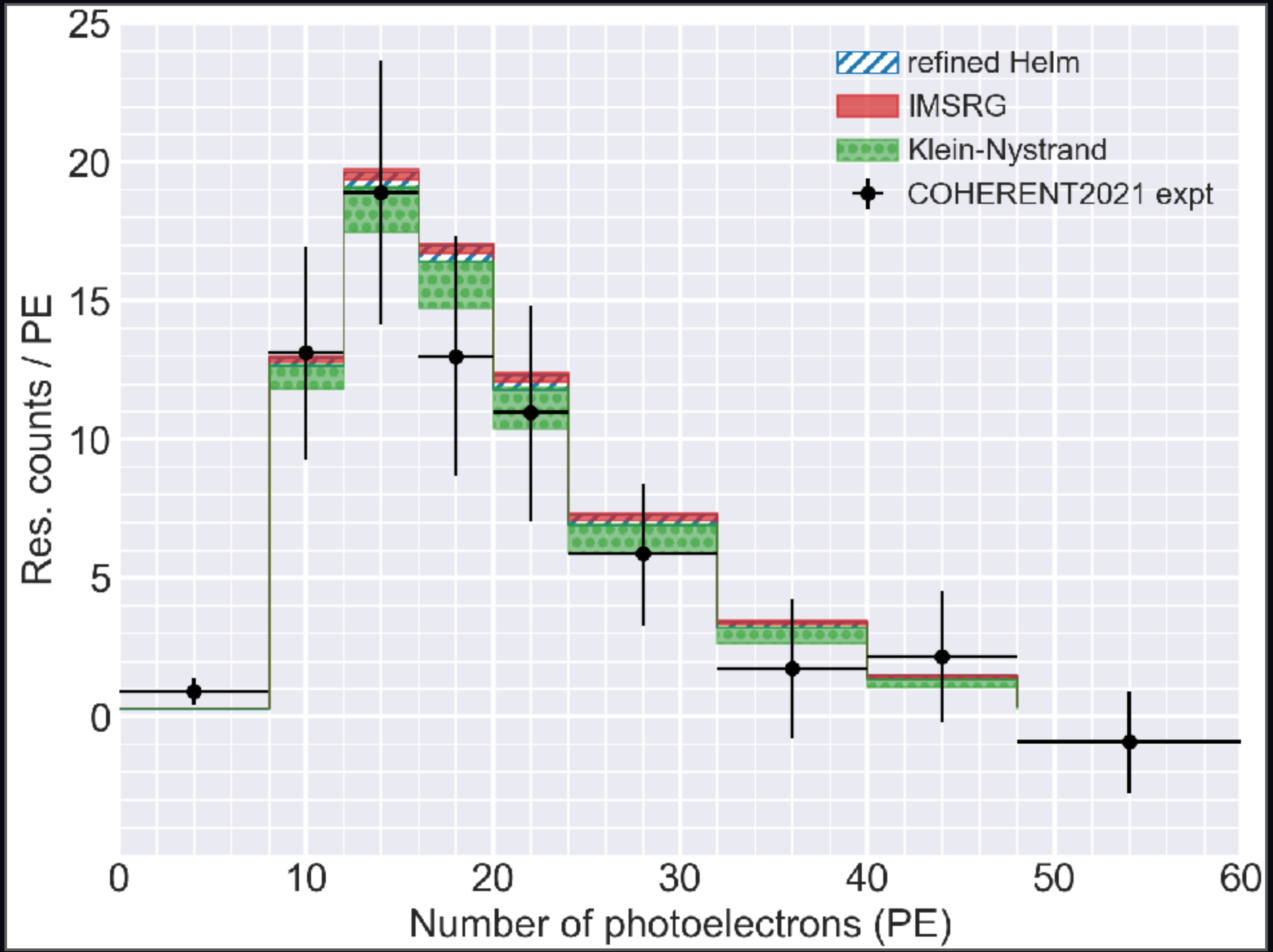


ΔNNLO_GO(394)
NNLO_sat
1.8/2.0(EM)
Helm
Klein-Nystrand
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
127I
133Cs
|F_W(q^2)|^2
0
20
40
60
80
100
120
140
160
q (MeV)

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



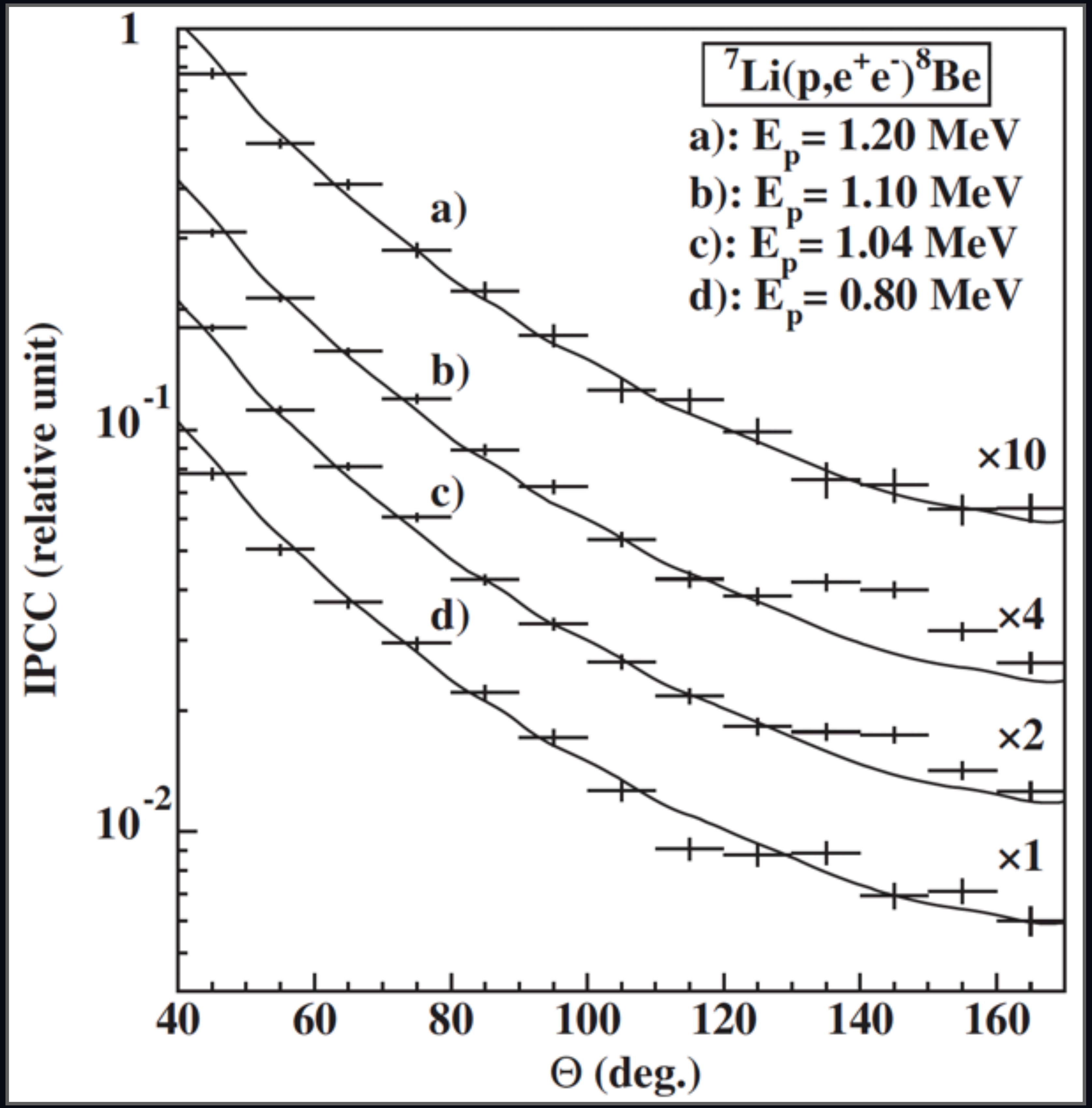
D. Akimov et al. (COHERENT). Phys Rev Lett 129, 081801 (2022)



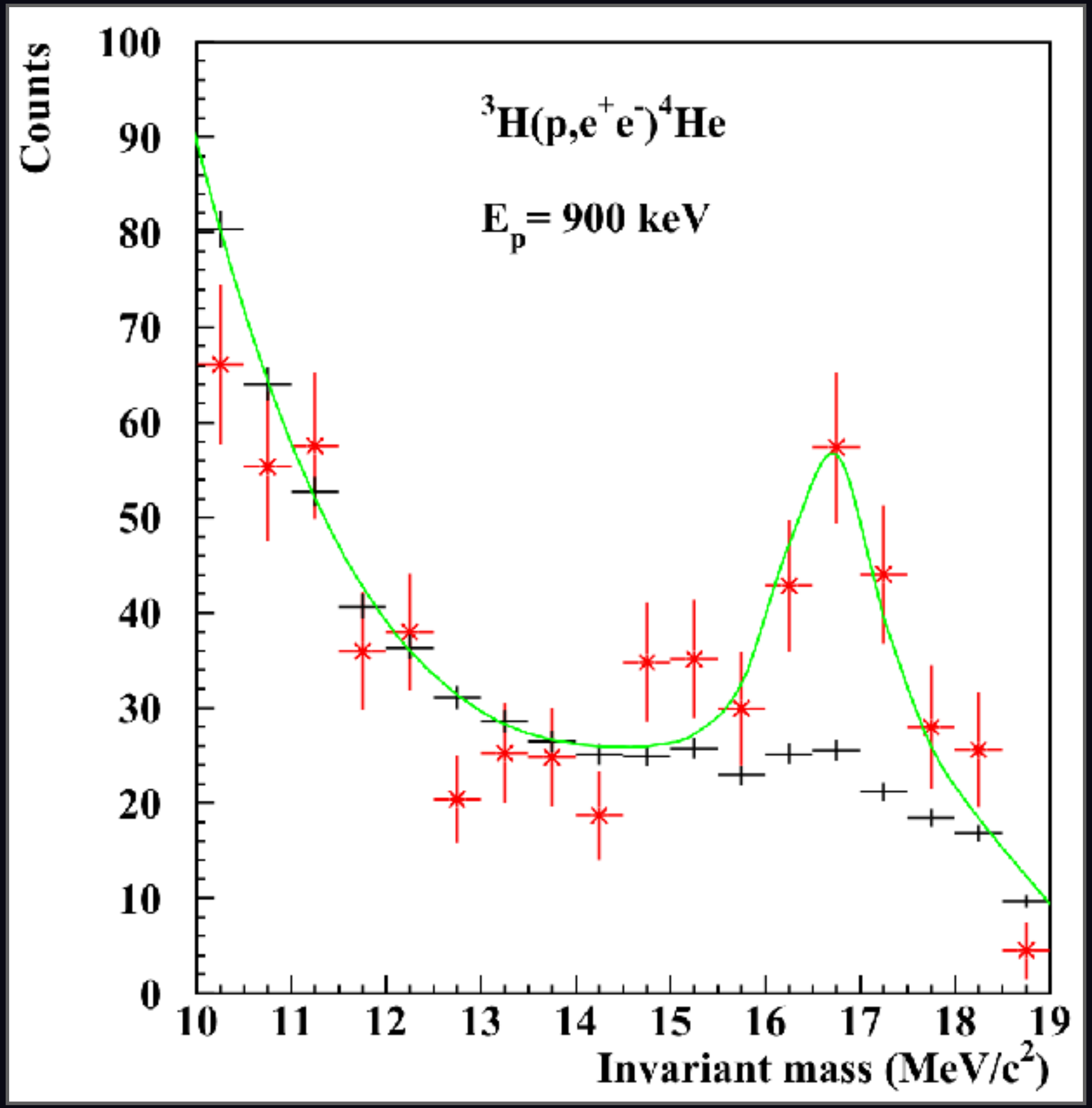
BSHu, et al., In preparation (2024)

II. A novel investigation of the ATOMKI anomaly

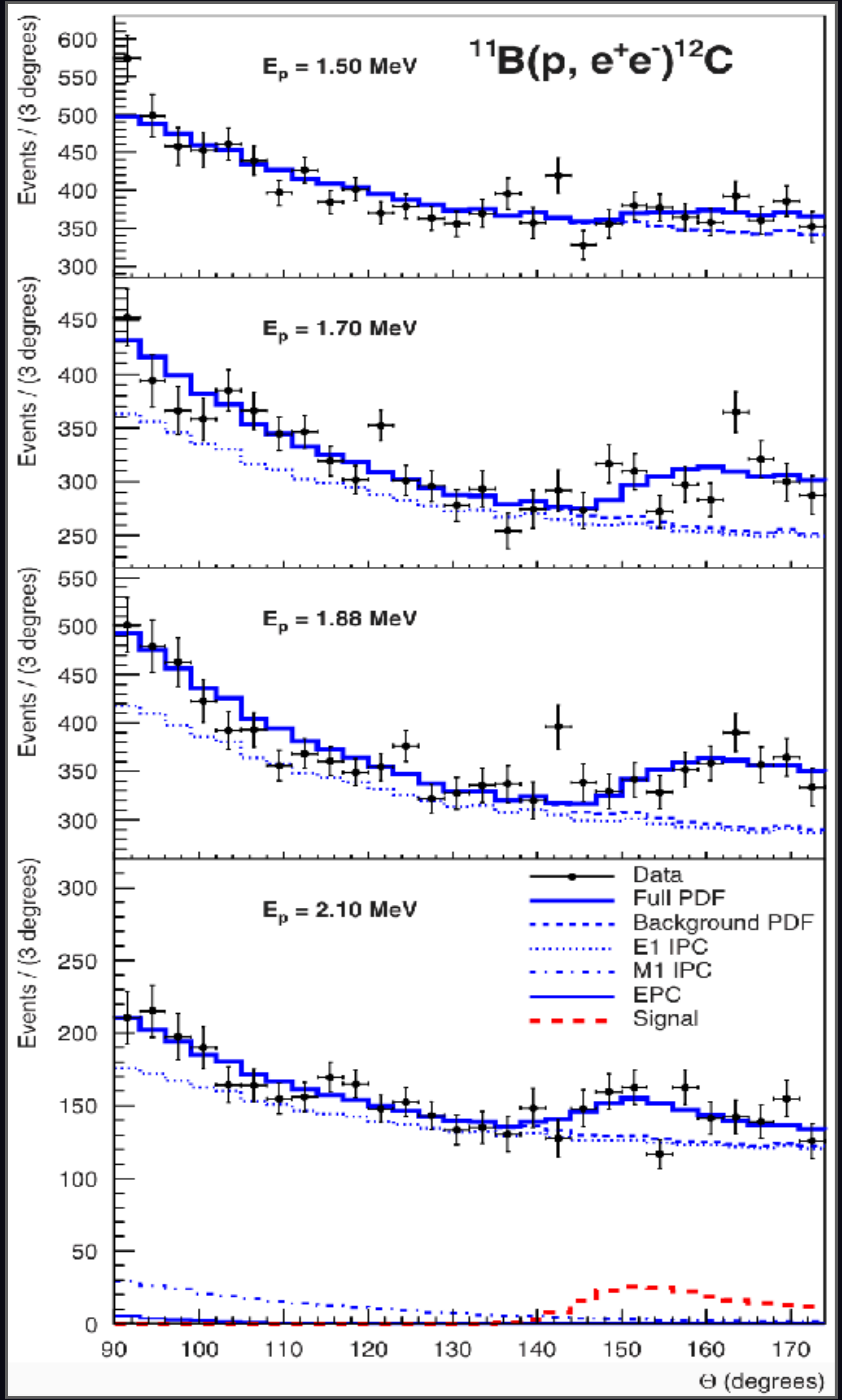
ATOMKI anomaly suggests a new BSM boson X with mass ~ 17 MeV



A. J. Krasznahorkay, et al. Phys Rev Lett 116, 042501 (2016)



A. J. Krasznahorkay, et al. arXiv:1910.10459 (2019)



A. J. Krasznahorkay, et al. Phys Rev C 106, L061601 (2022)

A novel investigation of the ATOMKI anomaly

neutron scatters inelastically at the detector nuclei and produces the new boson X, which quickly decays into a $e^+ e^-$ pair

$$n + \mathcal{N} \to n + \mathcal{N}^* \qquad \mathcal{N}^* \to \mathcal{N} + \gamma/X \qquad X \to e^+ + e^-$$

$$\mathscr{L} = \epsilon_p \bar{p} \gamma^\mu \gamma^5 p X_\mu + \epsilon_n \bar{n} \gamma^\mu \gamma^5 n X_\mu$$

- Events $N_X = T \sum_i \phi_X^i$
- X flux produced by nuclear states *i* $\phi_X^i = \phi_\gamma^i \frac{\Gamma_X^i}{\Gamma_\gamma^i}$
- photon flux from the inelastic neutron scattering $\phi_\gamma = nw \frac{N_A}{M_s} \frac{\Gamma_\gamma}{\Gamma_{tot}} \int \sigma_n(E_n) \frac{d\phi_n}{dE_n} dE_n$

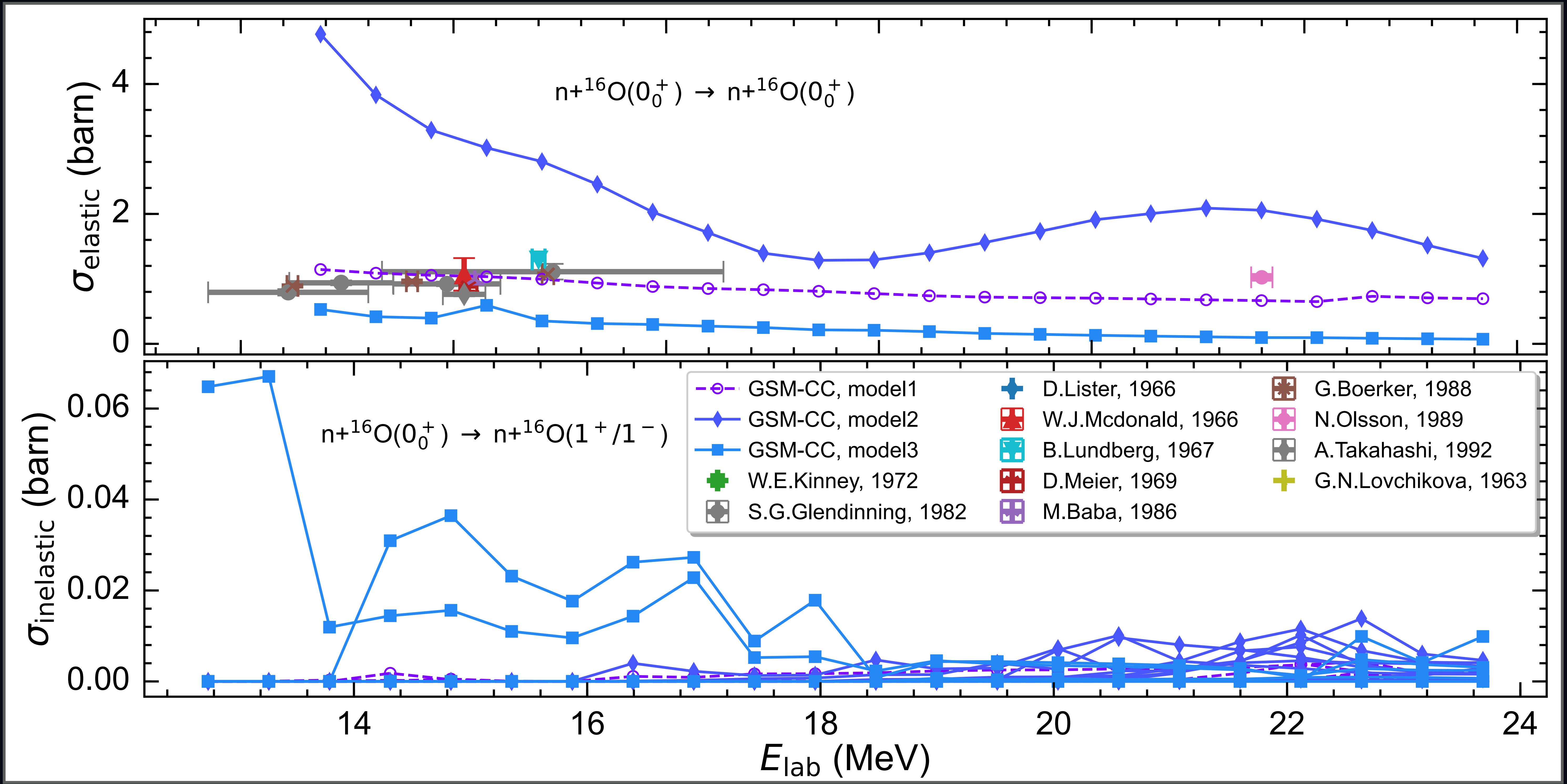
Variable	Definition	CCM	PIP2-BD	JSNS^2
ϕ_n	Neutron flux	$\mathcal{O}(10^{-4}) - \mathcal{O}(10^{-2})$ cm^{-2}s^{-1}		
σ_n	Neutron cross section	$\mathcal{O}(10^{-7}) - \mathcal{O}(10^{-2})$ barn		
M_s	ATOMKI detector molar mass	60.08 (SiO_2)	60.08 (SiO_2)	14 (CH_2)
n	Number of nucleus per molecule	2 (SiO_2)	2 (SiO_2)	1 (CH_2)
w	ATOMKI detector weight	130 kg	841.1 kg	17 ton
$\Gamma_{\rm tot}$	$\mathcal{N}^* \to \mathcal{N}$ + any: Total decay width	$\mathcal{O}(10) - \mathcal{O}(10^2)$ keV		
Γ_γ	$\mathcal{N}^* \to \mathcal{N} + \gamma$: Photon decay width	$\mathcal{O}(10^{-2}) - \mathcal{O}(10^{-1})$ keV		
N_A	Avogadro constant	6×10^{23}		

Nuclear calculations

- Coupled-channels Gamow shell model (GSM-CC)

  cross section σ_n of inelastic neutron scattering reactions: $^{12}C(n,n')$ and $^{16}O(n,n')$

$$\phi_\gamma = nw\frac{N_A}{M_s}\frac{\Gamma_\gamma}{\Gamma_{tot}}\int \sigma_n\left(E_n\right)\frac{d\phi_n}{dE_n}dE_n$$

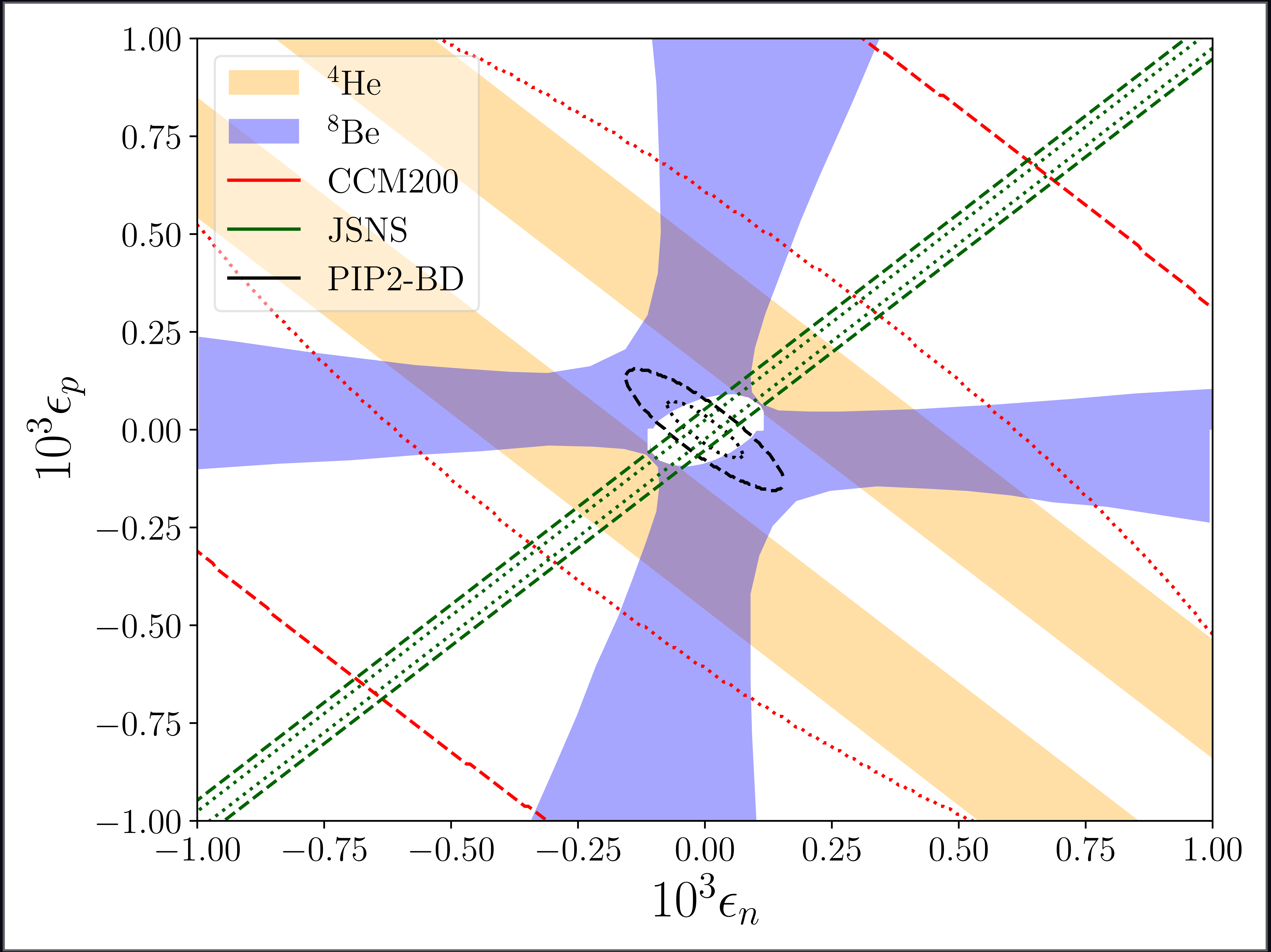


- Nuclear shell model

  Multipole expansion for nuclear X decay rate:

$$\Gamma_X = \frac{2q}{2J_i+1}\left\{\sum_{J>0}\left|\left\langle J_f\left\|\left[\frac{q}{m}\mathscr{M}_J-\frac{\omega}{m}\mathscr{L}_J\right]\right\|J_i\right\rangle\right|^2+\sum_{J\geq1}\left[\left|\left\langle J_f\|\mathscr{T}_J^{el}\|J_i\right\rangle\right|^2+\left|\left\langle J_f\left\|\mathscr{T}_J^{mag}\right\|J_i\right\rangle\right|^2\right]\right\}$$

Limits of ATOMKI for 2.3 events (dotted) and 10 events (dashed)



B. Dutta, W. C. Huang, BSHu, R. G. Van de Water, In preparation (2024)

- ^{4}He and ^{8}Be limits are from D. Barducci and C. Toni. JHEP 07, 168 (2023)
- CCM200: T = 3 years
  JSNS^2: T = 3 years
  PIP2-BD: T = 5 years

Collaborators:

TEXAS A&M UNIVERSITY

Bhaskar Dutta
Louis Strigari
Jeremy Holt
Wei-Chih Huang
Yi Zhuang

TRIUMF

Jason Holt

UNIVERSITY OF NOTRE DAME

Ragnar Stroberg

OAK RIDGE National Laboratory

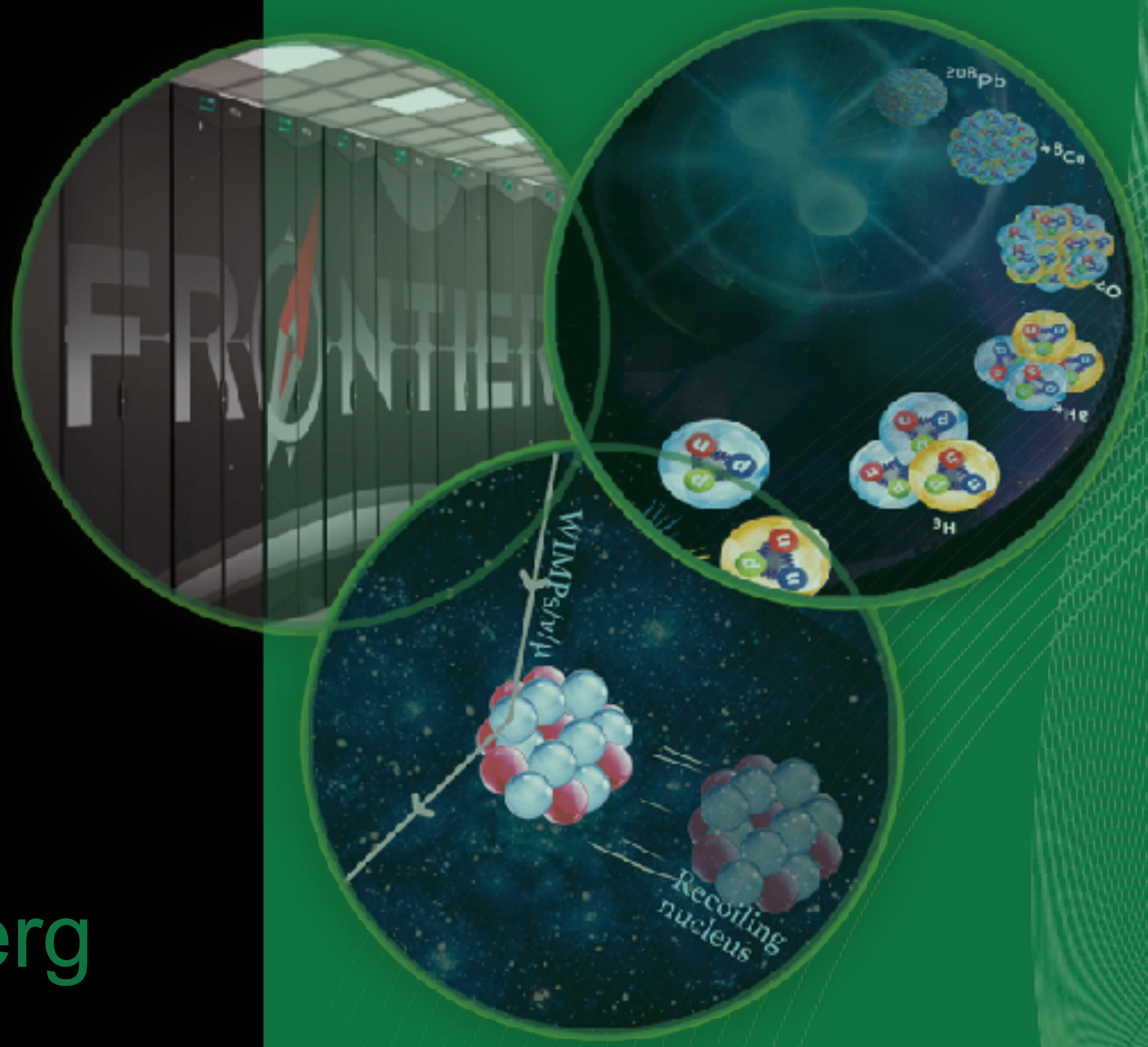
Gaute Hagen
Thomas Papenbrock

筑波大学 University of Tsukuba

Takayuki Miyagi

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 !

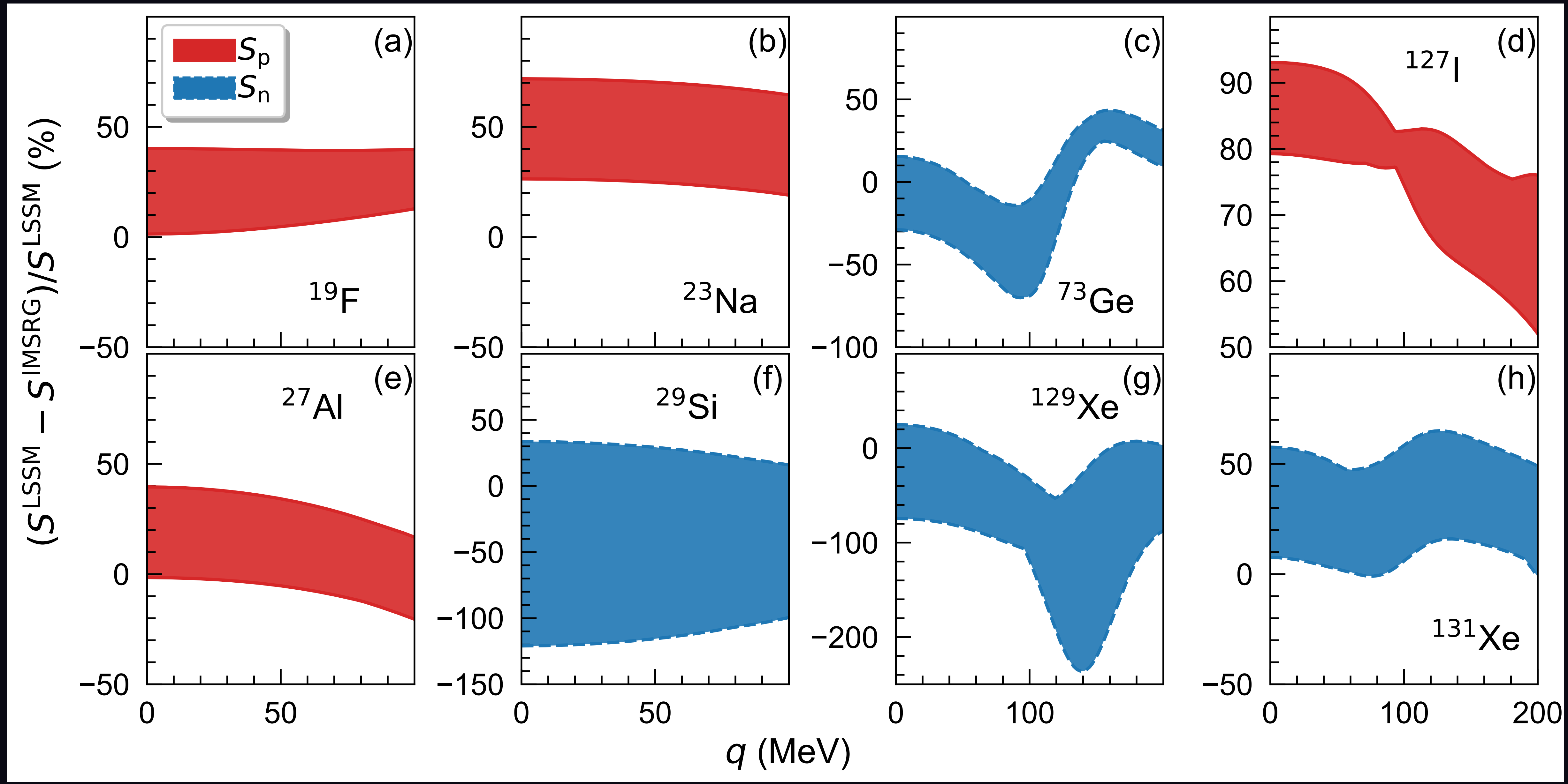


OAK RIDGE National Laboratory

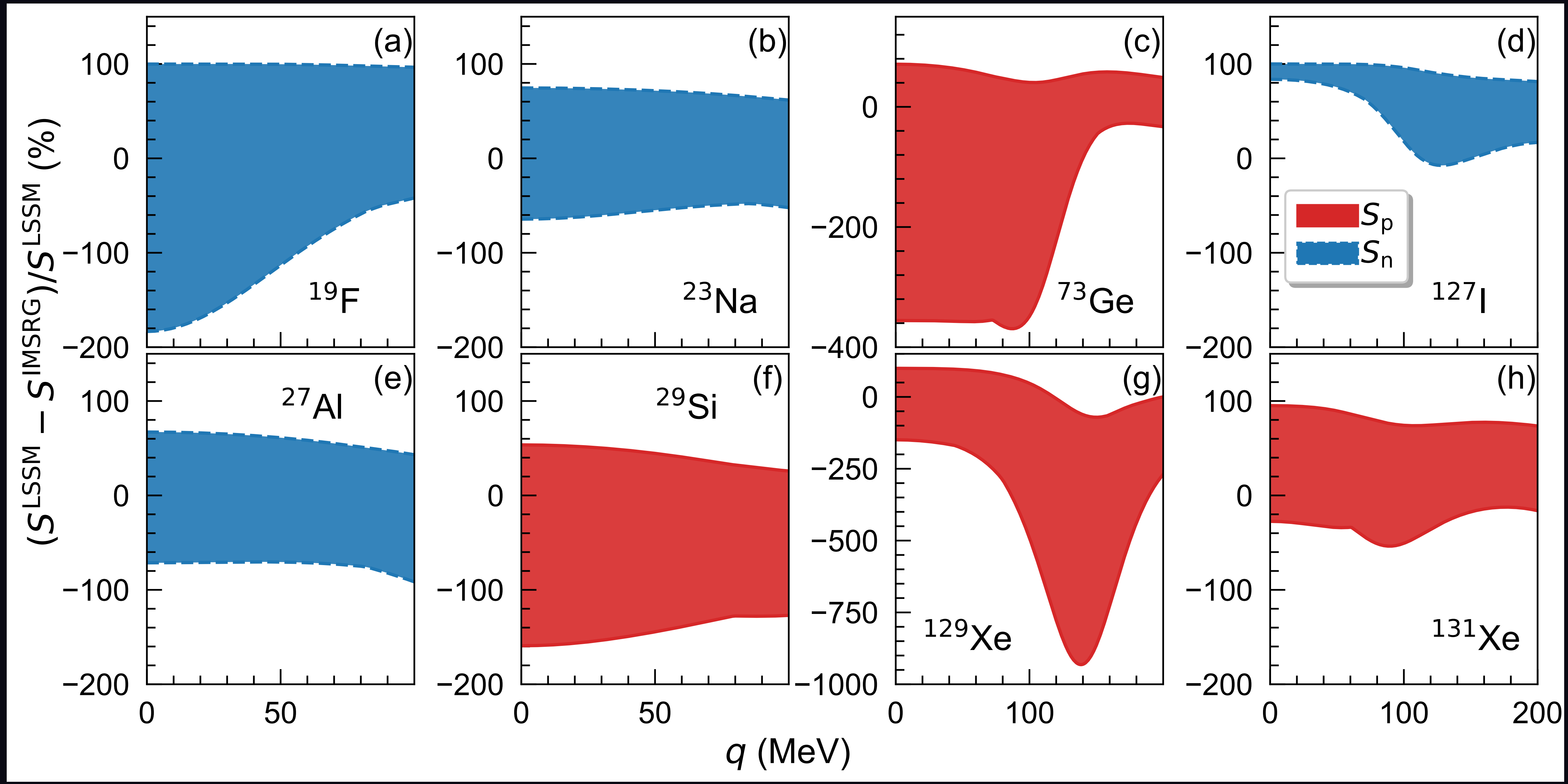
Backup

Discrepancy between LSSM and IMSRG

Dominant structure factor



Non-dominant structure factor



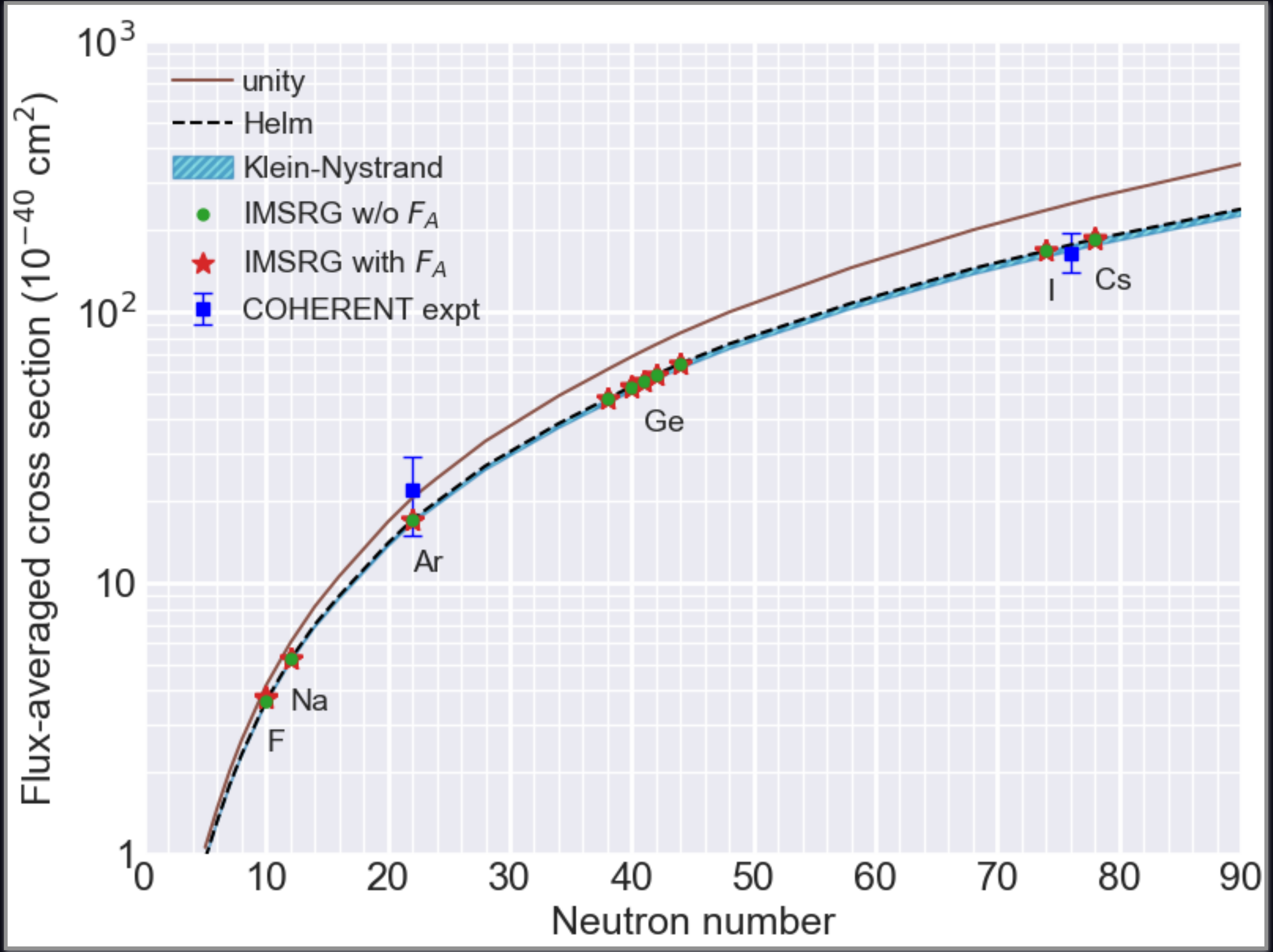
N	N^*	S^π	I	Γ(keV)	Γ_γ(eV)
^{8}Be		0^+	0	5.57 ± 0.25	
	^{8}Be(18.15)	1^+	0^*	138 ± 6	1.9 ± 0.4
	^{8}Be(17.64)	1^+	1^*	10.7 ± 0.5	15.0 ± 1.8
^{4}He		0^+	0	Stable	
	^{4}He(21.01)	0^-	0	0.84	0
	^{4}He(20.21)	0^+	0	0.50	0
^{12}C		0^+	0	Stable	
	^{12}C(17.23)	1^-	1	1150	44

Table 1. Spin-parity J^π and isospin I quantum numbers, total decay widths Γ and γ-decay widths $\Gamma_\gamma = \Gamma(N^* \to N\gamma)$ for the nuclei used in the ATOMKI experiment: ^{8}Be [7], ^{4}He [8, 9] and ^{12}C [10, 11] nuclei. Asterisks on isospin assignments indicate states with significant isospin mixing.

Process	**X boson spin parity**			
$N^* \to N$	$S^\pi = 1^-$	$S^\pi = 1^+$	$S^\pi = 0^-$	$S^\pi = 0^+$
^{8}Be(18.15) $\to$ ^{8}Be	1	0, 2	1	/
^{8}Be(17.64) $\to$ ^{8}Be	1	0, 2	1	/
^{4}He(21.01) $\to$ ^{4}He	/	1	0	/
^{4}He(20.21) $\to$ ^{4}He	1	/	/	0
^{12}C(17.23) $\to$ ^{12}C	0, 2	1	/	1

Table 2. Relative angular momentum between the X boson and N in the various decays, based on its possible parity-spin assignments. Note that parity conservation prohibits a pure scalar solution to the Beryllium anomaly.

D. Barducci and C. Toni. JHEP 07, 168 (2023)



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

$$Q_W^p = 0.0714,\ Q_W^n = -0.9900$$

$$Q_W^n = -1,\ Q_W^p = 1 - 4\sin^2\theta_W \qquad \sin^2\theta_W = 0.23122 \pm 0.00003$$

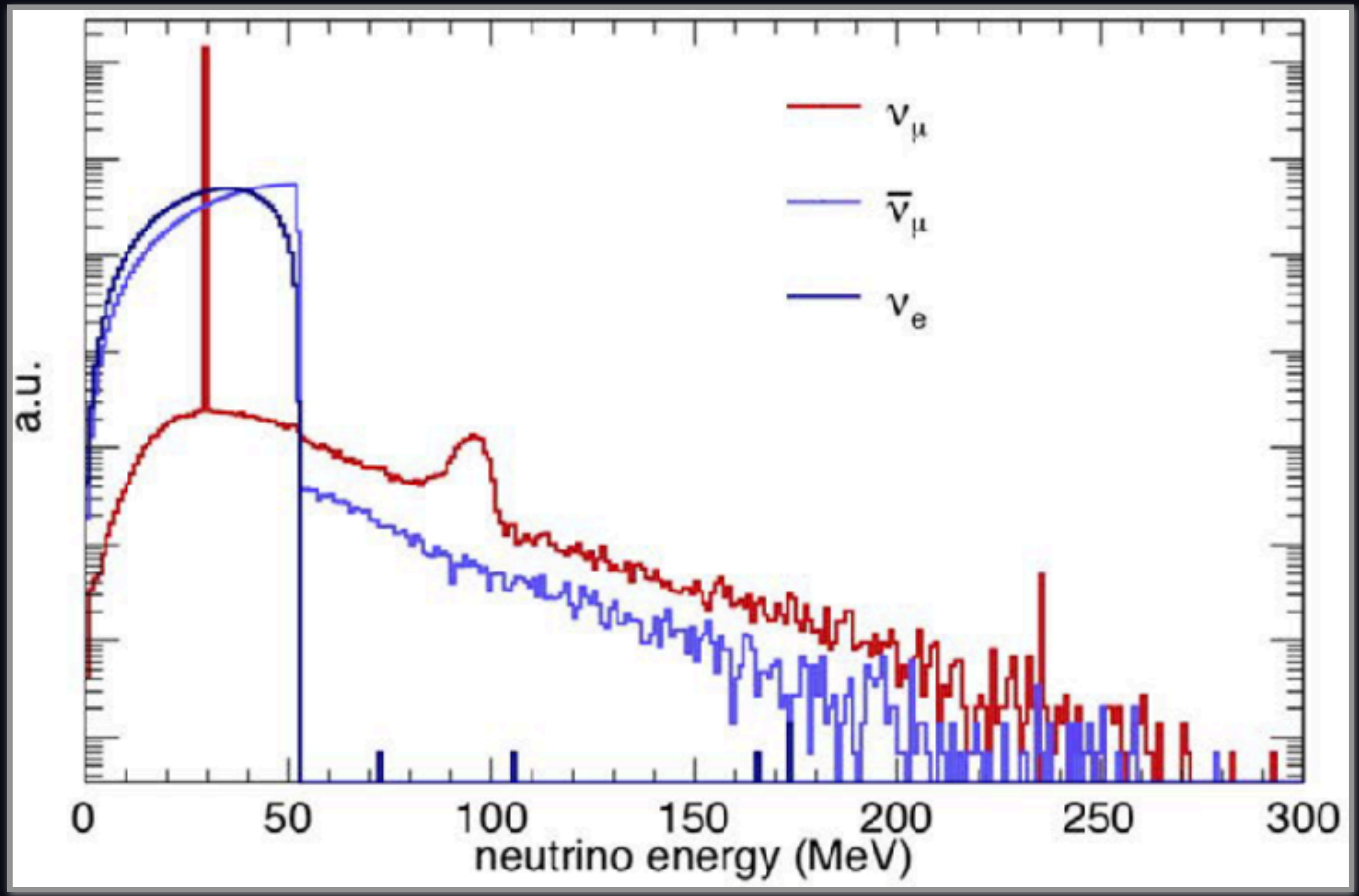
Spin-orbit current $\mathcal{F}_\tau^{\Phi''}$:

less than 10^(-6)%

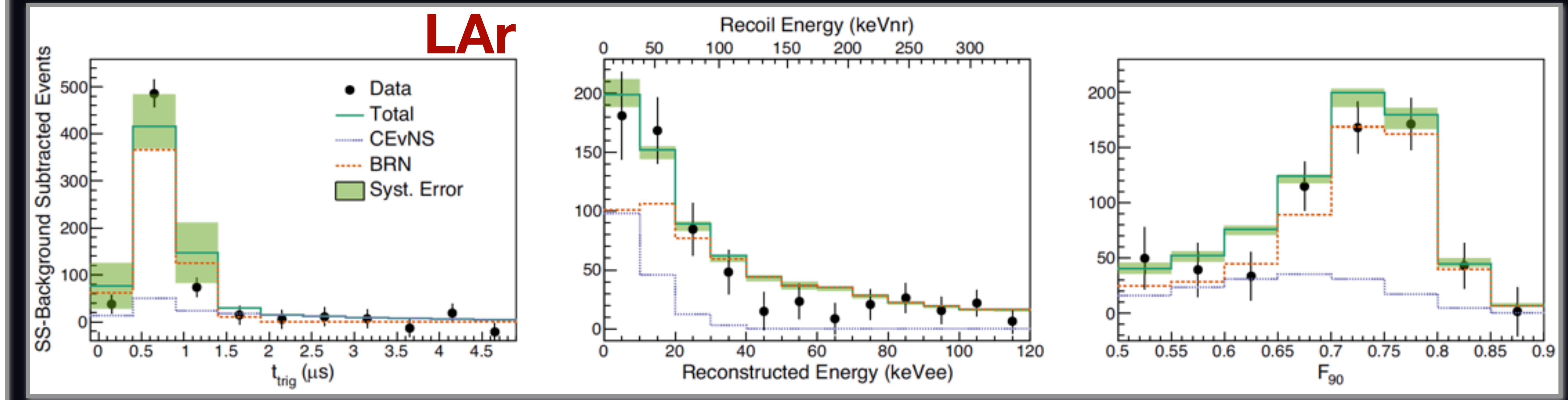
Axial-vector form factor F_A:

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

COHERENT experiment



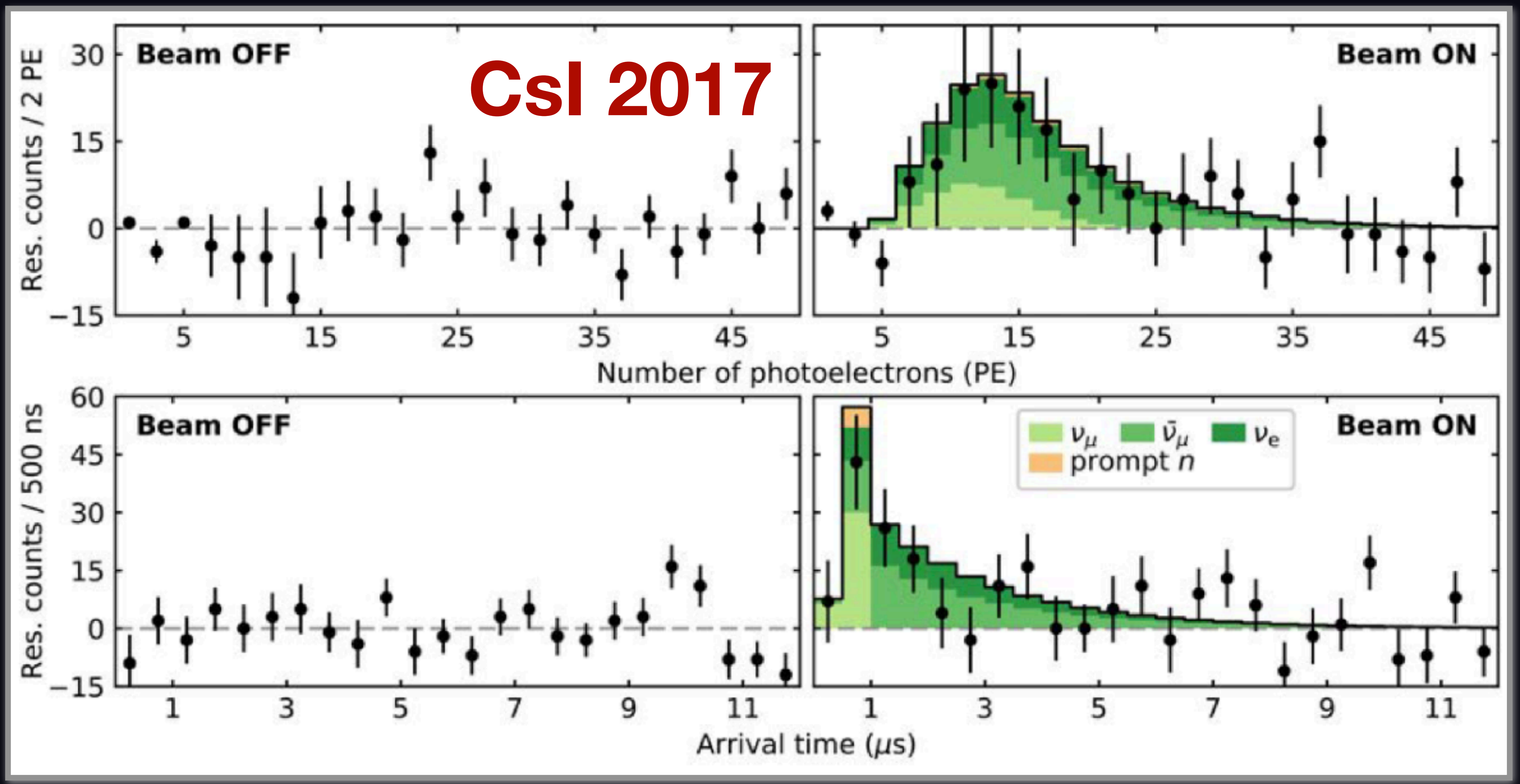
D. Akimov et al. (COHERENT). Science 357 (2017) 1123

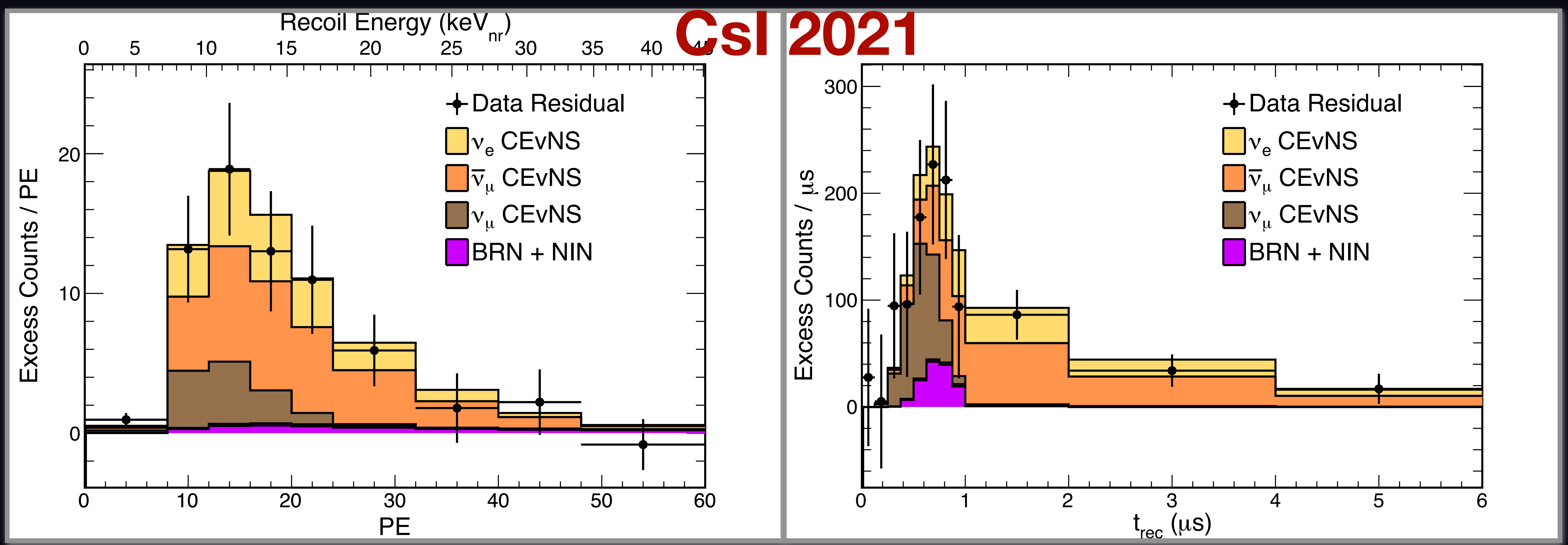


D. Akimov et al. (COHERENT). Phys. Rev. Lett. 126 (2021) 012002

SNS as a neutrino source

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

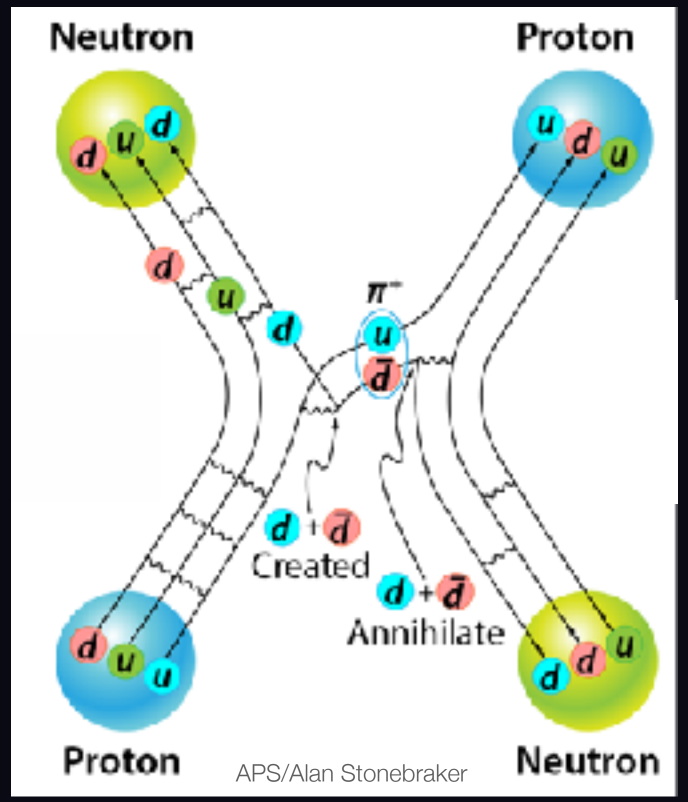




D. Akimov et al. (COHERENT). arXiv:2110.07730 (2021)

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

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

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

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

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

Ex: 300 orbits to study ^{12}C

The total number of Slater determinants is:

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

Numerical budgets:

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

Scale exponentially with mass A

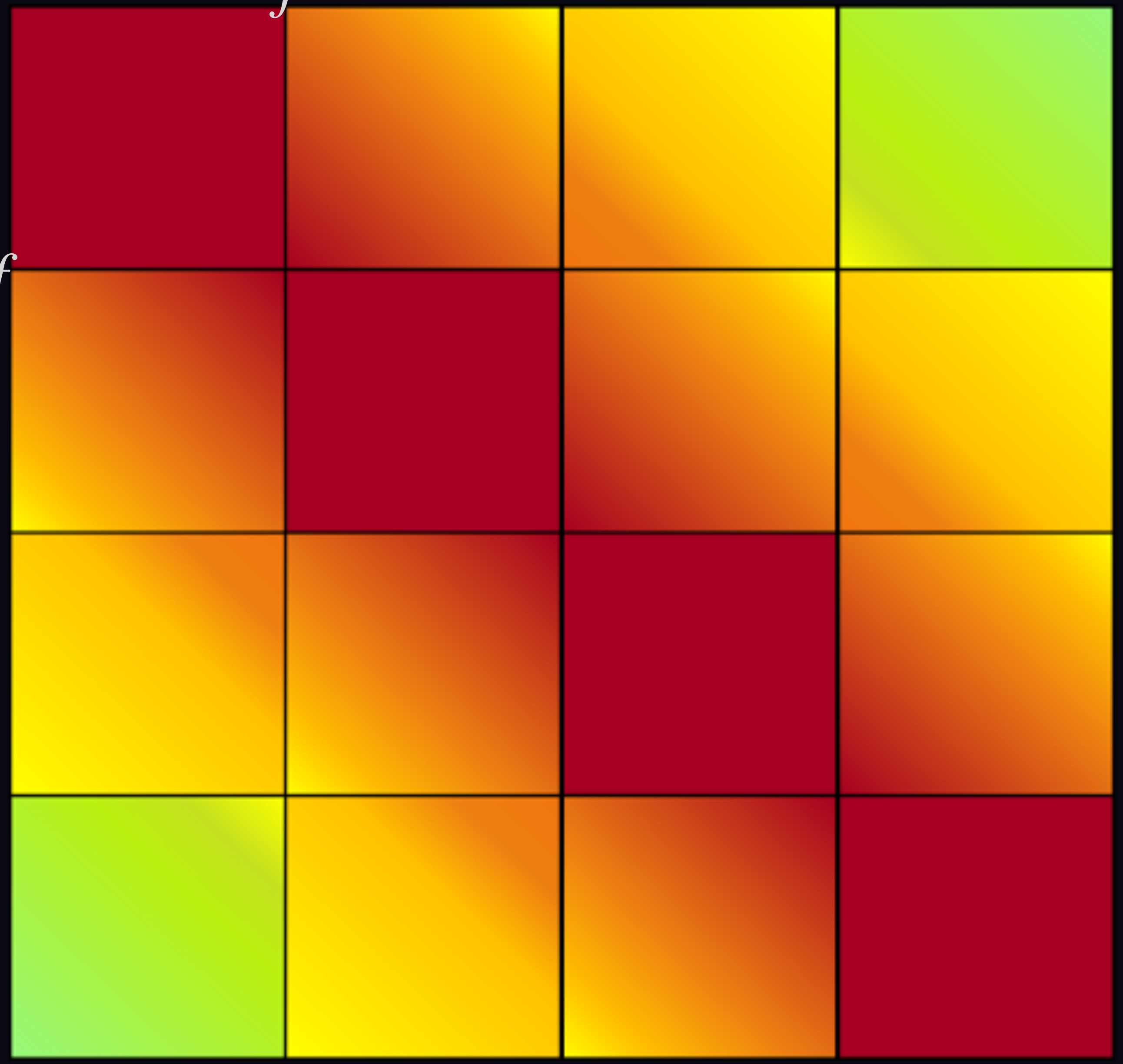
Polynomially scaling methods

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

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

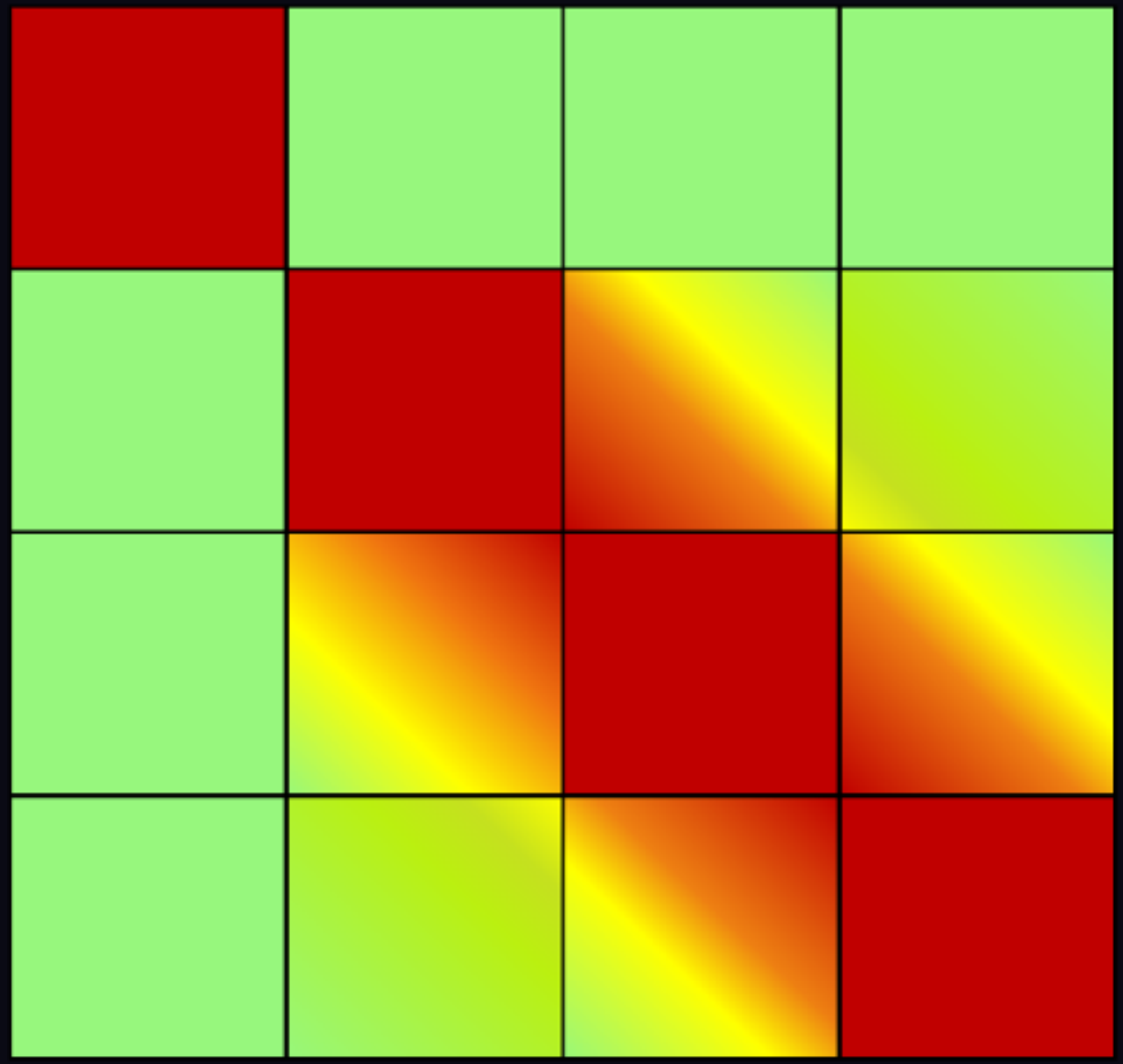
ϵ_f ϵ_f



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

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

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



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

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)