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Ab initio overlap integrals for $\mu \rightarrow e$ conversion in nuclei

MH, Hoferichter, Miyagi, Noël, Schwenk, arXiv:2412.04545

Matthias Heinz, ORNL

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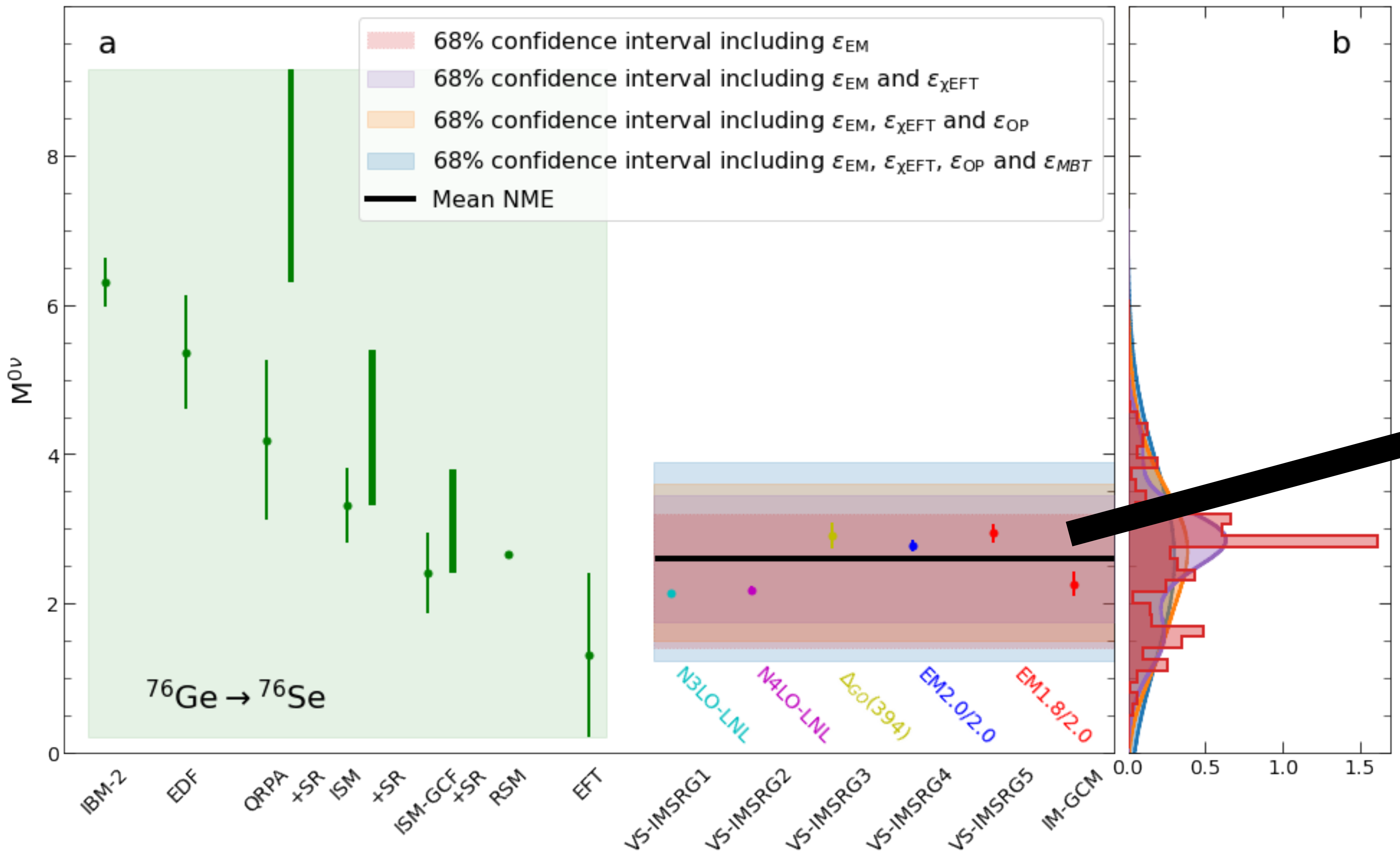
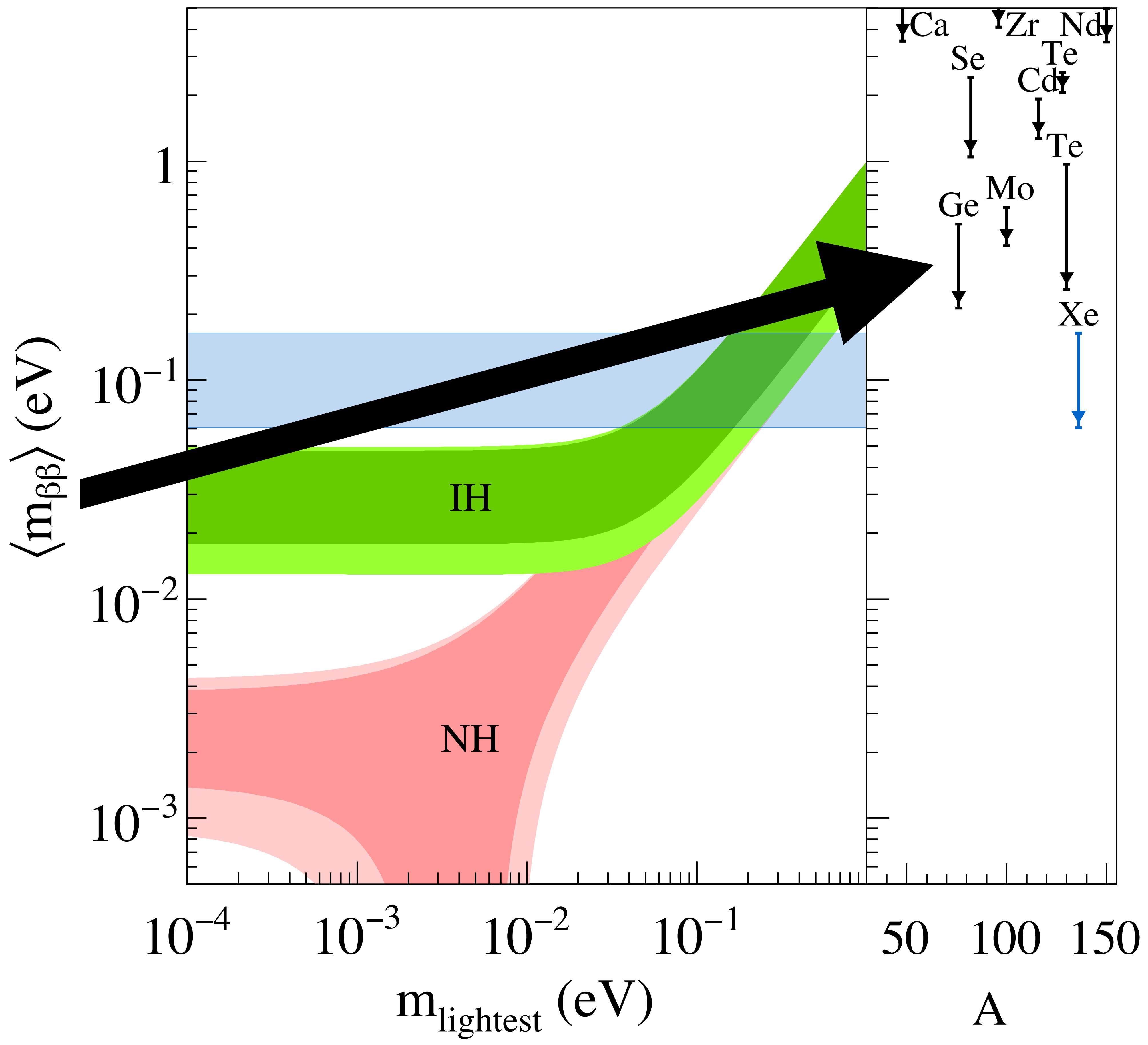
New physics in nuclei requires nuclear theory



Belley et al., PRL **132** (2024)



Engel, Menéndez, RPP **80** (2016)

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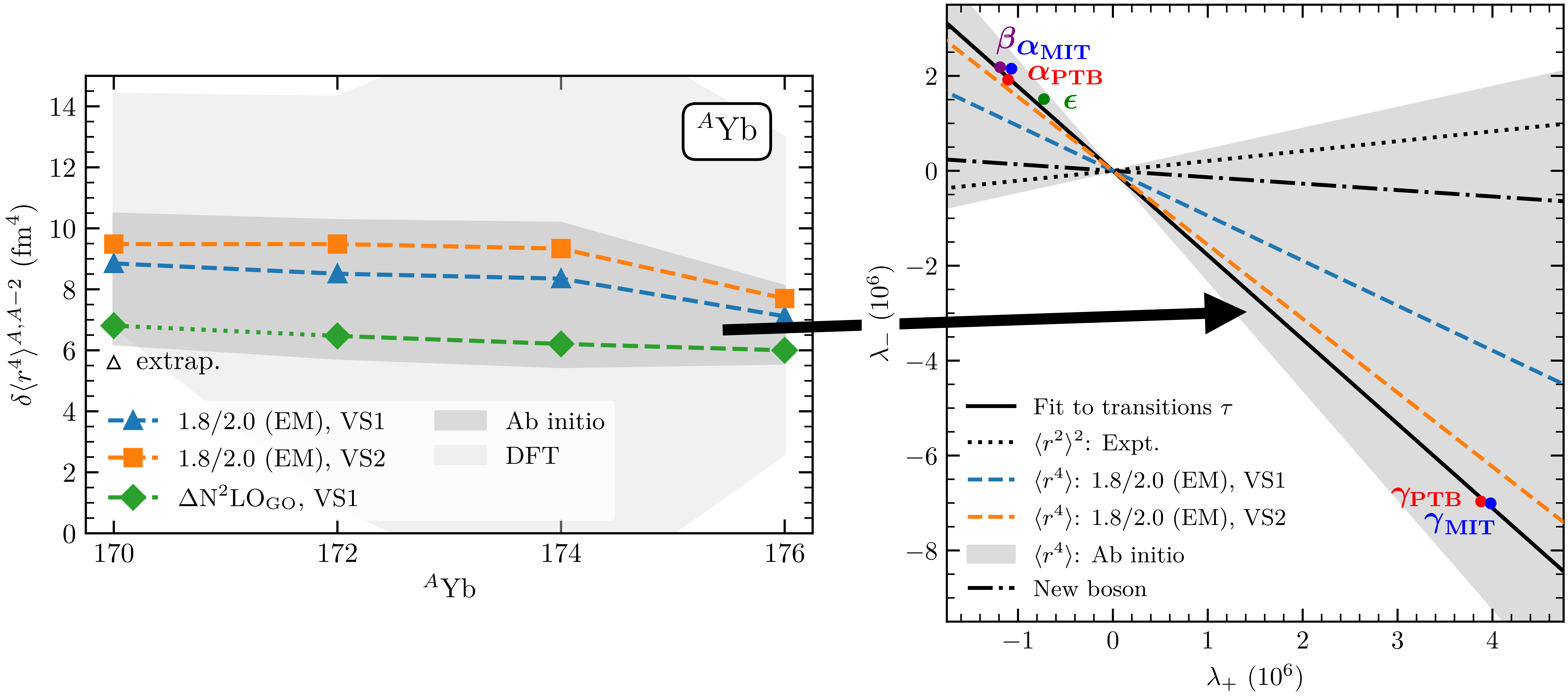
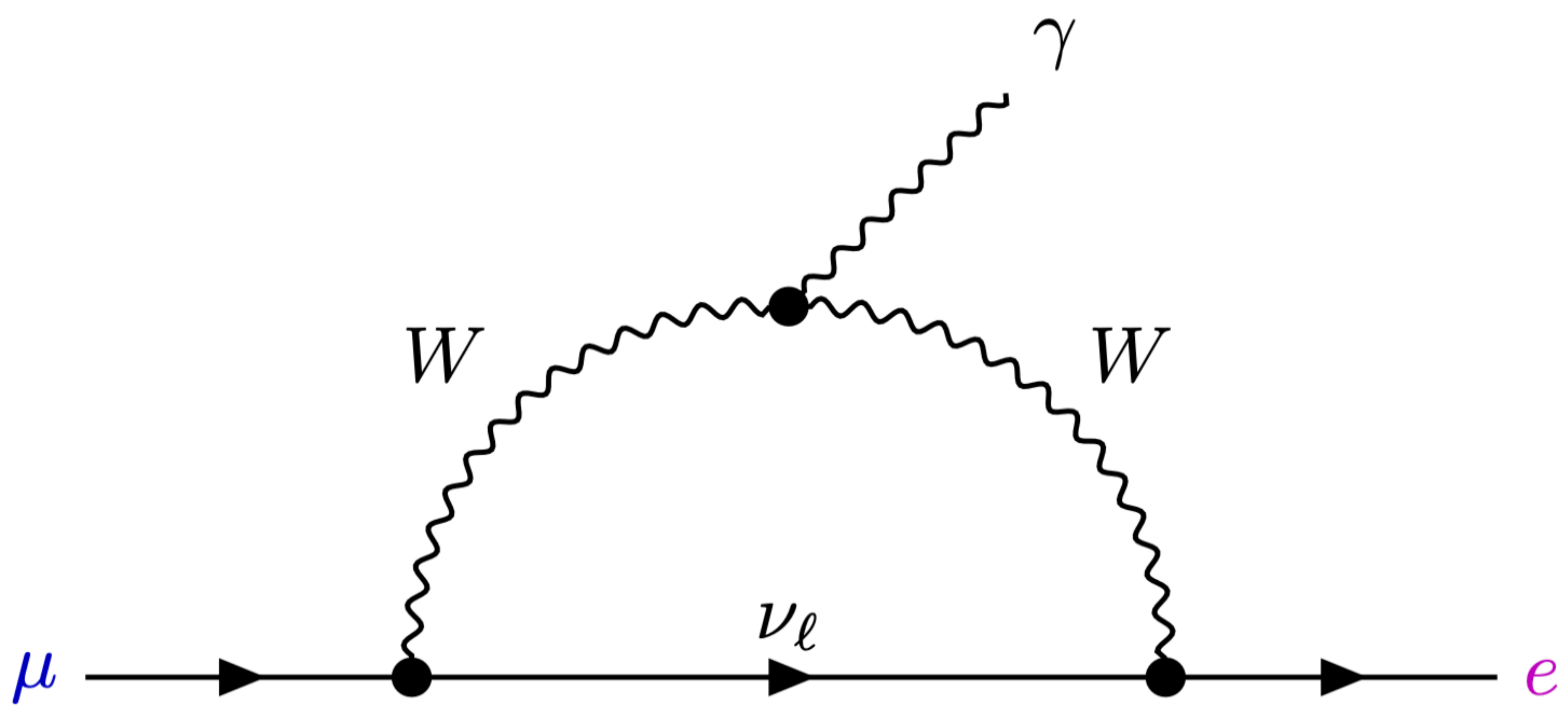
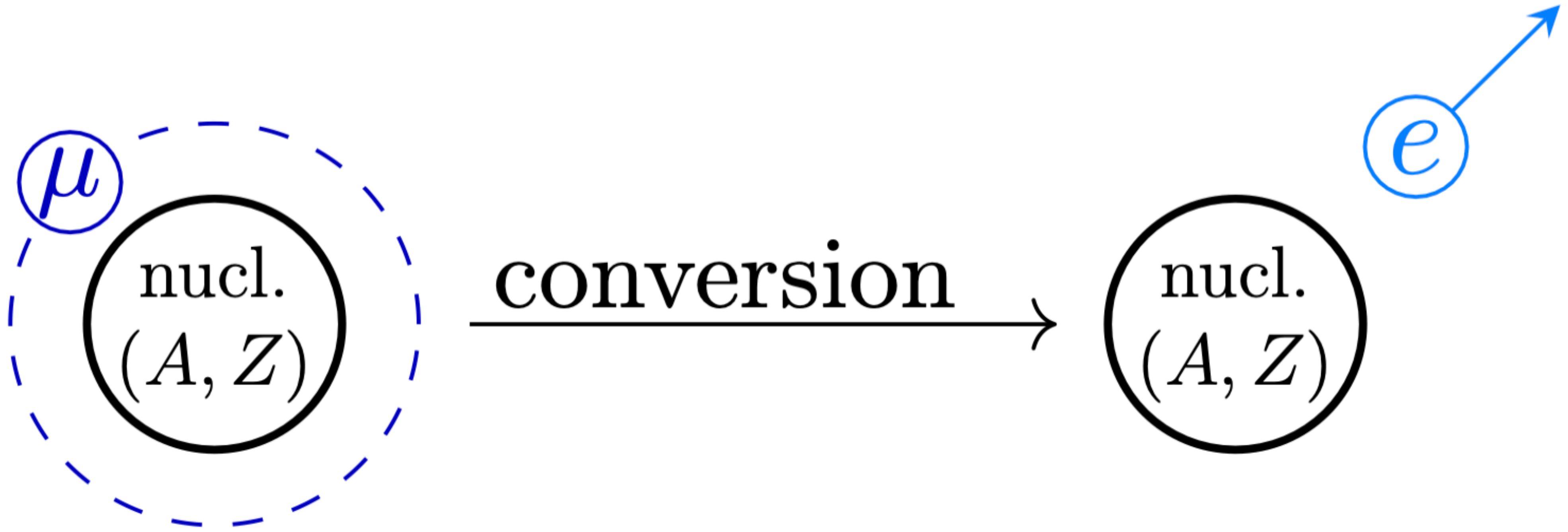


Door, Yeh, **MH**, Kirk, Lyu, Miyagi, et al., PRL **134** (2025)

Muon to electron conversion

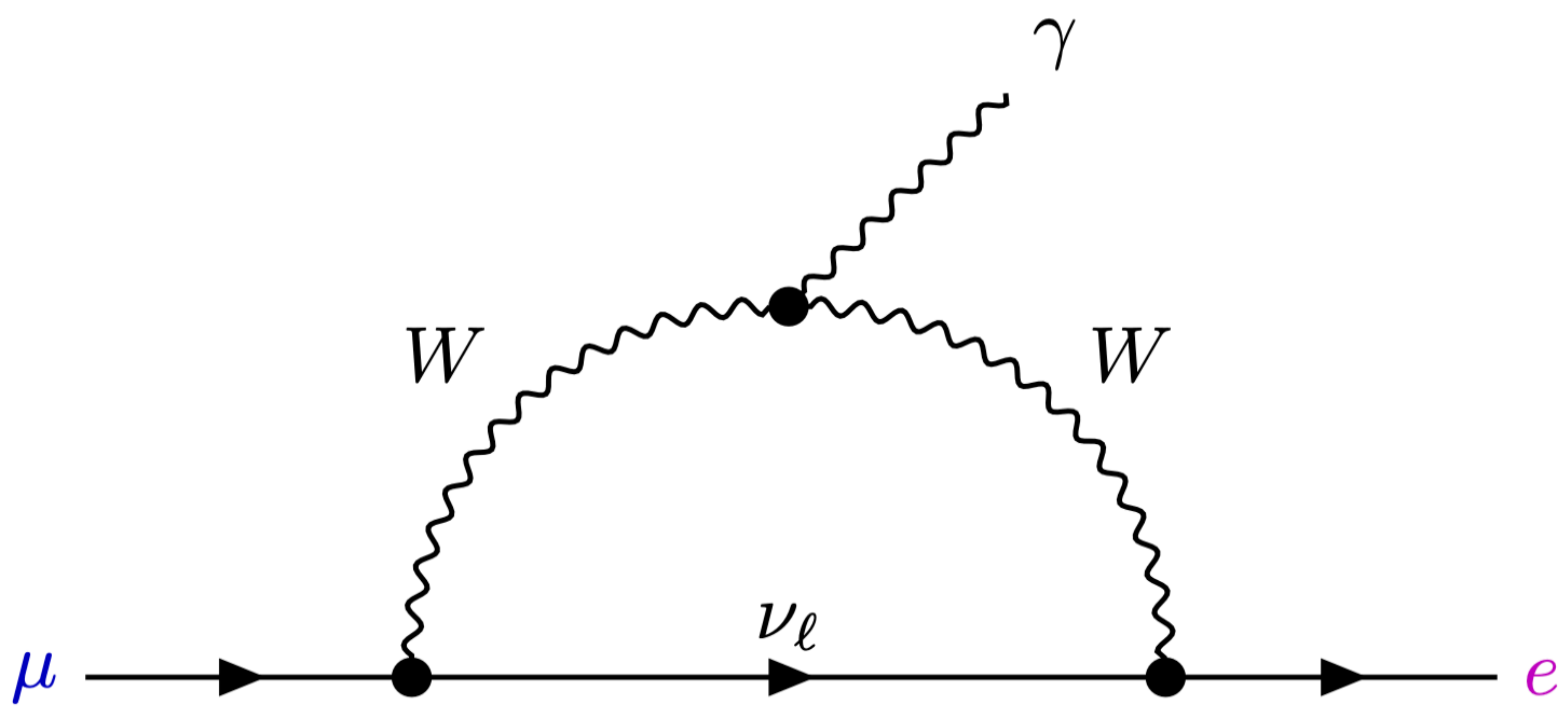


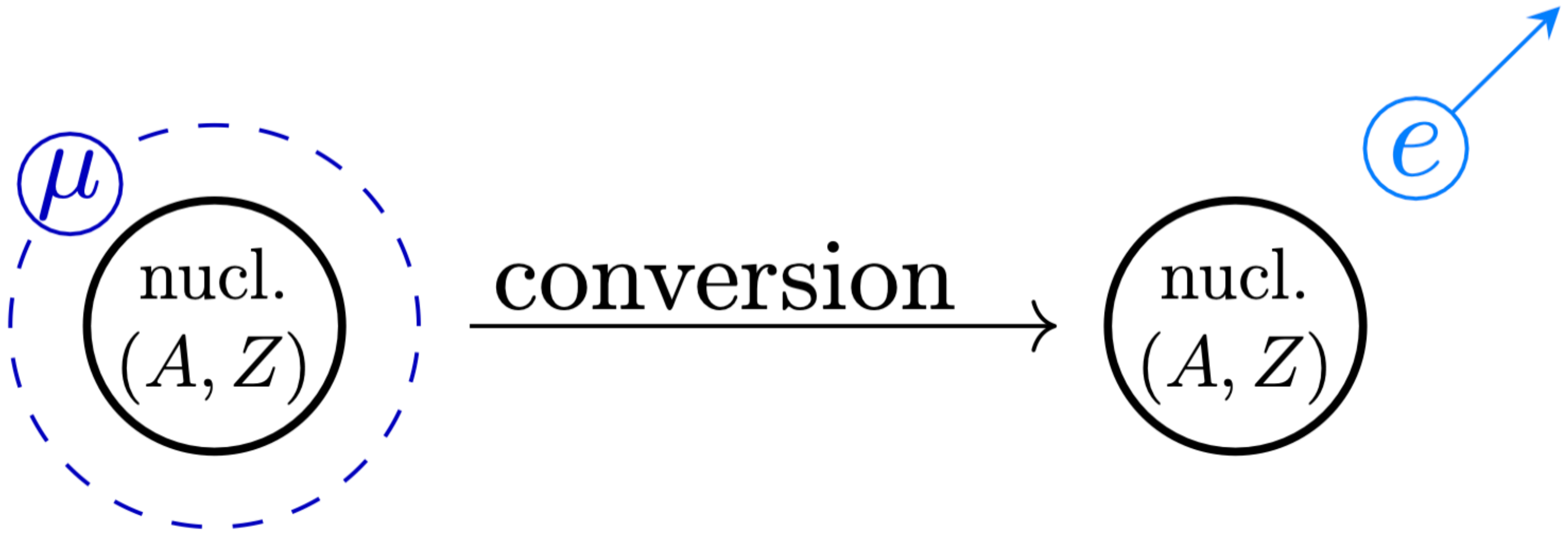


Figures: F. Noël

- Lepton flavor violation in the standard model suppressed by $\left(\Delta m_\nu / m_W\right)^4 \sim 10^{-50}$
- Searches for $\mu \to e$ conversion constrain new lepton flavor violating interactions
- Complementary channels: $\mu \to e\gamma$; $\mu \to 3e$; $\mu \to e$ [nucl.]

Muon to electron conversion





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Our focus: ^{27}Al, ^{48}Ti

What has been done so far?

- Microscopic theories mapped to nonrelativistic effective theory operators

See talks by, e.g., Kaori Fuyuto, Evan Rule, William McNulty

- Treatment of leptonic part varies;
Key challenge: **Coulomb distortion**
    - Coulomb Dirac solution
    $\rightarrow$ Overlap integrals
    - Free Dirac with effective electron momentum $q_{\rm eff}$ $\rightarrow$ plane-wave formalism
- Neutron density contribution important, but **not well understood** with **unquantified uncertainties**

Method 1. First, we take the proton density from electron scattering experiments given in Appendix A and assume that the neutron density is the same as the proton density. For

Kitano, Koike, Okada, PRD **66** (2002)

explore uncertainties associated with alternative schemes for fitting the effective interaction. The uncertainties associated with the SM itself—the basis truncation and the choice of single particle basis—are more difficult to assess. Shell model

Haxton, Rule, McElvain, Ramsey-Musolf, PRC **107** (2022)

Kitano, Koike, Okada, PRD **66** (2002)

Revisiting the overlap integrals

$$\mu \to e \text{ decay rate } \sim \sum_i \left| \bar{C}^{I_i} \times I_i \right|^2$$

- Knowing overlap integrals constrains Wilson coeffs of underlying theories
- Overlap integrals combine nuclear densities and lepton wave functions

$$S^{(n)} \sim \int_0^\infty dr\, r^2 \rho_n(r)\, s(r)$$

- Full set for spin-independent formalism: D, $S^{(p)}$, $V^{(p)}$, $S^{(n)}$, $V^{(n)}$
- Charge, point-proton, and point-neutron densities required

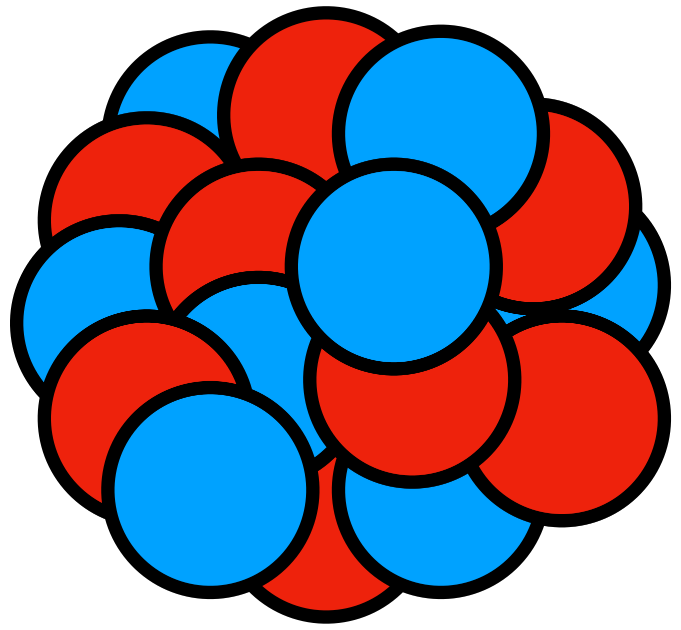
Ab initio nuclear structure theory

Ab initio nuclear structure

N **neutrons**

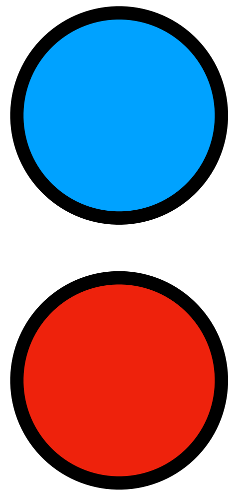
Z **protons**

A **nucleons**



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

Ab initio nuclear structure



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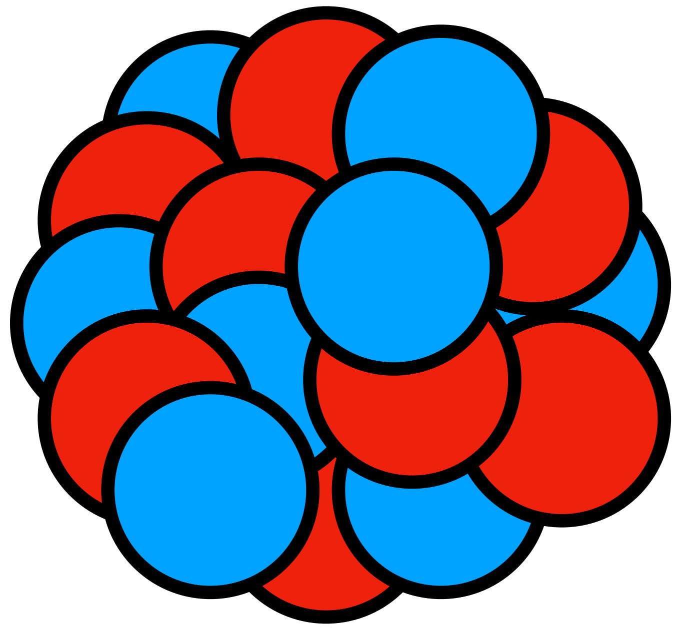
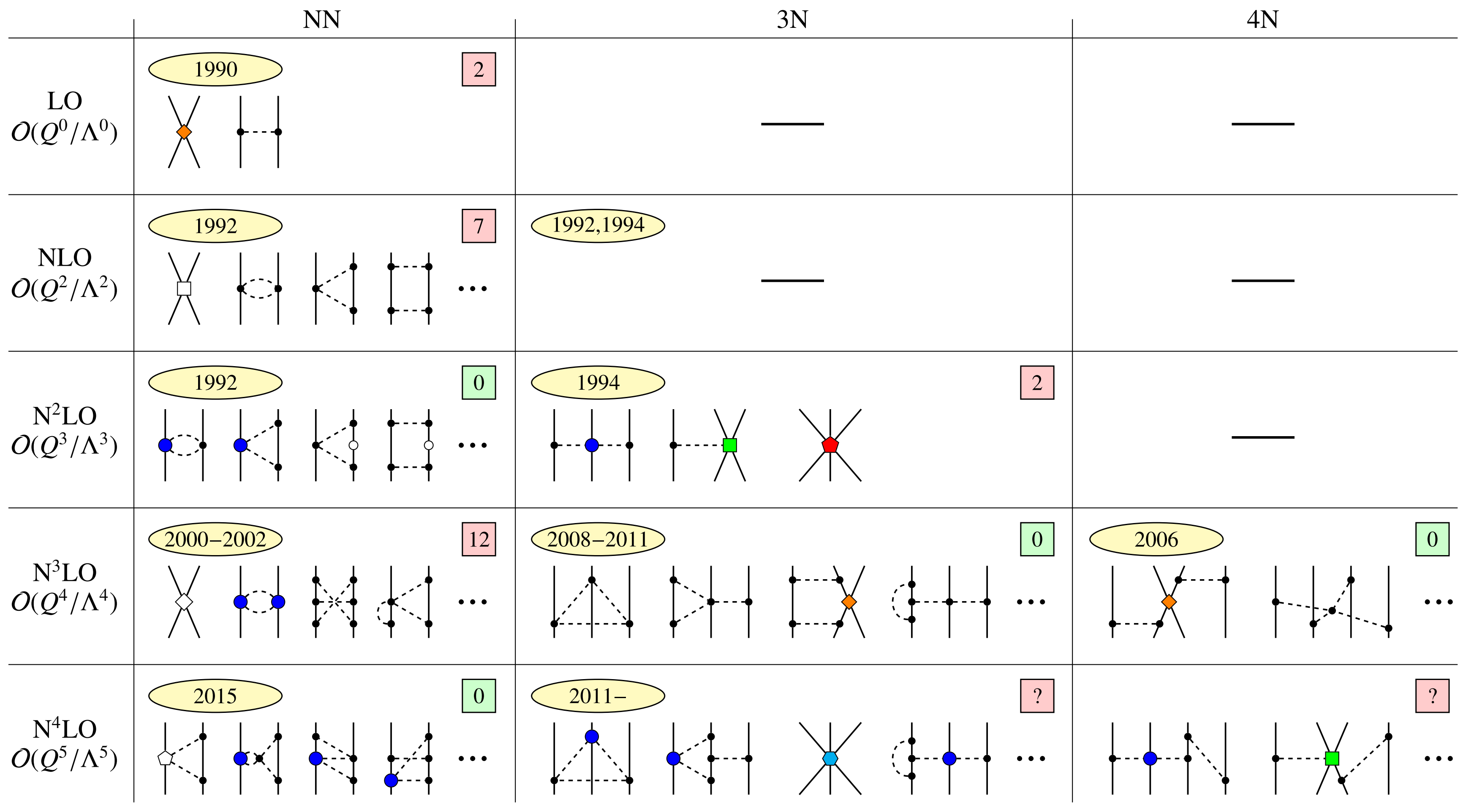


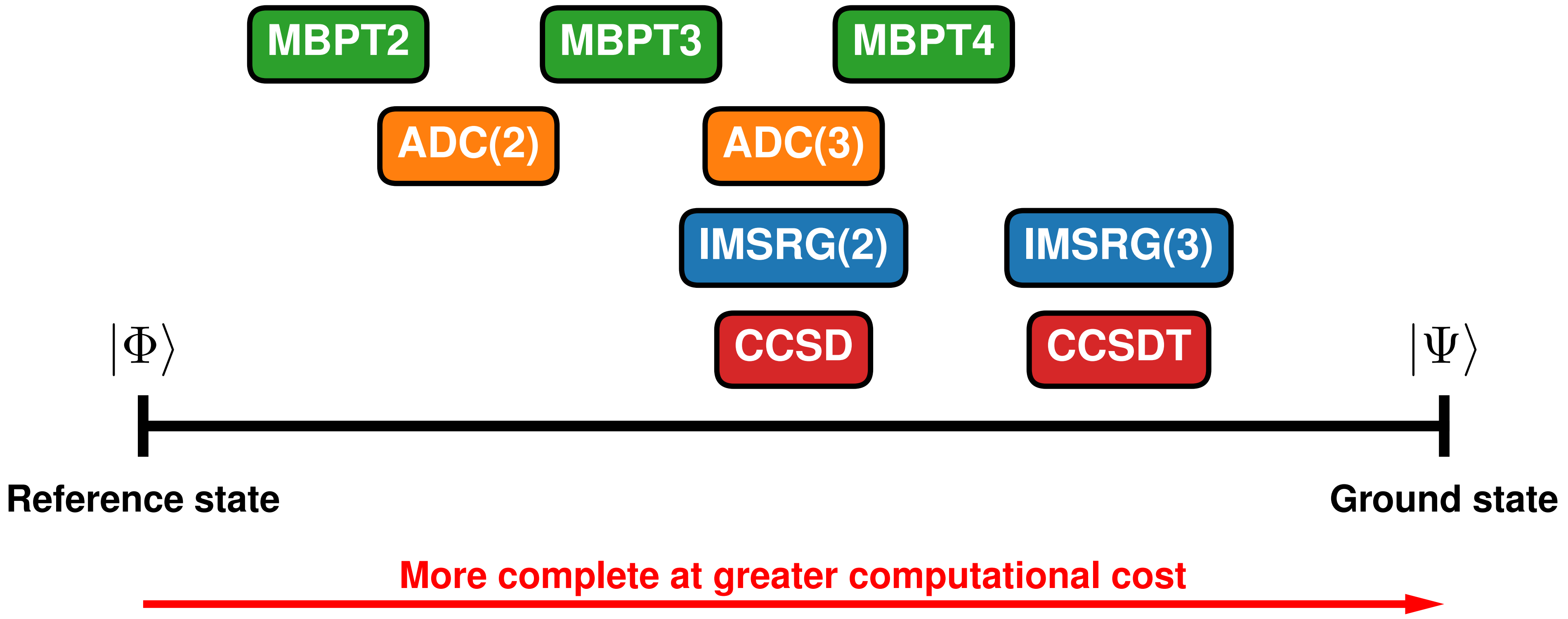
$$H|\Psi\rangle = E|\Psi\rangle$$

Nuclear forces



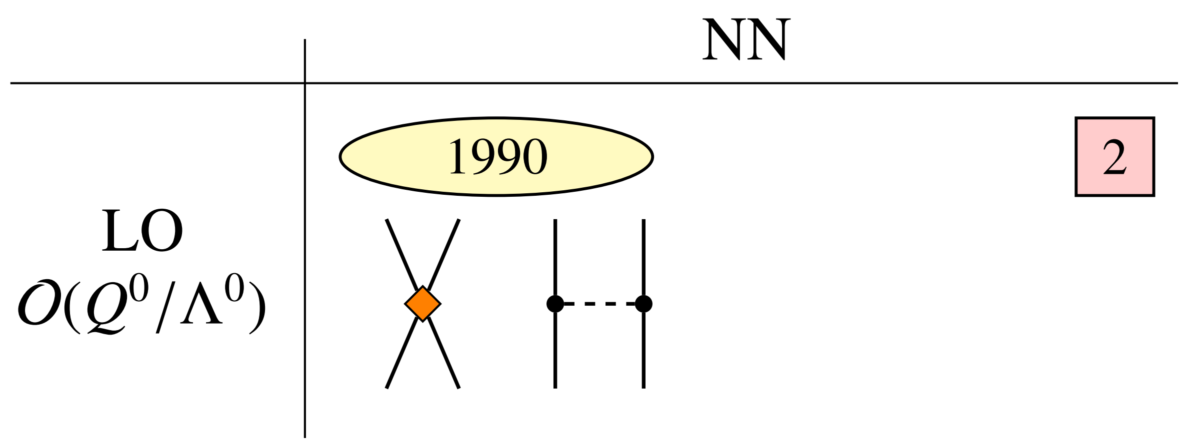
Hebeler, Phys. Rep. **890** (2021)

Many-body methods



Nuclear forces from chiral EFT

effective field theory



- **Nuclear forces are uncertain**
- Chiral EFT:
  Low-energy expansion of QCD
- Long distances: pion exchanges
- Short distances: contact expansion

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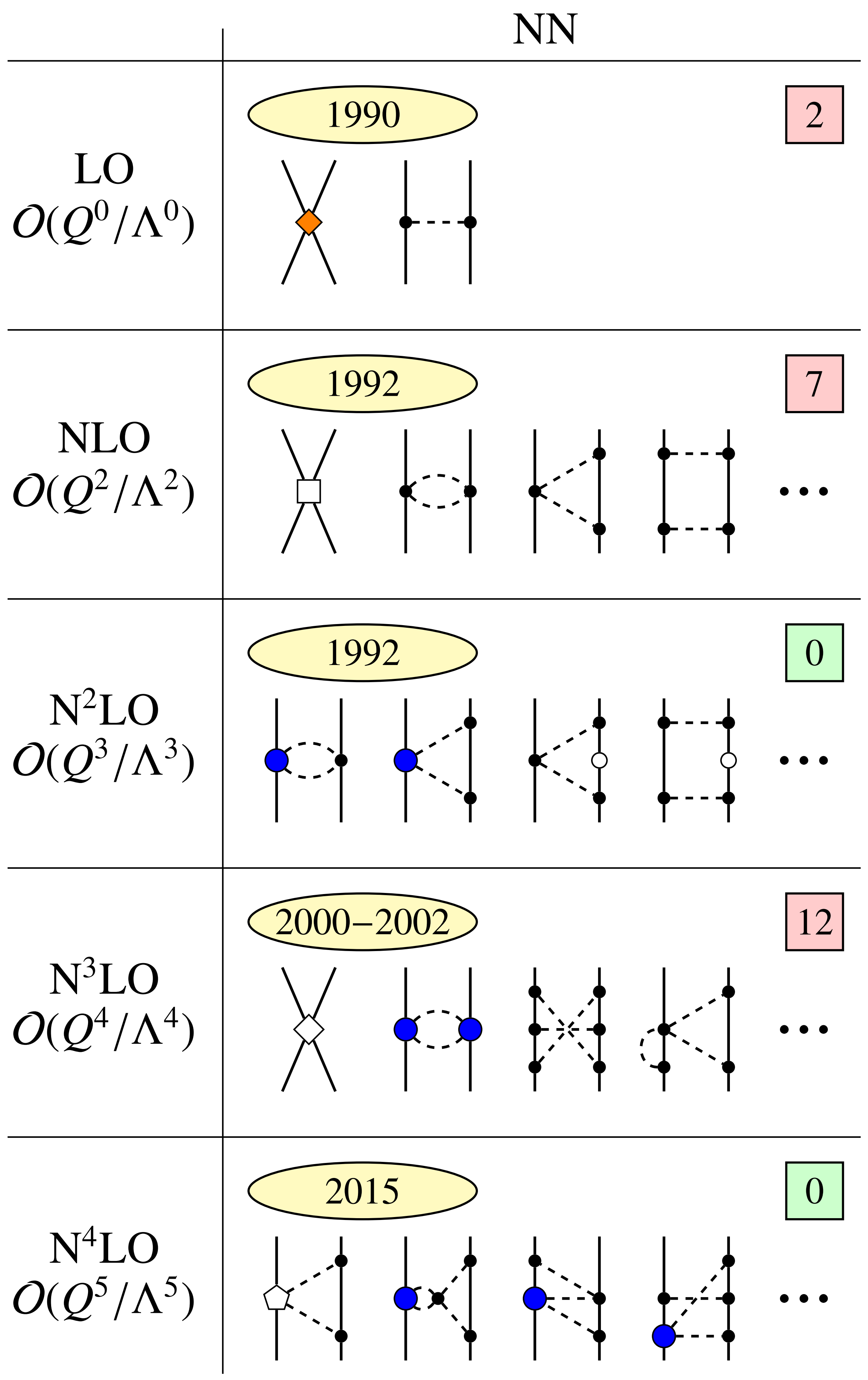

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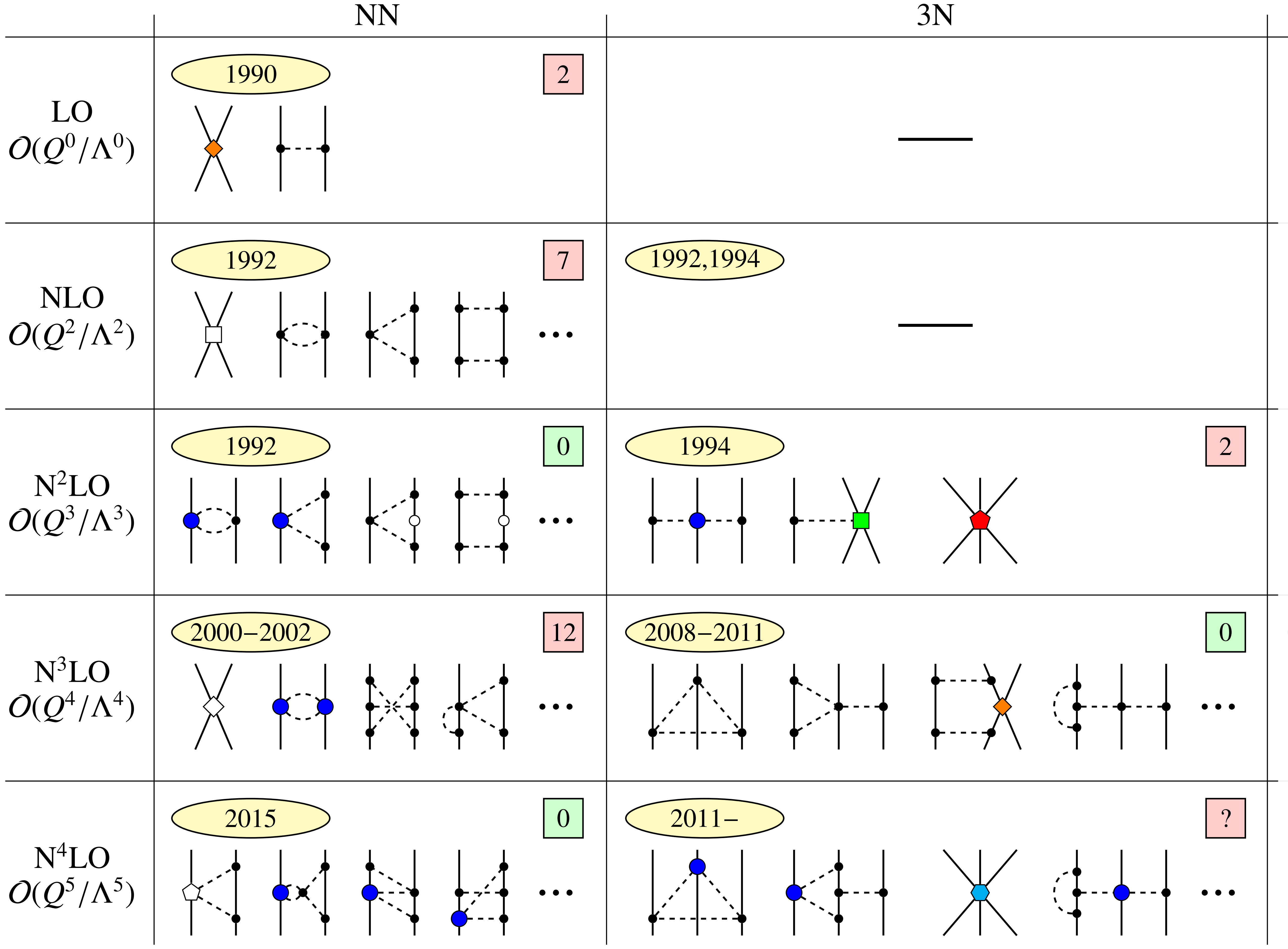

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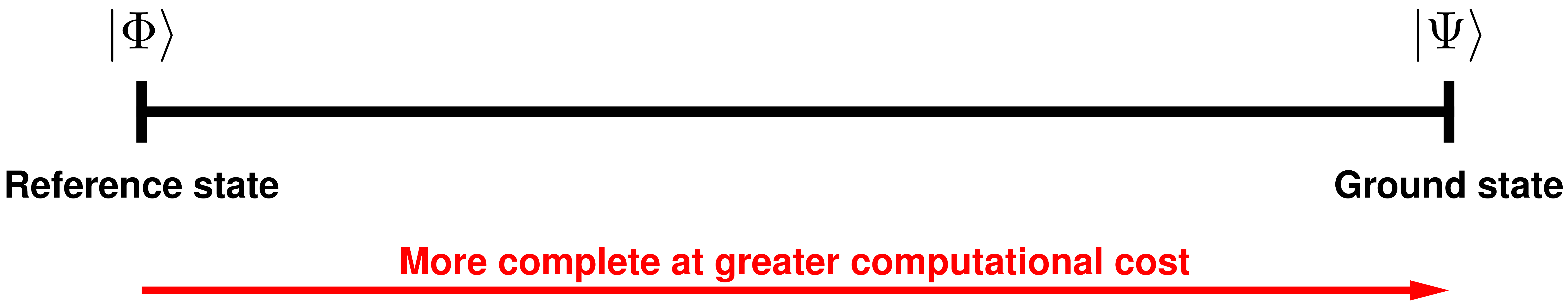
- **Nuclear forces are uncertain**
- Chiral EFT:
  Low-energy expansion of QCD
- Long distances: pion exchanges
- Short distances: contact expansion
- Natural inclusion of 3B forces
- Truncation &
  systematic improvement
- **Uncertainty quantification**
- **Consistent prediction of currents to describe external probes**

Many-body expansion methods



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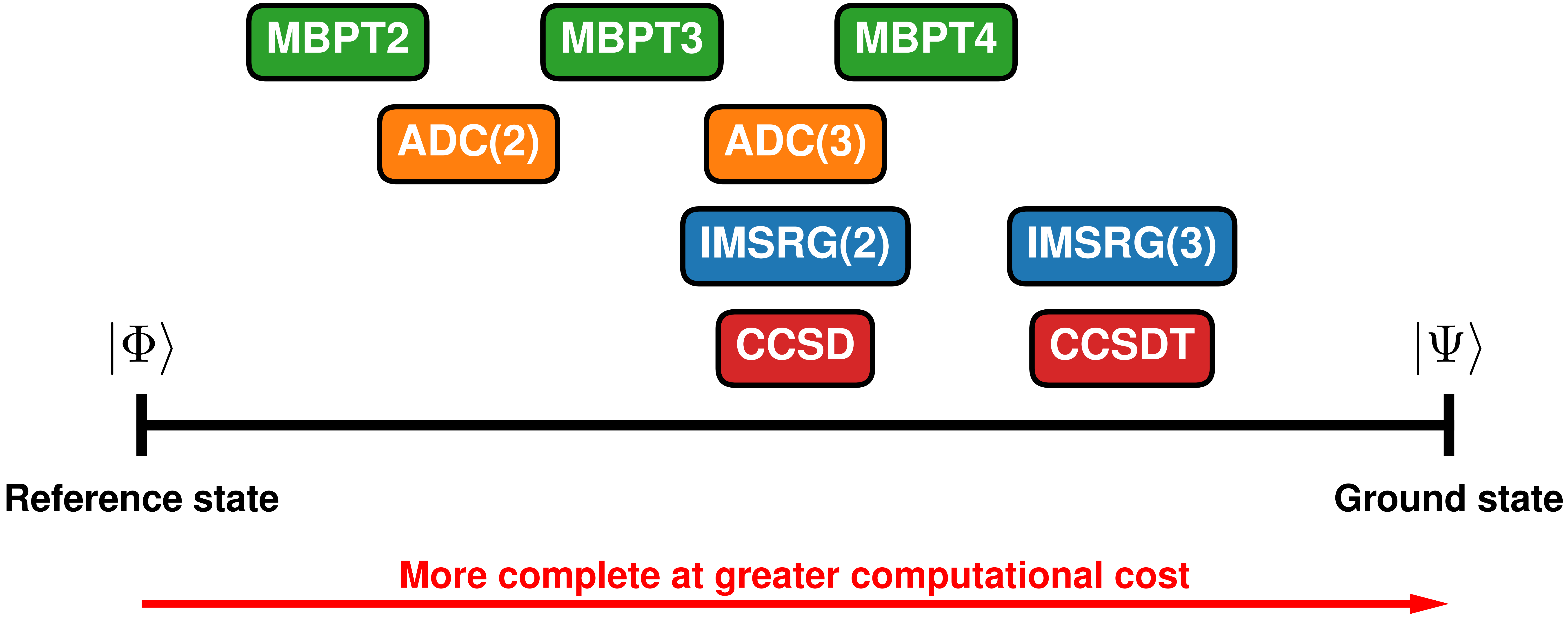
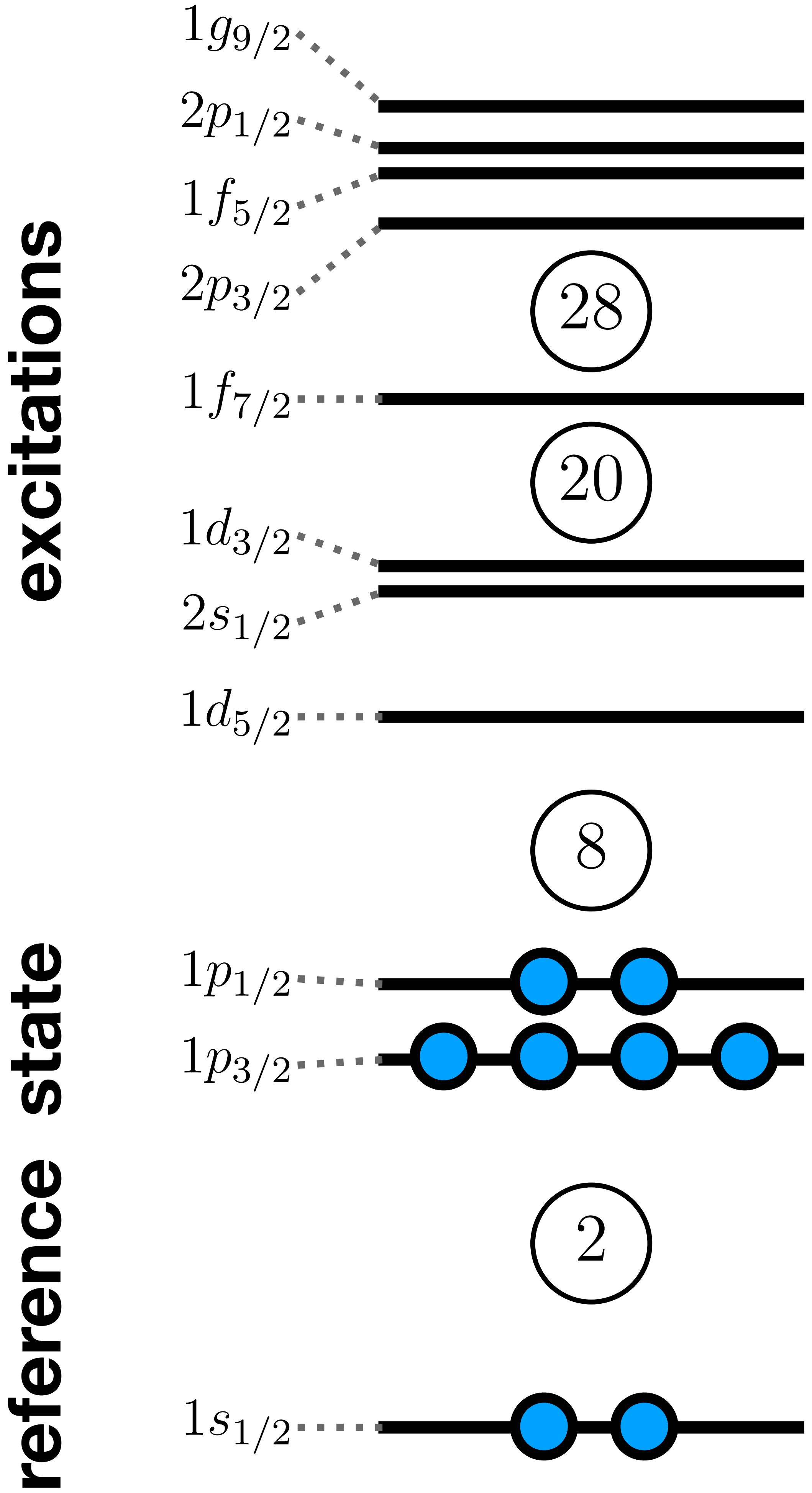


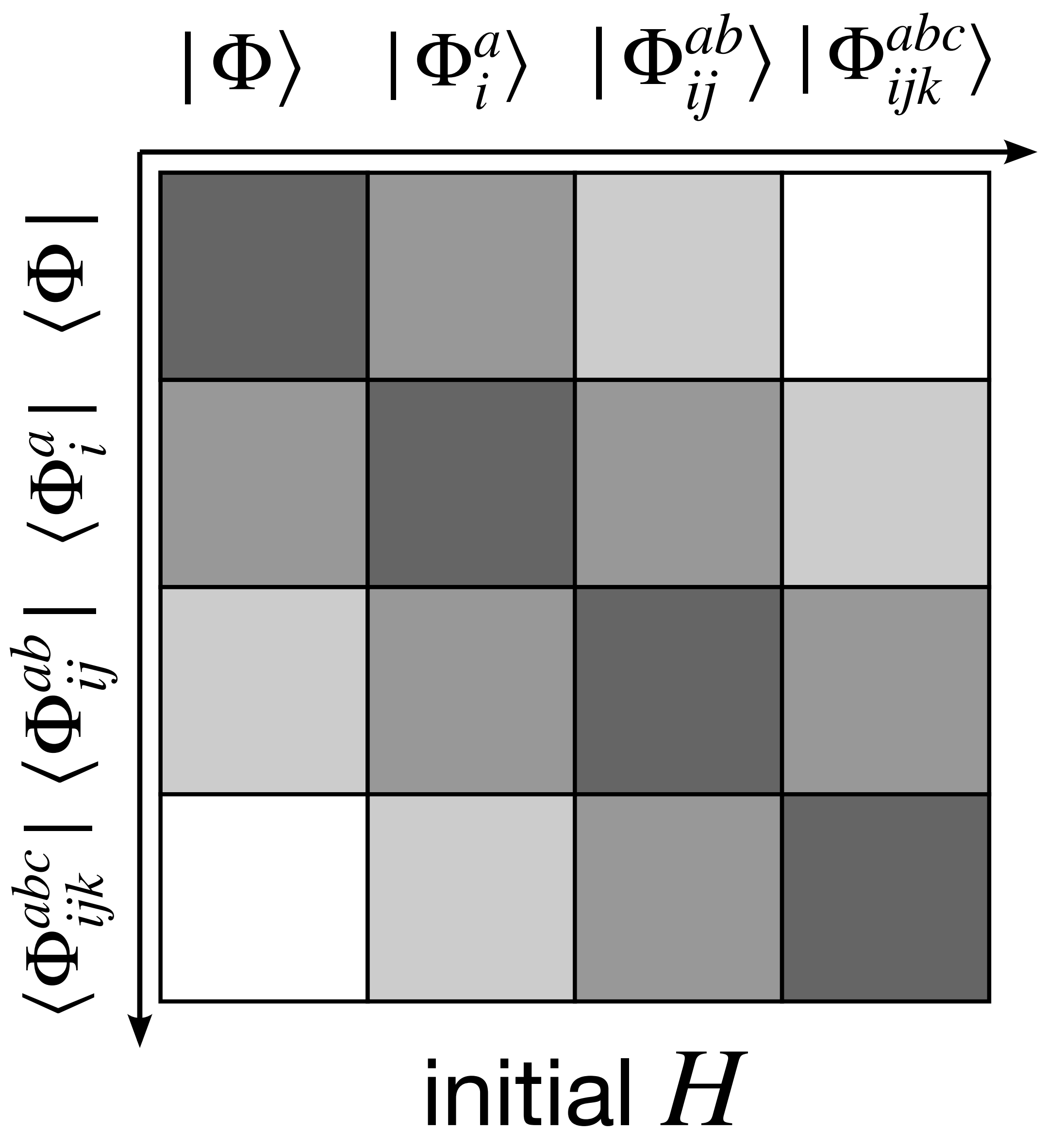
- **Systematically improvable expansion** around reference state $|\Phi\rangle$
- **Tractable computational cost** in larger nuclei
- Approximate many-body solution with **quantifiable uncertainty**

Tsukiyama et al., PRL **106** (2011)
Hergert et al., Phys. Rep. **621** (2016)

The IMSRG

in-medium similarity renormalization group





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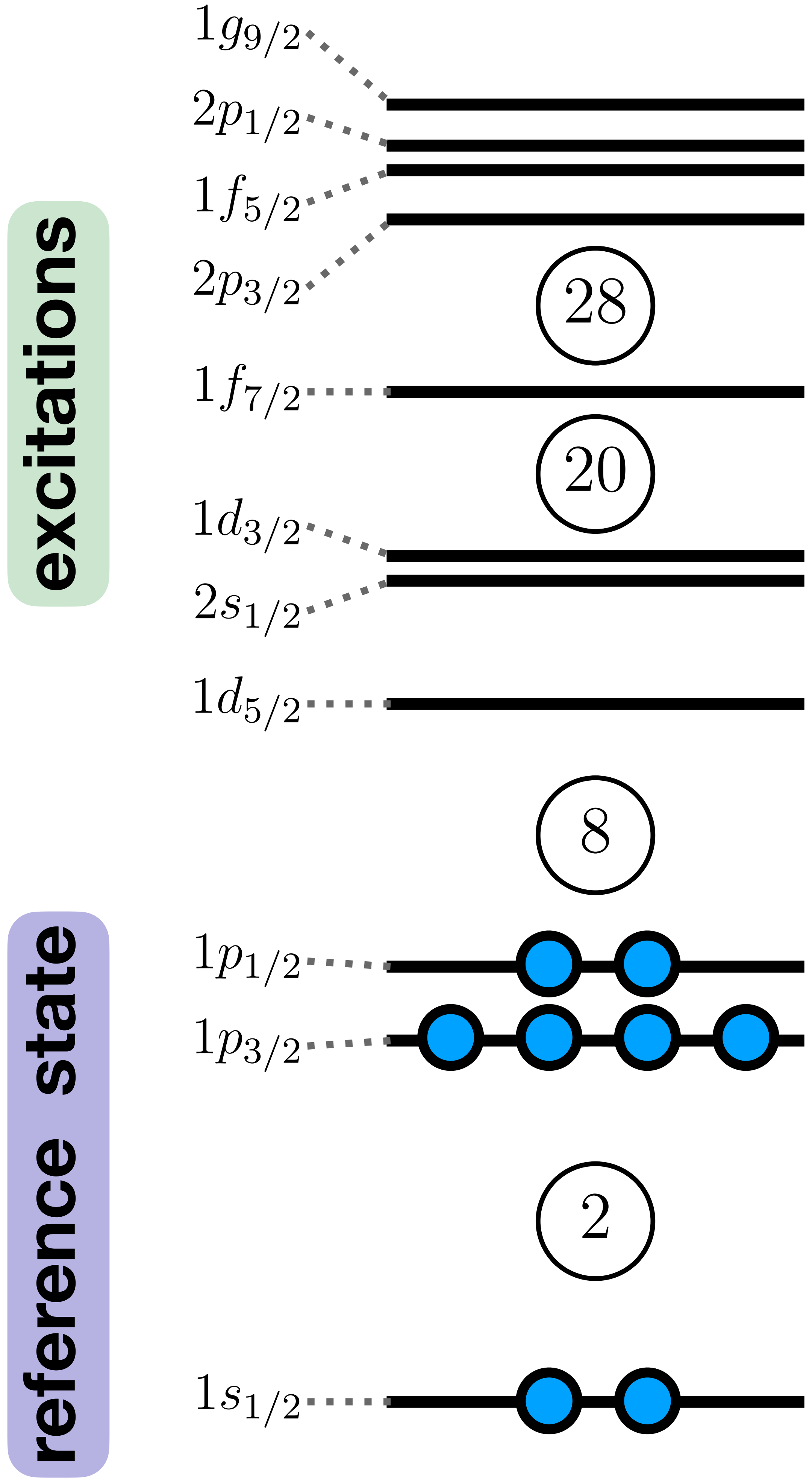

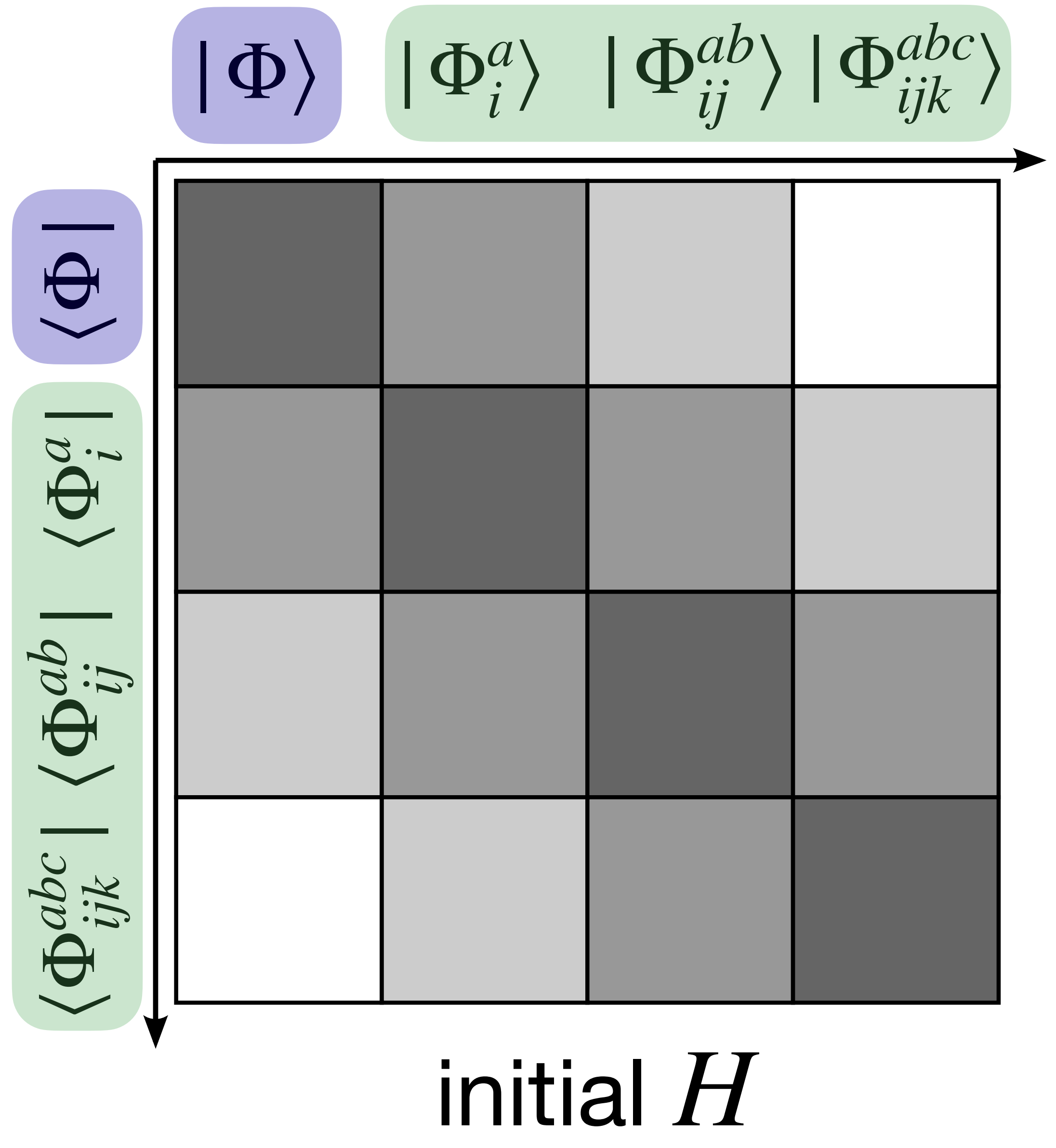

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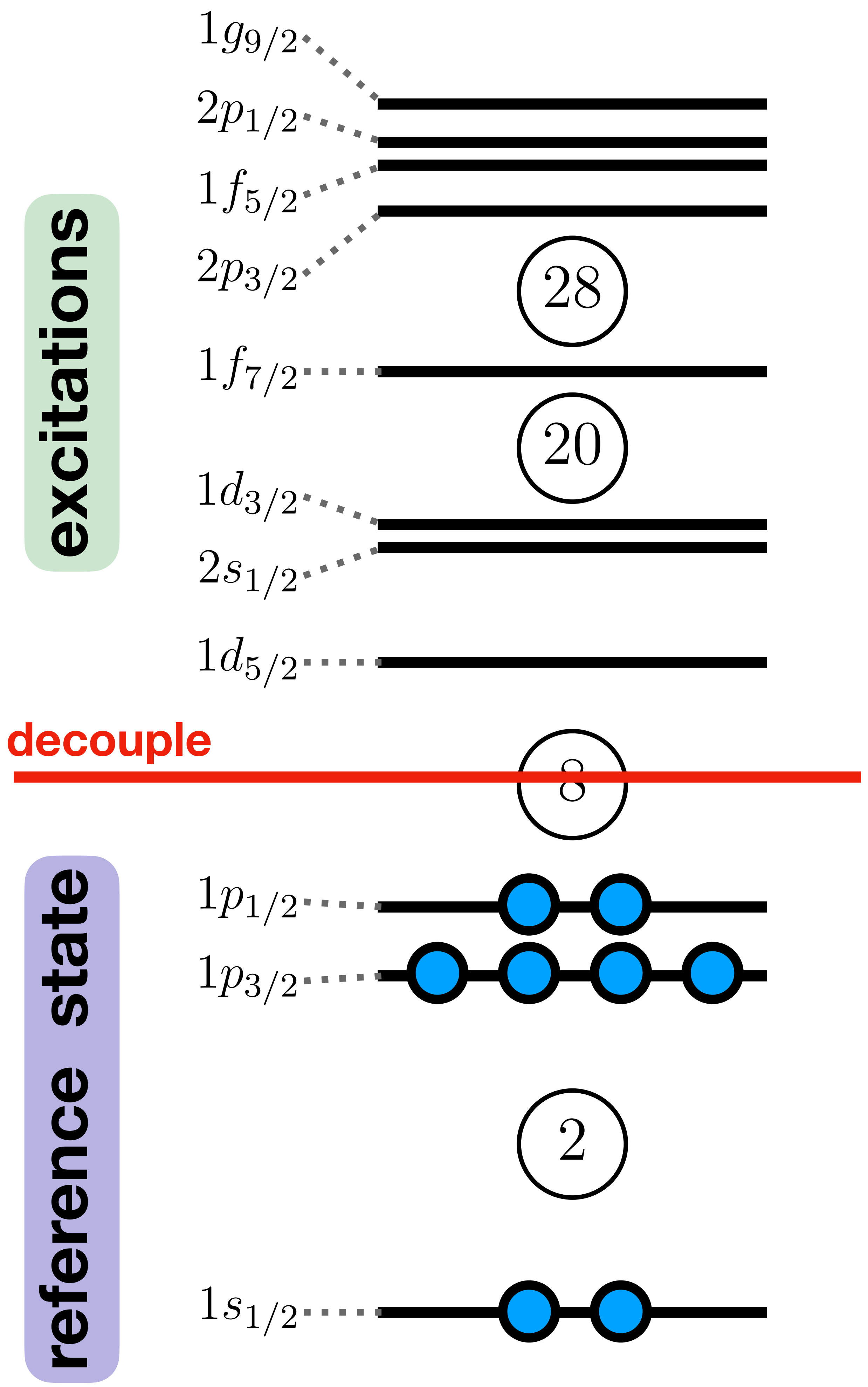

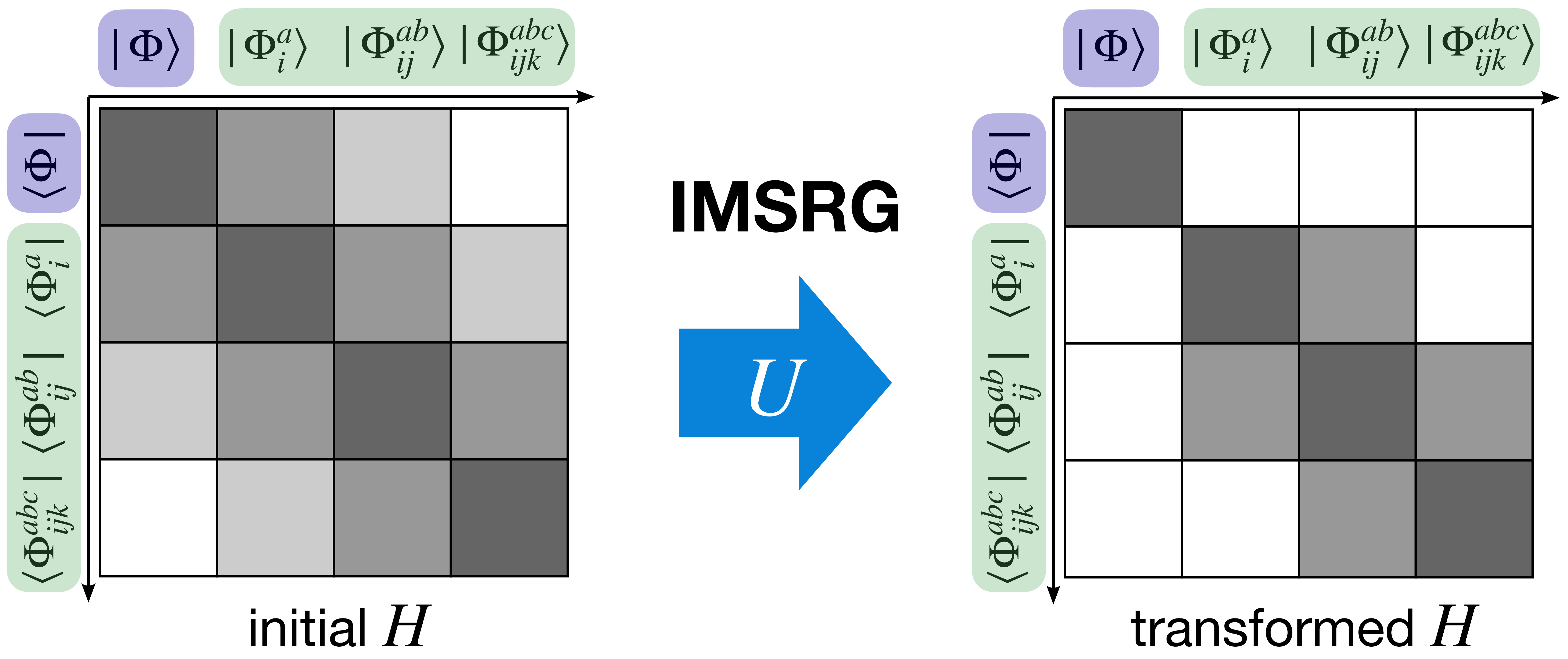

Hergert et al., Phys. Rep. **621** (2016)

- **IMSRG**: Unitary transformation $U = e^{\Omega}$ to decouple reference state from excitations

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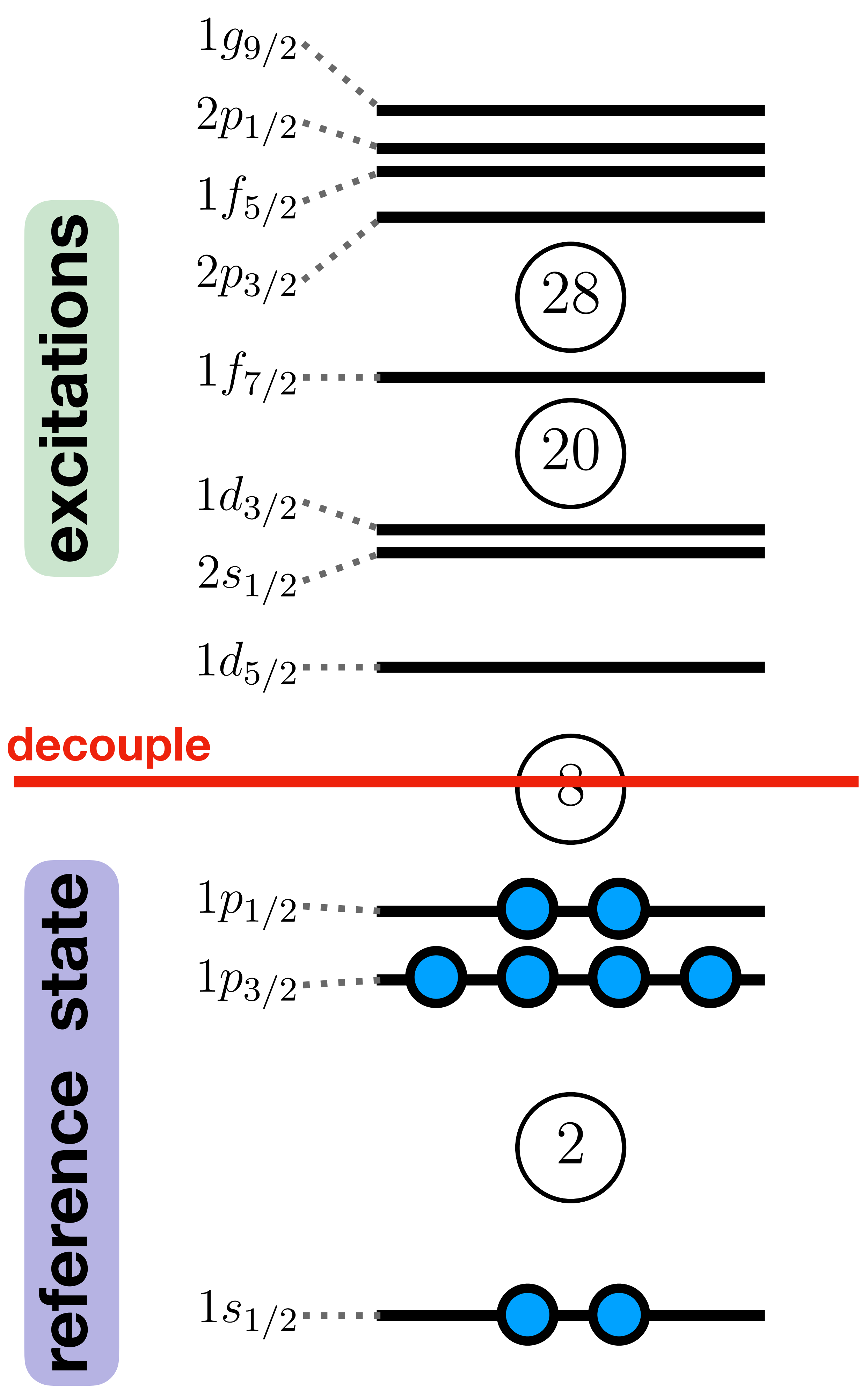
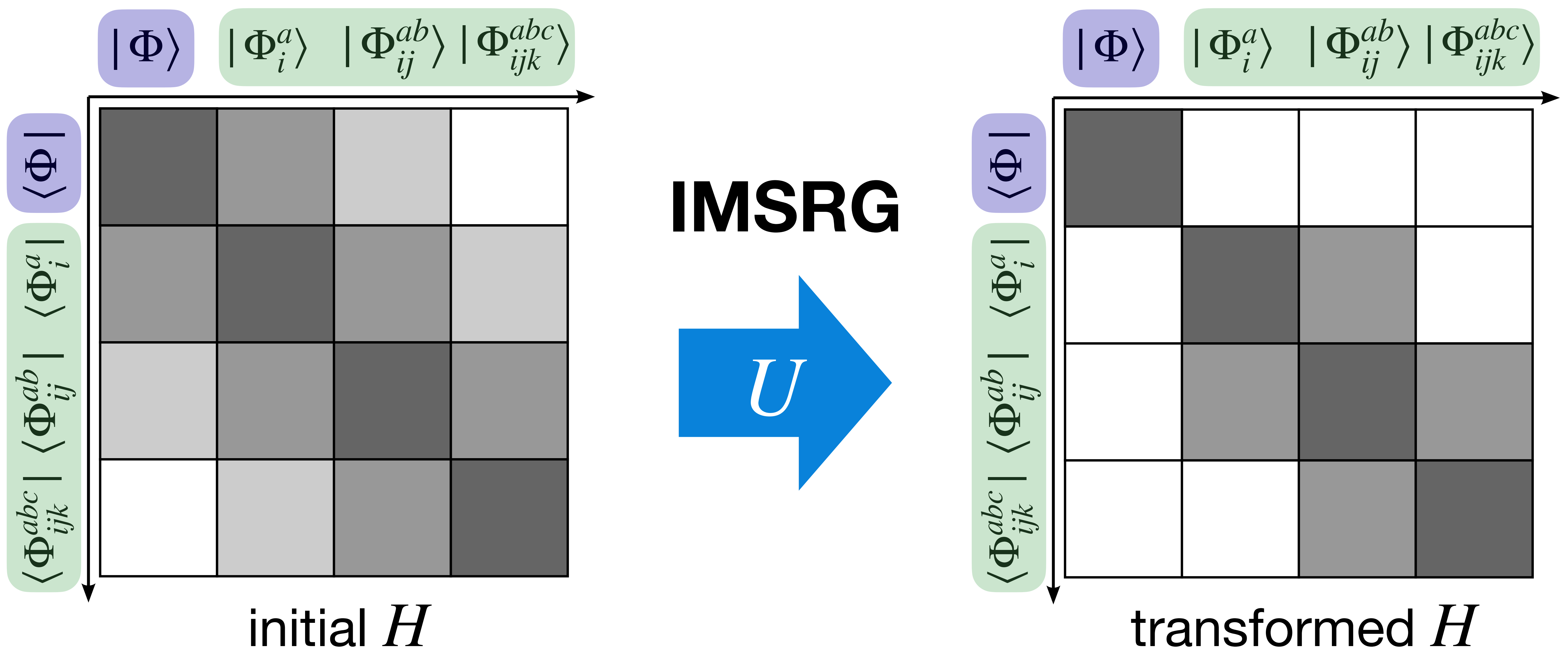




Hergert et al., Phys. Rep. **621** (2016)

- **IMSRG**: Unitary transformation $U = e^{\Omega}$ to decouple reference state from excitations
- Expansion and truncation in **many-body operators**

$$U = e^{\Omega} = e^{\Omega_1 + \Omega_2 + \Omega_3 + \dots}$$

MH et al., PRC **103** (2021)
PRC **111** (2025)
Stroberg, He (2024)

- **IMSRG(3)** for **precision** and **uncertainty quantification**

Also relevant for neutrino scattering and direct dark matter detection, see talk by Baishan Hu

See, e.g., Fitzpatrick et al., JCAP **2013** (2013)

Computed nuclear responses

Nuclear response notation: $X_{J,p/n}(q)$

Spin-independent:

- $M_{0,p}$, $M_{0,n}$: coherent, related to point-proton, point-neutron densities

Semi-coherent:

- $\Phi''_{0,p}$, $\Phi''_{0,n}$: spin-orbit effects

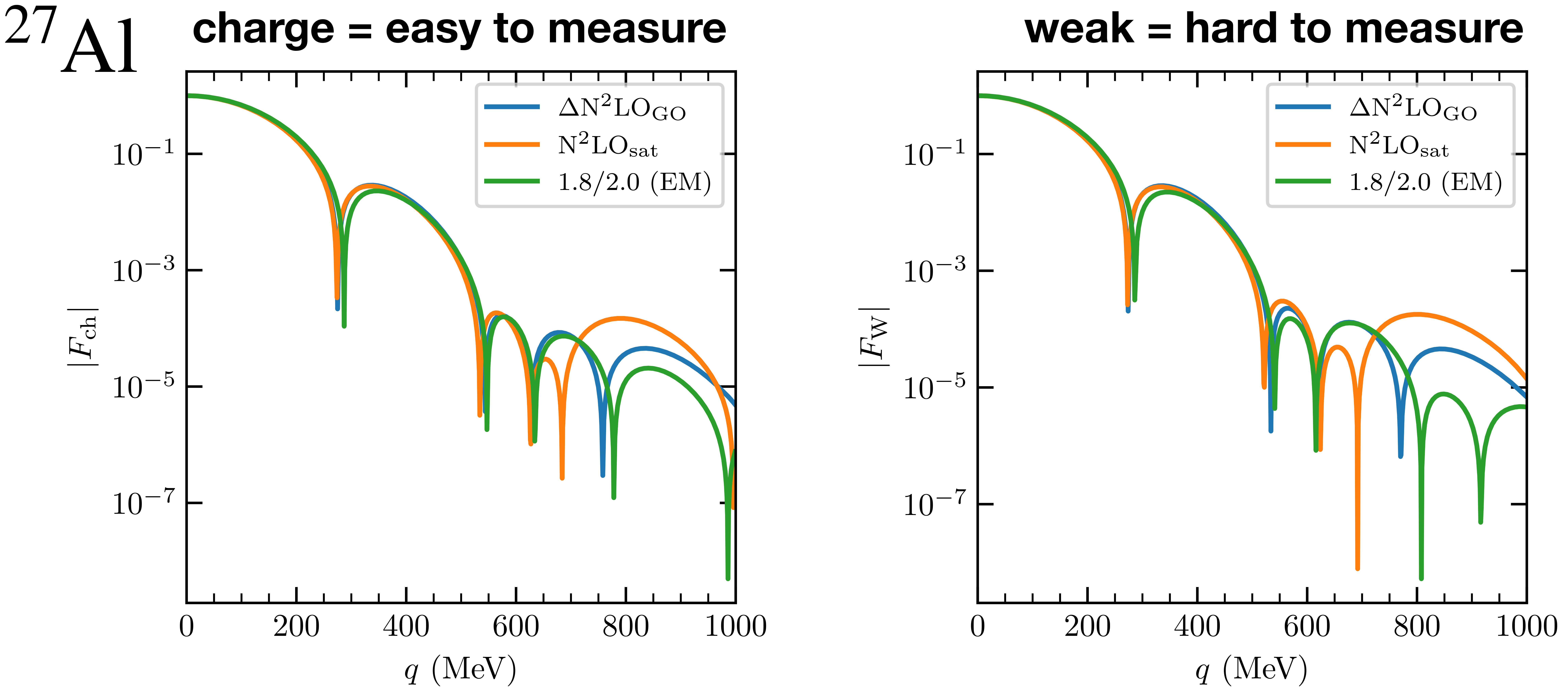
Incoherent:

orb. ang. mom. **spin**

- $M_{J,p/n}$, $\Phi''_{J,p/n}$, $J = 2,\ldots$; $\Delta_{J,p/n}$, $\Sigma'_{J,p/n}$, $\Sigma''_{J,p/n}$, $J = 1,\ldots$
- No obvious hierarchy for incoherent responses → need up to $J = 5$ for $^{27}\mathrm{Al}$

Ab initio $\mu \to e$ overlap integrals

Charge and weak responses are correlated



- **Approach**: Correlations between $\rho_{\mathrm{ch}}(r), \rho_n(r), \rho_p(r)$ constrain overlap integrals

The correlation

Ensemble of 42 Hamiltonians:

- “Magic” 4 [1.8/2.0 (EM), …]

  Hebeler et al., PRC **83** (2011)
- $\mathrm{N^2LO_{sat}}$

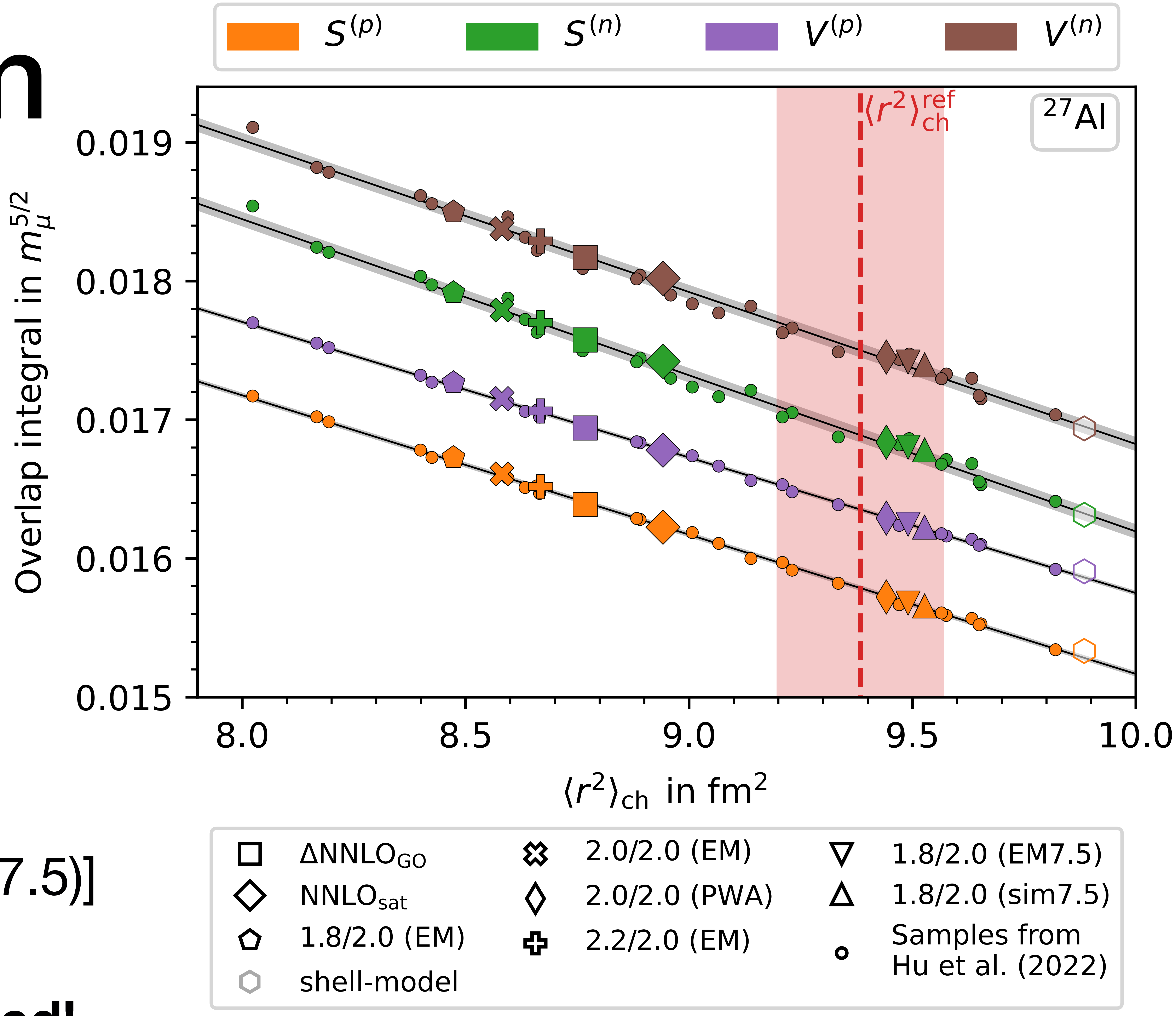
  Ekström et al., JPG **42** (2015)
- $\Delta\mathrm{N^2LO_{GO}}$ ($\Lambda = 394$ MeV)

  Jiang et al., PRC **102** (2020)
- 34 nonimplausible samples

  Hu et al., Nat. Phys. **18** (2022)
- Refit “magic” [1.8/2.0 (EM7.5/sim7.5)]

  Arthuis et al., arXiv:2401.06675

Tight correlations with R^2_{ch} observed!



MH, Hoferichter, Miyagi, Noël, Schwenk, arXiv:2412.04545

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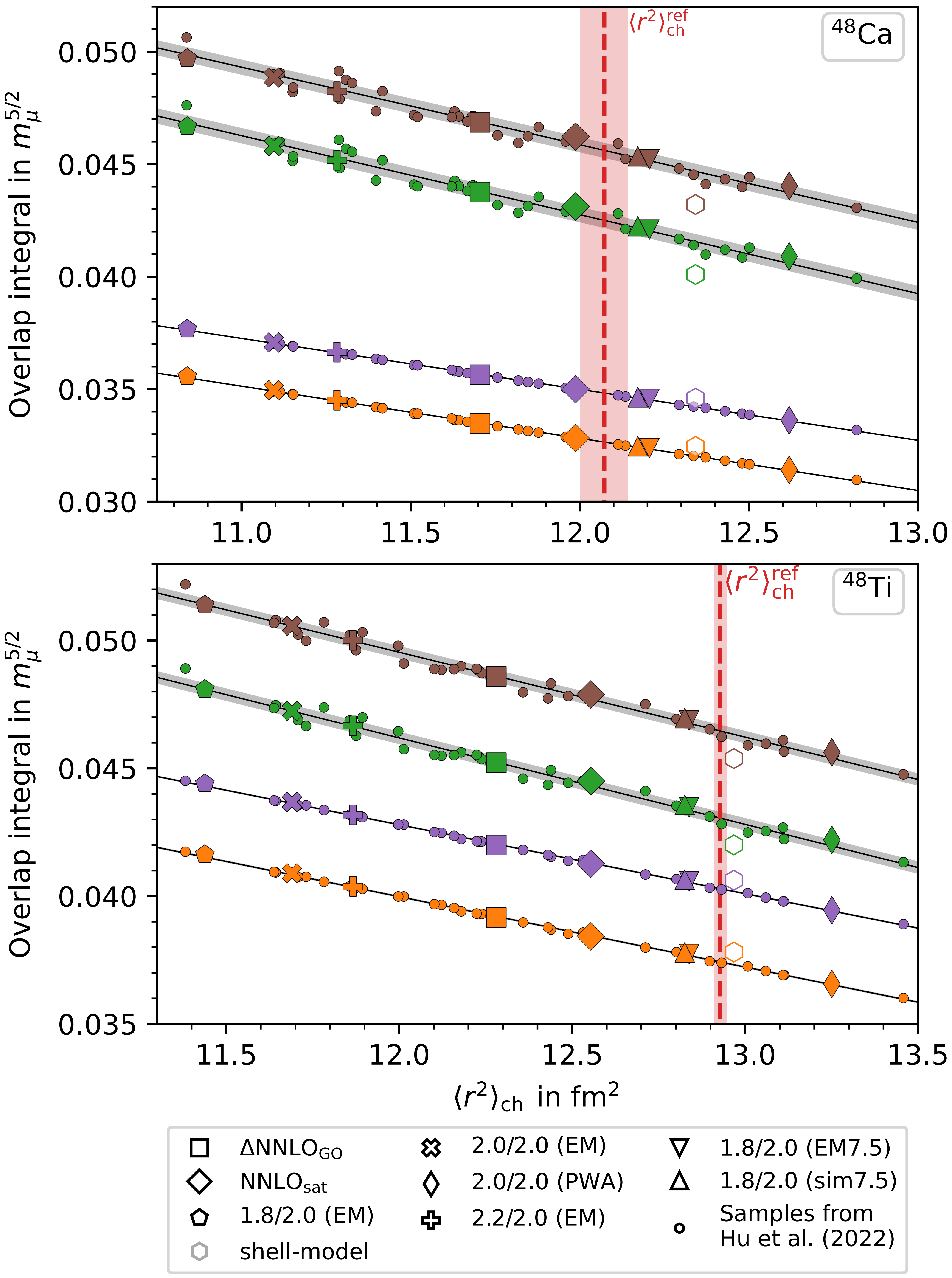
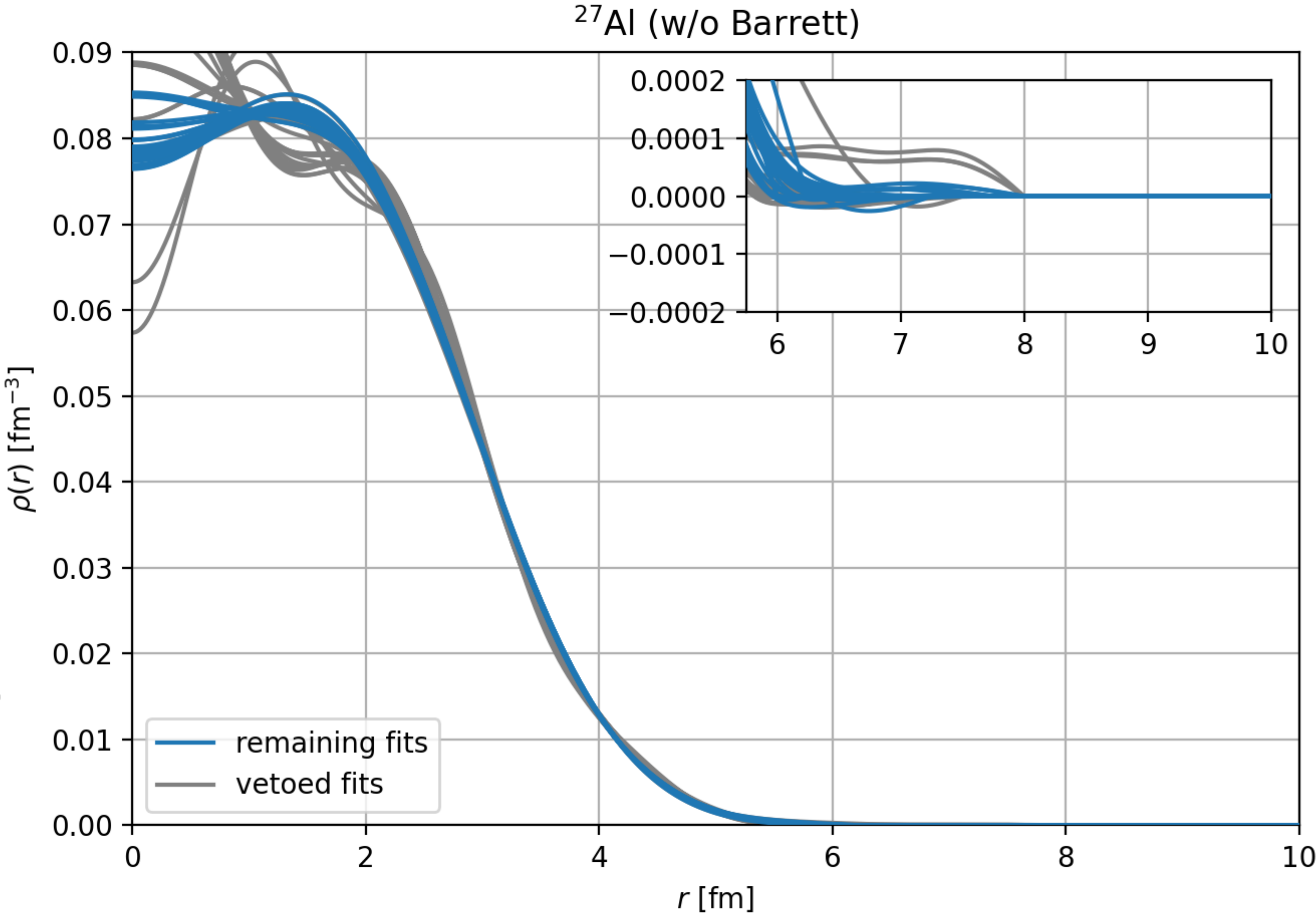


Charge distribution uncertainties

- Re-analysis of electron-scattering data
- Improved evaluation of uncertainties (more conservative for $^{27}\mathrm{Al}$)
- Goes into uncertainty for R_{ch}^2 and D (overlap integral)

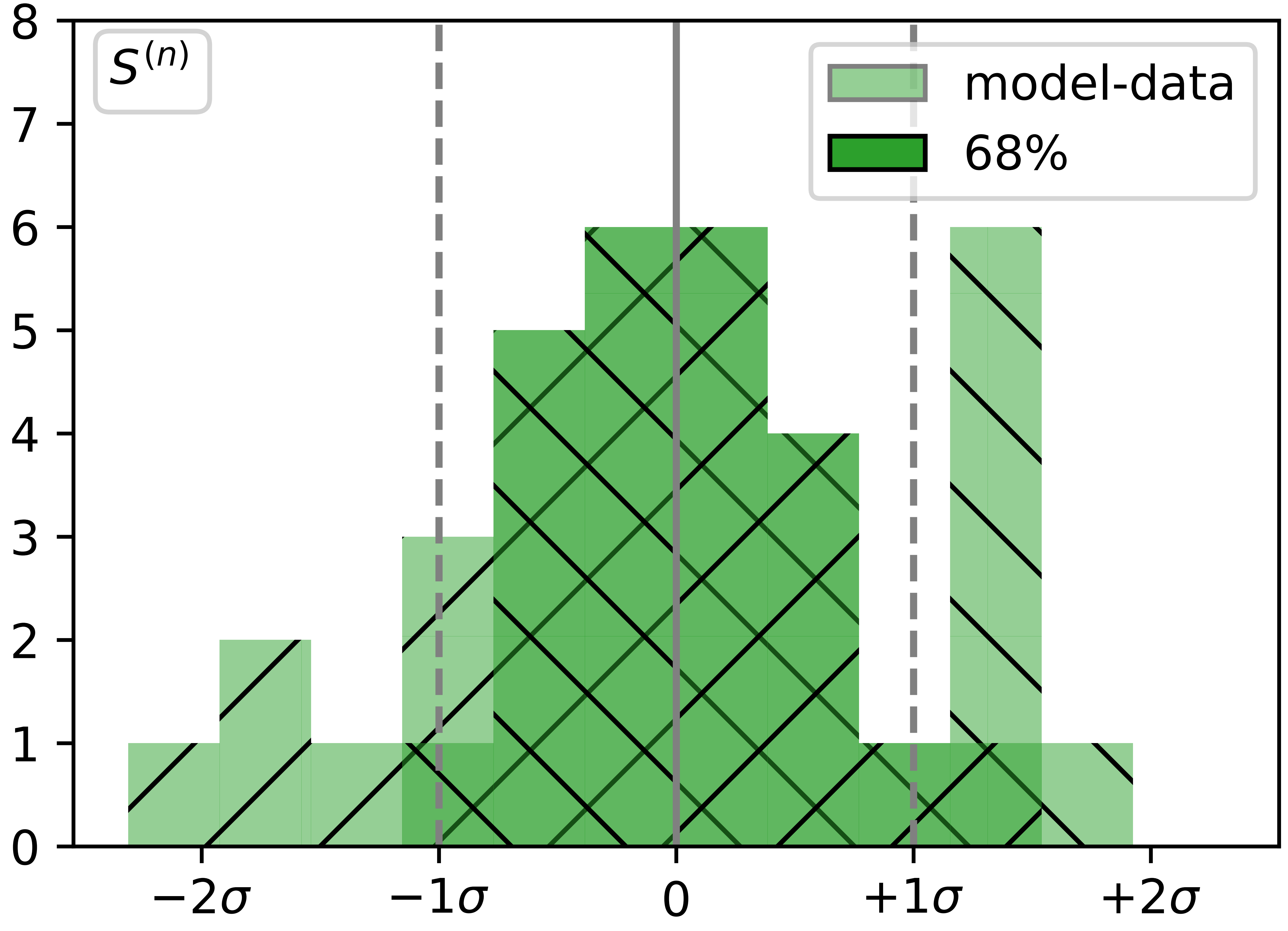


Noël, Hoferichter, JHEP **08** (2024)

Nuclear structure uncertainties

$^{27}\mathrm{Al}$

Remaining scatter around correlation



- Correlation → simple linear fit

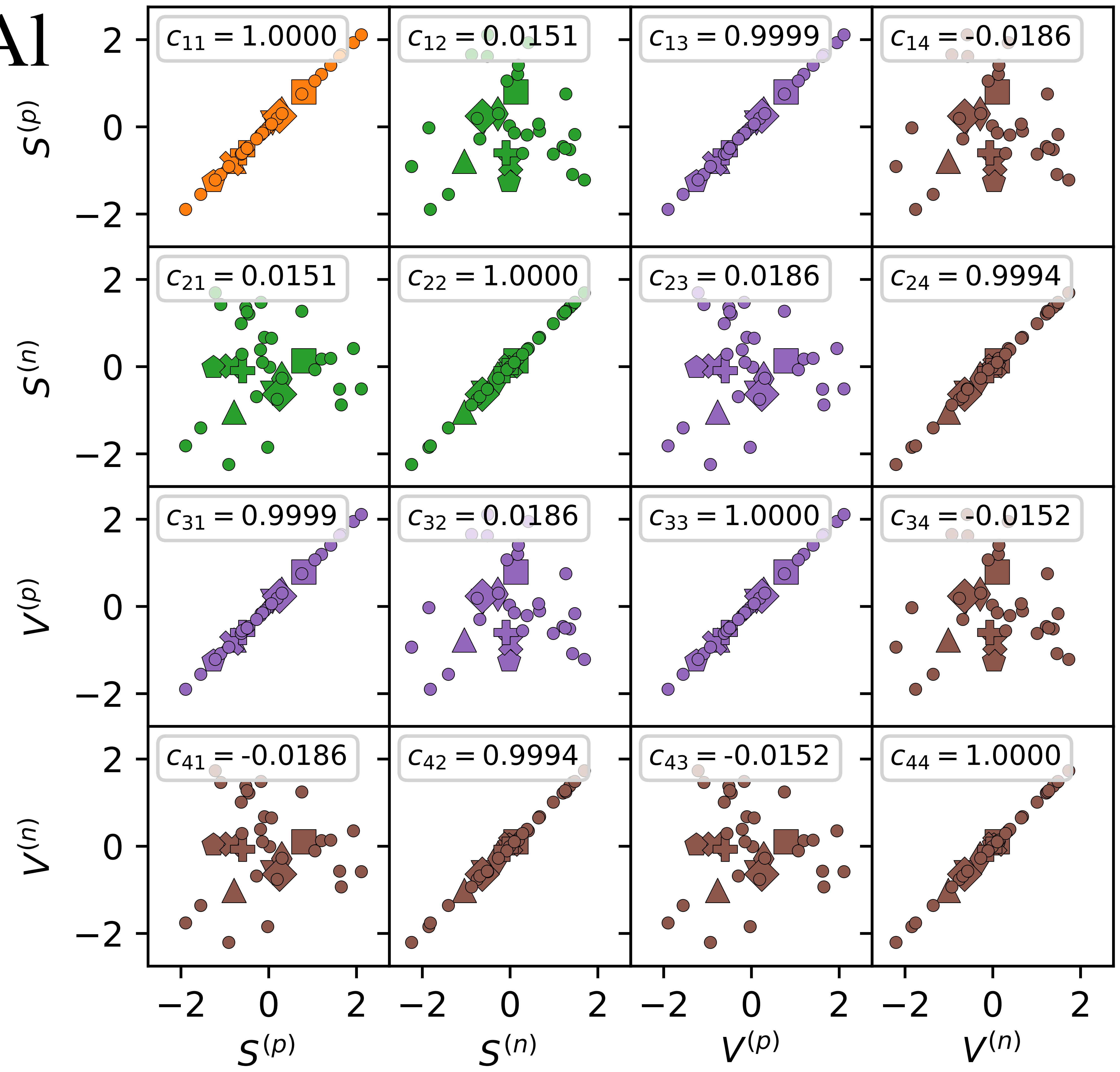
$$S^{(n)}_{i,\mathrm{corr}} = a\,(R^2_{\mathrm{ch,i}} - R^2_{\mathrm{ch,ref}}) + b$$

- **How to assess correlation uncertainties?**
- Residuals $S^{(n)}_{i} - S^{(n)}_{i,\mathrm{corr}}$ approximately normally distributed
- Include variance σ^2 in b
- Can also consider **covariance** between overlap integrals

MH, Hoferichter, Miyagi, Noël, Schwenk, arXiv:2412.04545

Nuclear structure uncertainties

^{27}Al



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Ab initio overlap integral predictions

Predictions + uncertainties

		Our result	Kitano et al.
^{27}Al	D	0.0359(2)	0.0362
	$S^{(p)}$	0.01579(2)(19)	0.0155
	$S^{(n)}$	0.01689(5)(21)	0.0167
	$V^{(p)}$	0.01635(2)(18)	0.0161
	$V^{(n)}$	0.01750(5)(21)	0.0173

Covariance matrix

^{27}Al

	D	$S^{(p)}$	$S^{(n)}$	$V^{(p)}$	$V^{(n)}$
D	1.0000	0.7205	0.7030	0.7210	0.7028
$S^{(p)}$		1.0000	0.9656	1.0000	0.9645
$S^{(n)}$			1.0000	0.9664	1.0000
$V^{(p)}$				1.0000	0.9654
$V^{(n)}$					1.0000

- ^{27}Al: Uncertainties from e scattering dominate → strong correlations among overlap integrals
- ^{48}Ti: Correlation analysis uncertainties dominate for neutrons

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	D	0.08640(11)	0.0864
	$S^{(p)}$	0.03742(05)(5)	0.0368
^{48}Ti	$S^{(n)}$	0.04305(25)(6)	0.0435
	$V^{(p)}$	0.04029(04)(5)	0.0396
	$V^{(n)}$	0.04646(24)(5)	0.0468

Covariance matrix

^{48}Ti

	D	$S^{(p)}$	$S^{(n)}$	$V^{(p)}$	$V^{(n)}$
D	1.0000	0.4657	0.1169	0.5003	0.1163
$S^{(p)}$		1.0000	0.1118	0.9991	0.0916
$S^{(n)}$			1.0000	0.1176	0.9997
$V^{(p)}$				1.0000	0.0978
$V^{(n)}$					1.0000

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	$V^{(p)}$	$0.04029(04)(5)$	0.0396
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^{48}Ti

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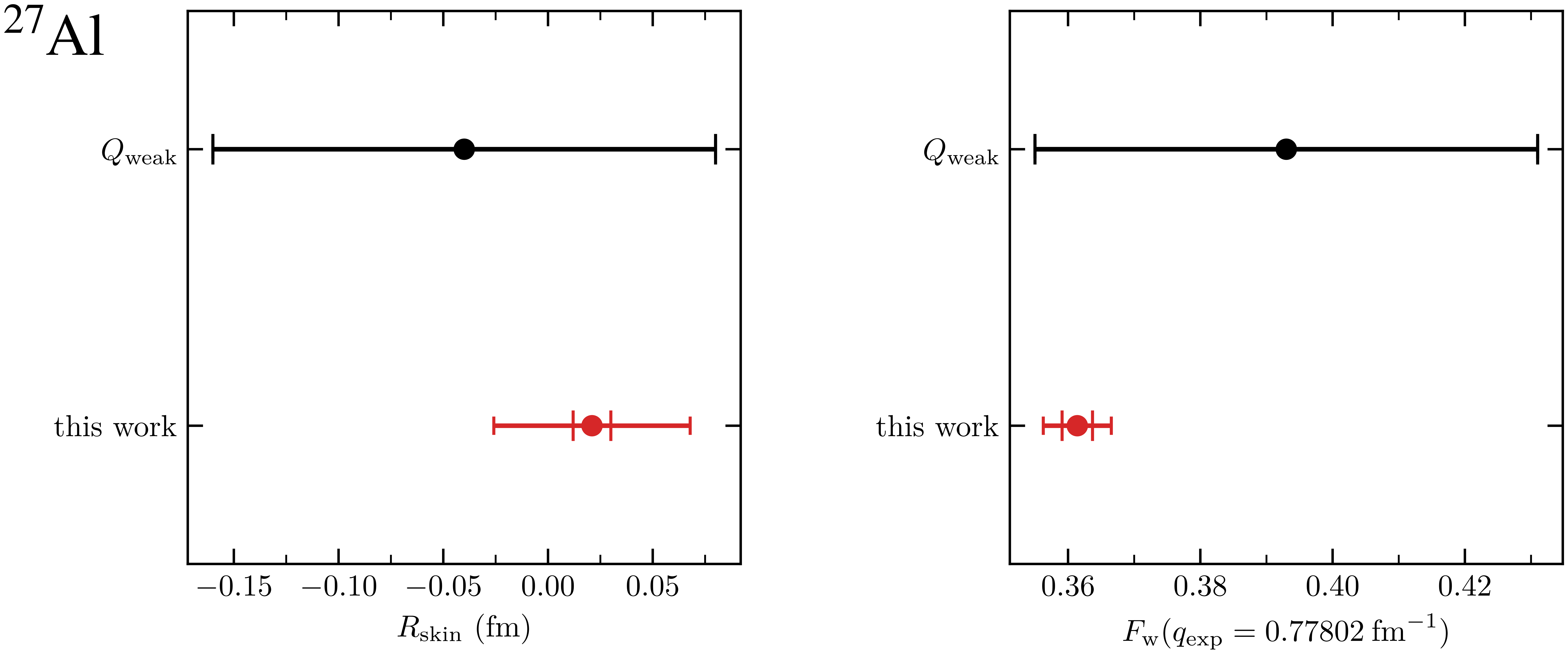
Bonus: Predictions for weak scattering



Q_{weak}, PRL **128** (2022), CREX, PRL **129** (2022), Hagen et al., Nat. Phys. **12** (2016)
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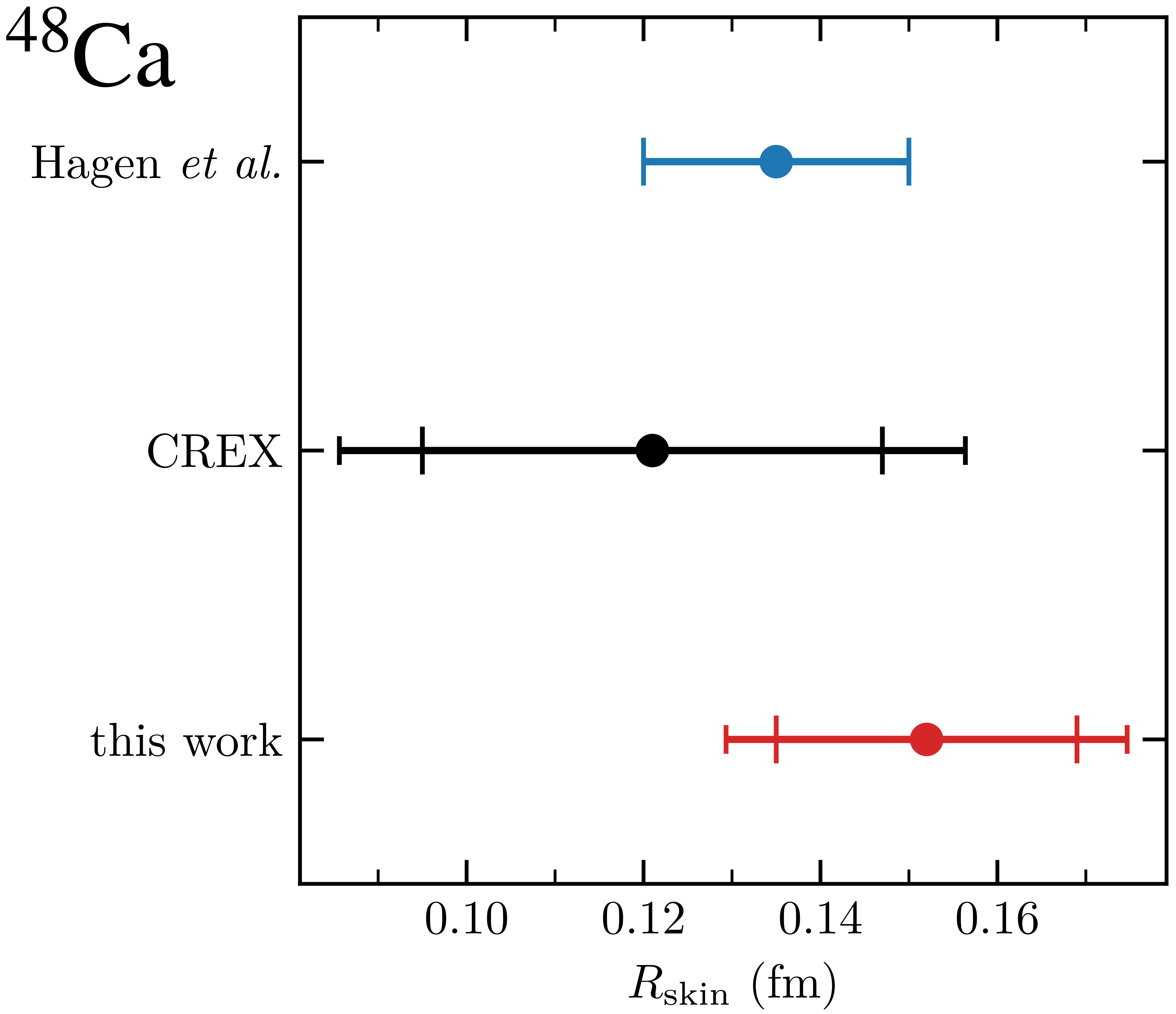

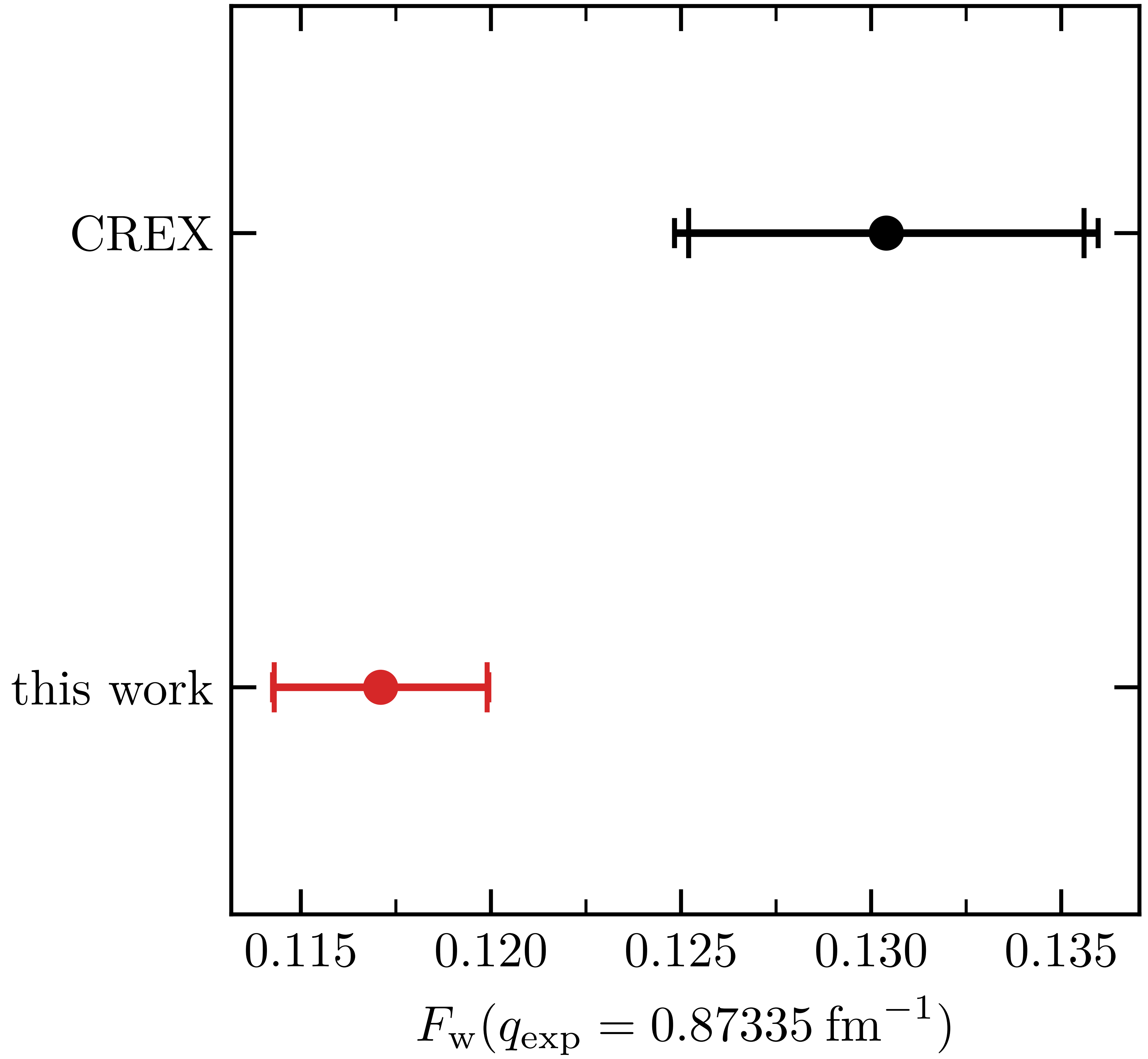

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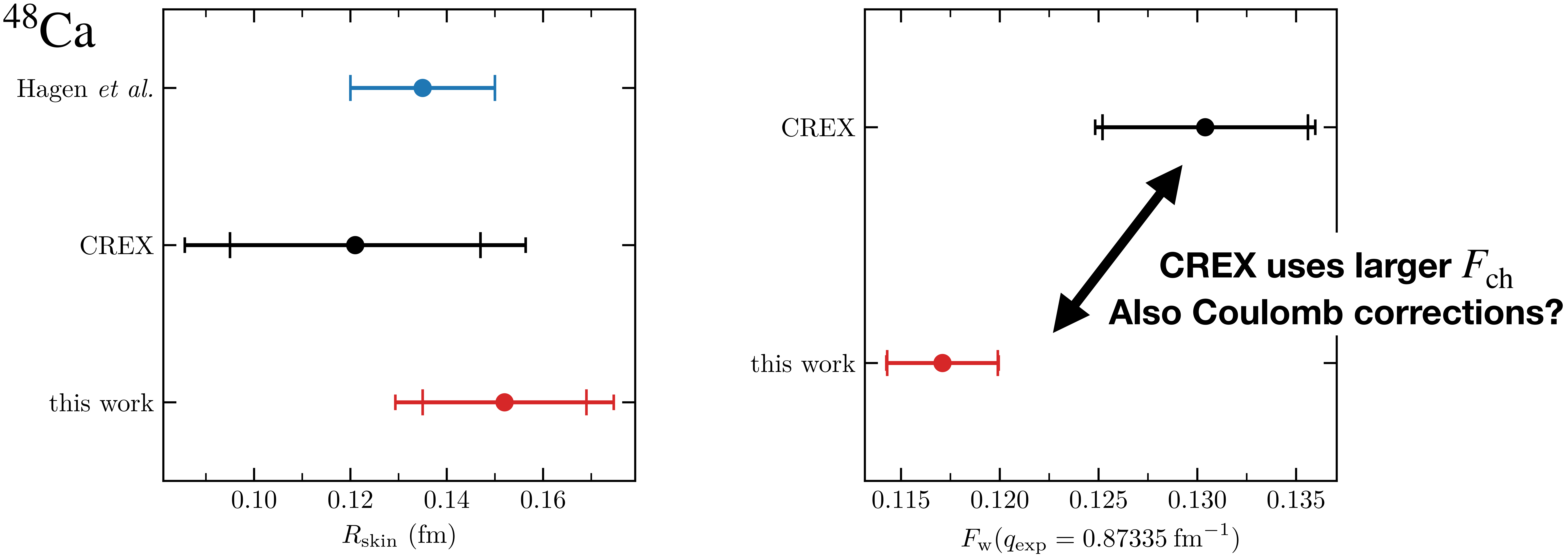

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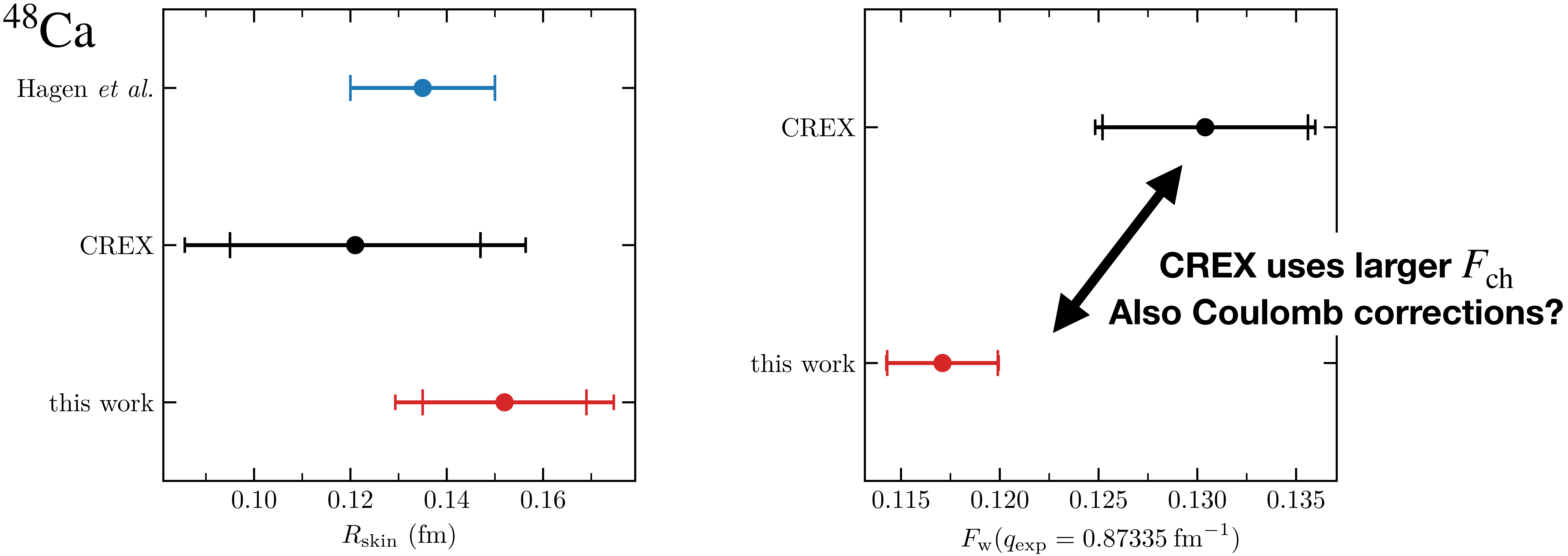
Bonus: Predictions for weak scattering

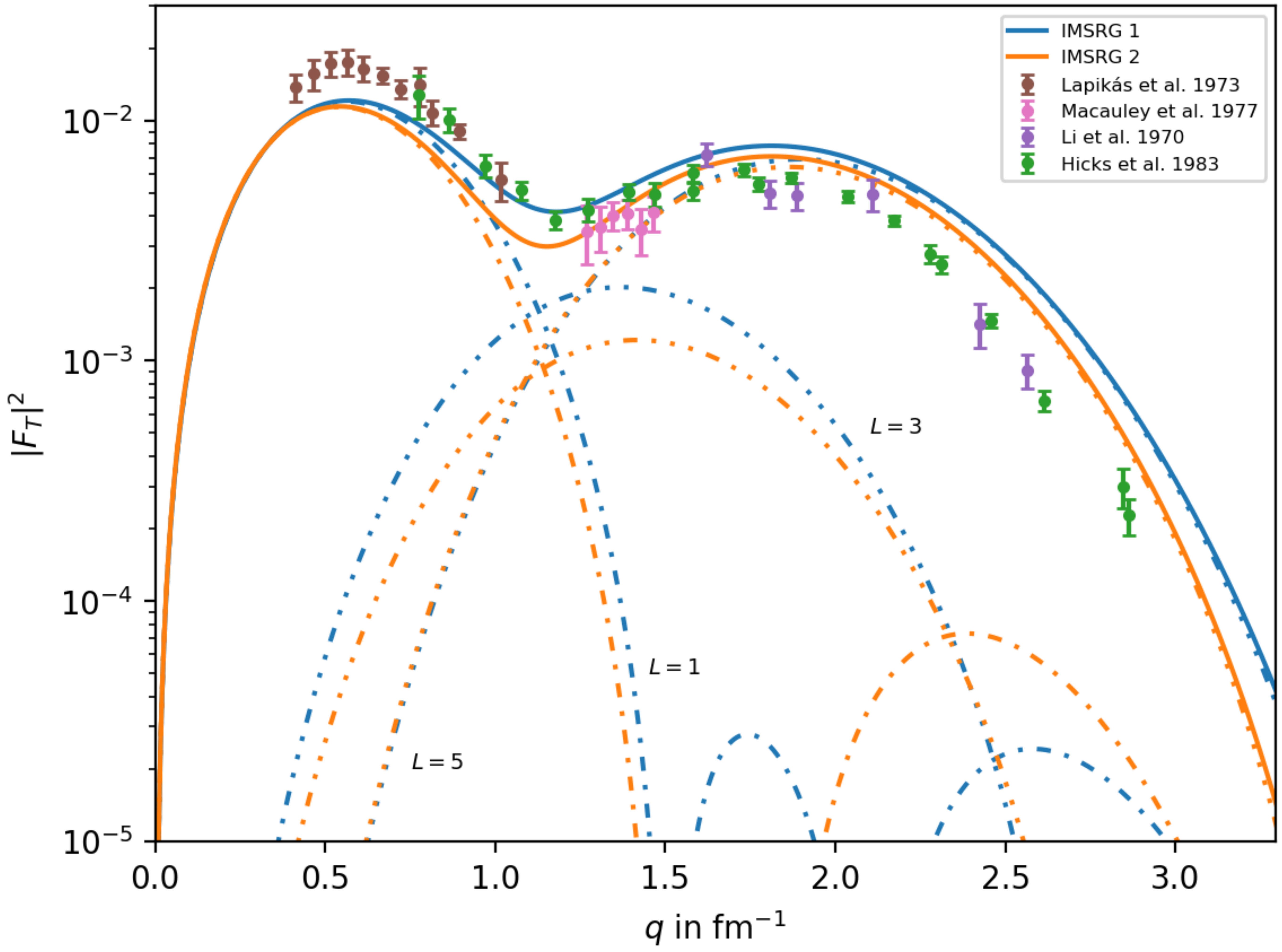


- Apparent tension with CREX partially resolved by accounting for Coulomb corrections and comparing with measured $A_{\rm PV}$

$Q_{\rm weak}$, PRL **128** (2022), CREX, PRL **129** (2022), Hagen et al., Nat. Phys. **12** (2016)
MH, Hoferichter, Miyagi, Noël, Schwenk, arXiv:2412.04545

What next?

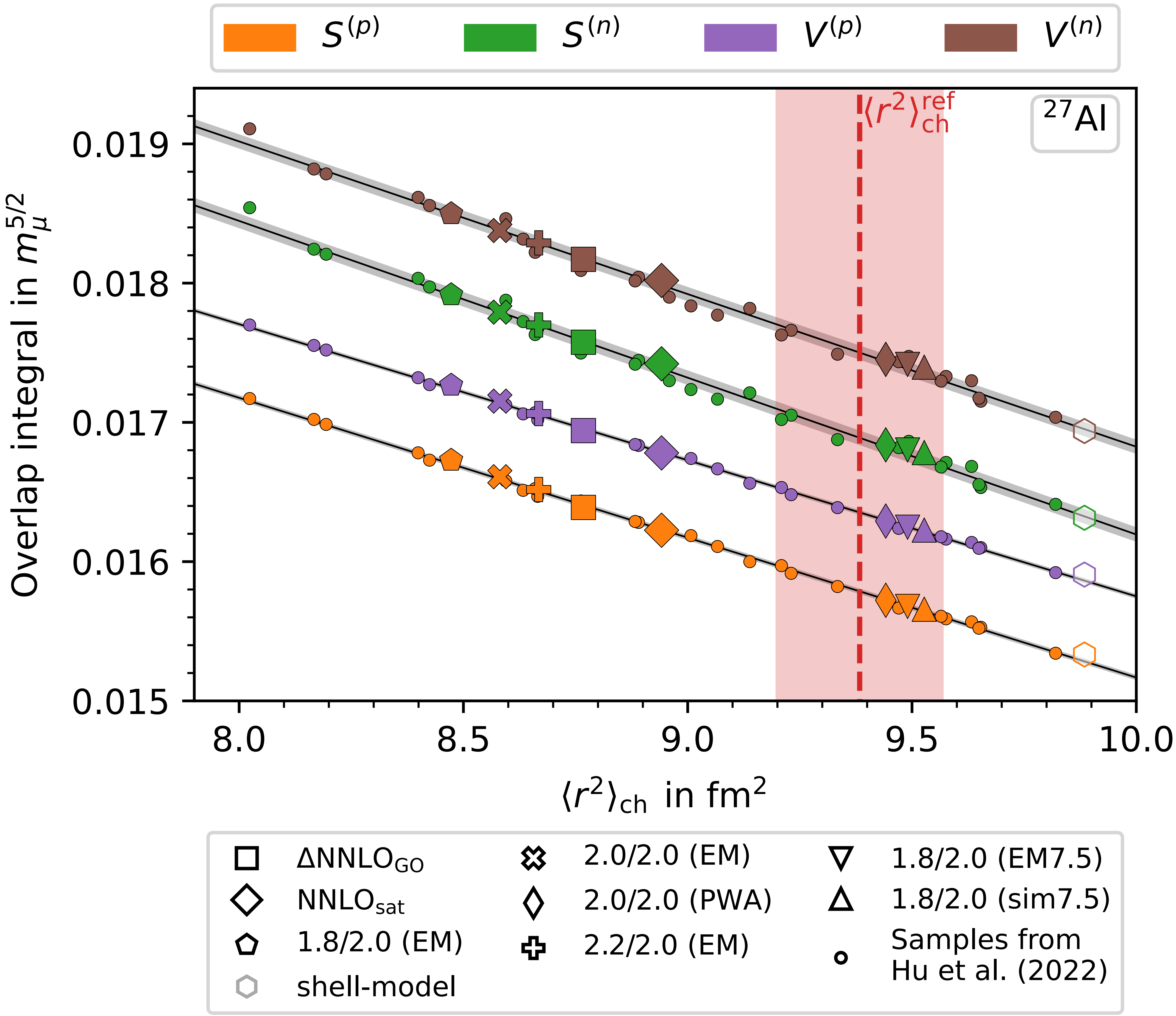
- **Incoherent spin-dependent** responses also contribute
  - Naively subleading contribution, but may be important for some microscopic theories
- **Understand impact of uncertainties** on analyses constraining Wilson coefficients of SMEFT operators



Noël, Hoferichter, JHEP **08** (2024)

Conclusion

- Ab initio predictions of overlap integrals for spin-independent $\mu \rightarrow e$ conversion
- **Comprehensive treatment** of Hamiltonian (and many-body) uncertainties
- **Correlation analysis** accounts for correlated uncertainties
- Consistent with past work on weak scattering
- **Key input for inferences** of implications for BSM physics from $\mu \rightarrow e$ decay rate



MH, Hoferichter, Miyagi, Noël, Schwenk, arXiv:2412.04545

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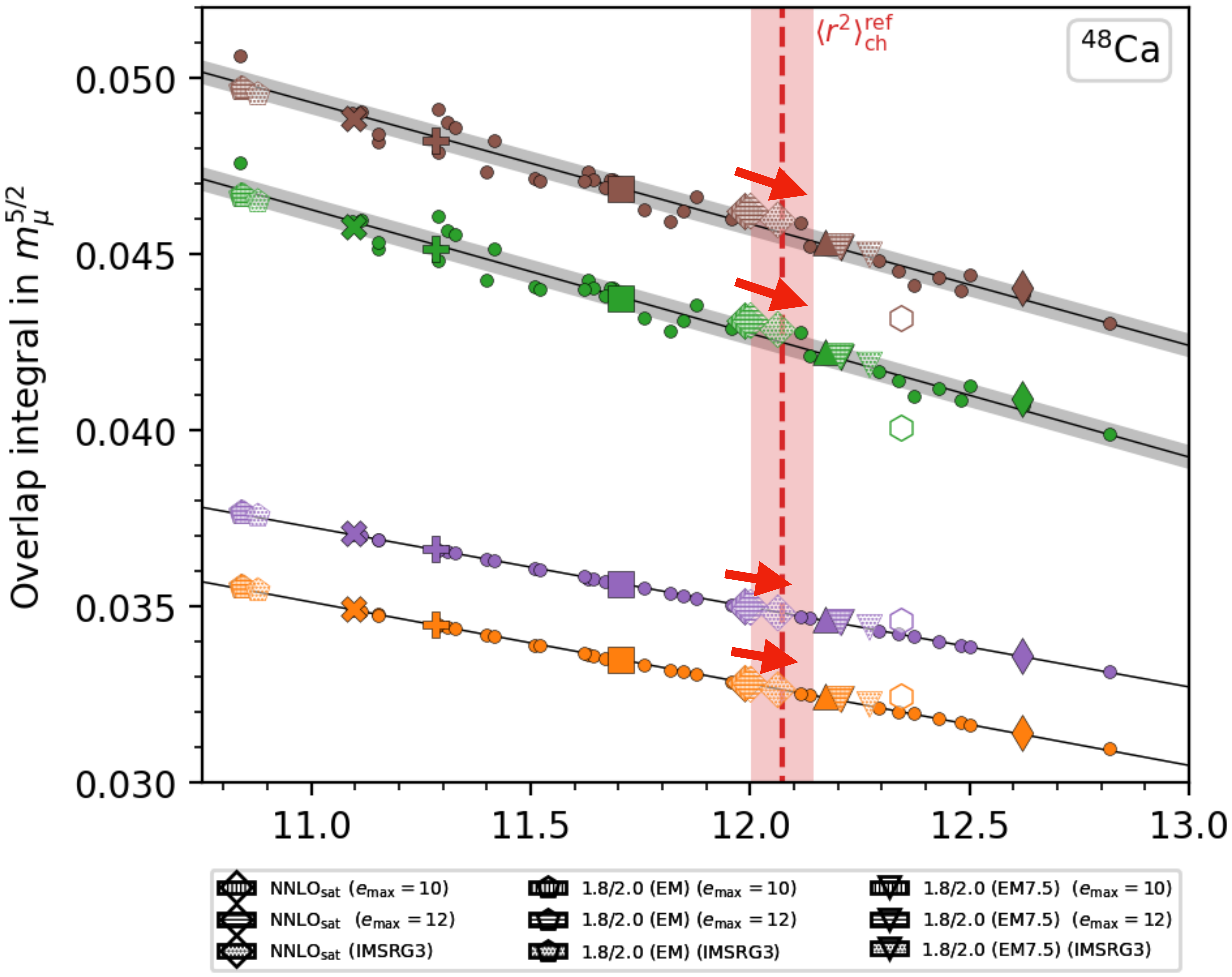
What about many-body uncertainties?

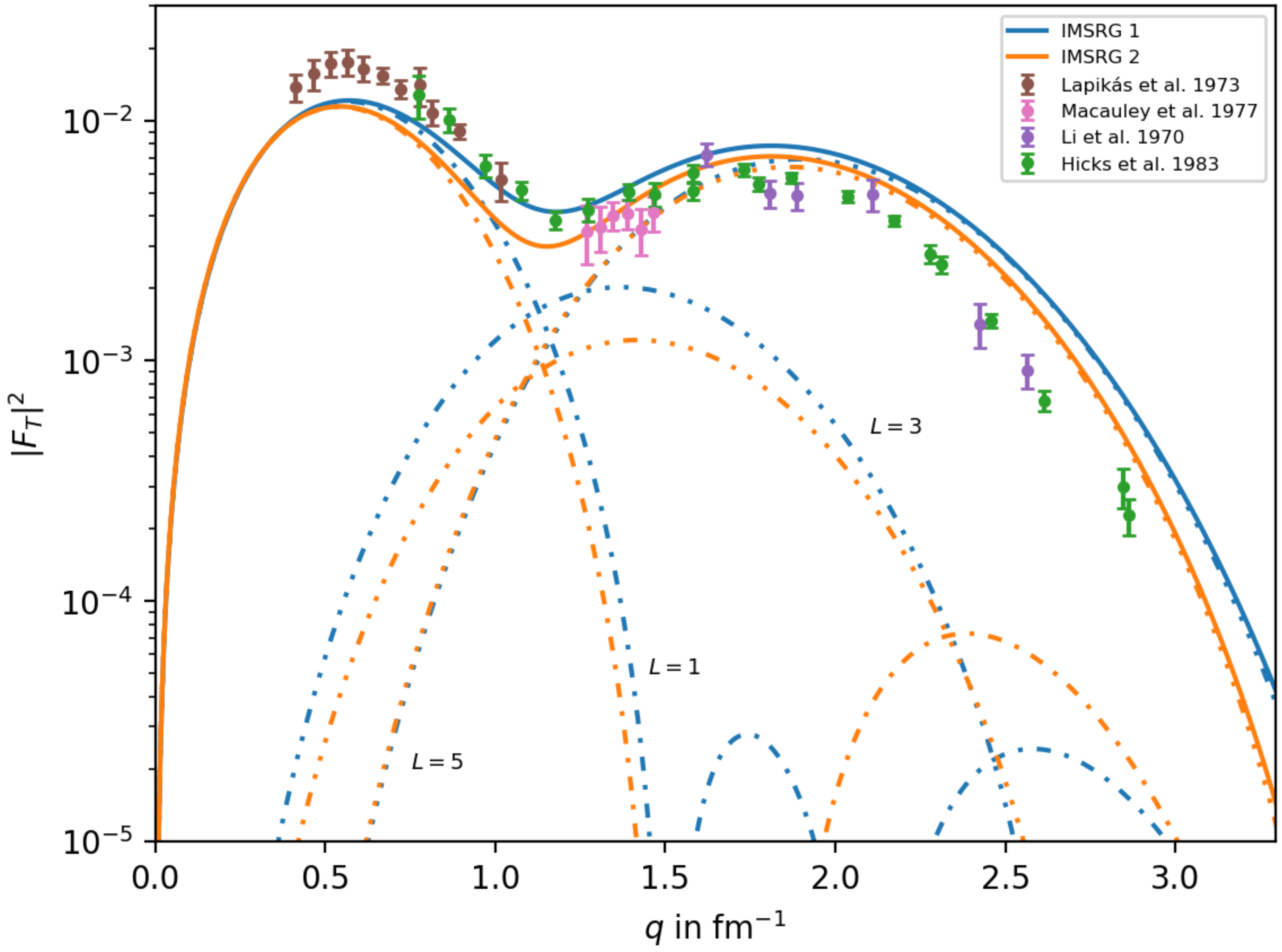
- Adjusted both model-space and many-body truncations
- Resulting points still lie on the correlation
- Correlation encompasses both diverse Hamiltonian uncertainties and many-body uncertainties



IMSRG(3) = IMSRG(3)-N^7 with restricted 3B operators

Can we resolve subleading responses?

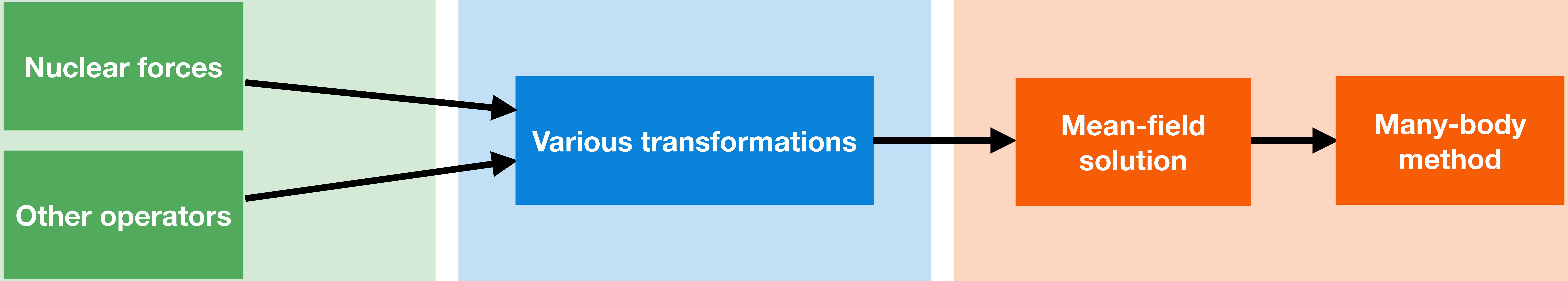
- Incoherent spin-dependent responses also contribute
- Challenges:
  - Many more responses to evaluate: $M, \Phi'', \Delta, \Sigma', \Sigma''$ for $J \leq 5$
  - Overlap integral formalism not yet established
  - **Which observable to correlate with?**
  - **Can we actually resolve this given current uncertainties?**
  - **2BCs might be relevant?**



Noël, Hoferichter, JHEP **08** (2024)

Many-body calculation uncertainties

Operator determination | **Basis transformation** | **Many-body calculation**



Hamiltonian uncertainty:
- Nuclear force model
- Model error
- Fit strategy to experimental data

Model-space uncertainty:
- Basis truncation
  - $e_{\max}, E_{3,\max}$

Many-body uncertainty:
- Many-body method truncation
  - IMSRG(2), IMSRG(3)
- ...