



TECHNISCHE  
UNIVERSITÄT  
DARMSTADT

# ***Ab initio* calculations of nuclear structure factors for spin-dependent WIMP-nucleus scattering**

**– with full leading two-body current**

**Zhen Li (TU Darmstadt)**

PandaX-xT 2nd Open Meeting  
6-10 April 2026, Shanghai, China

# Acknowledgment

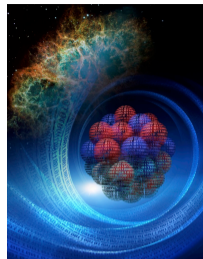
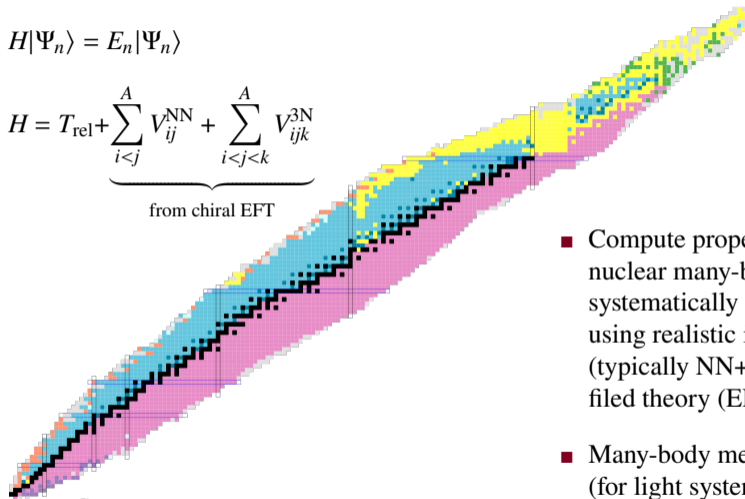
- C. Brase (TU Darmstadt)
- Y. Chiba (Tsukuba U.)
- T. Marrodán Undagoitia (Max-Planck-Institut für Kernphysik)
- J. Menéndez (Barcelona U.)
- T. Miyagi (Tsukuba U.)
- A. Schwenk (TU Darmstadt)

**for collaborations and discussions!**

# *Ab initio* calculation for atomic nuclei

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

$$H = T_{\text{rel}} + \underbrace{\sum_{i<j}^A V_{ij}^{\text{NN}} + \sum_{i<j<k}^A V_{ijk}^{\text{3N}}}_{\text{from chiral EFT}}$$



- Compute properties of nuclei by solving the nuclear many-body Schrödinger equation with systematically improvable many-body methods, using realistic inter-nucleon interactions (typically NN+3N) derived from chiral effective field theory (EFT)
- Many-body methods: NCSM, QMC, HH, ... (for light system  $A \lesssim 16$ ), and MBPT, CC, SCGF, IMSRG, ... (for heavier systems)

See e.g., *Hergert et al., Front. Phys. (2020)*  
*Hebeler, Phys. Rept. (2021)*  
and ref therein

# Chiral EFT for nuclear forces

	NN	3N
LO $\mathcal{O}(Q^0/\Lambda^0)$	1990 [151,152] <span style="border: 1px solid red; padding: 2px;">2</span> 	—
NLO $\mathcal{O}(Q^2/\Lambda^2)$	1992 [164,165] <span style="border: 1px solid red; padding: 2px;">7</span> 	1992,1994 [166-169] —
N <sup>2</sup> LO $\mathcal{O}(Q^3/\Lambda^3)$	1992 [164,165] <span style="border: 1px solid green; padding: 2px;">0</span> 	1994 [167,170] <span style="border: 1px solid red; padding: 2px;">2</span> 
N <sup>3</sup> LO $\mathcal{O}(Q^4/\Lambda^4)$	2000–2002 [179-182] <span style="border: 1px solid red; padding: 2px;">12</span> 	2008–2011 [183-185] <span style="border: 1px solid green; padding: 2px;">0</span> 
N <sup>4</sup> LO $\mathcal{O}(Q^5/\Lambda^5)$	2015 [188,189] <span style="border: 1px solid green; padding: 2px;">0</span> 	2011– [190-192] <span style="border: 1px solid red; padding: 2px;">?</span> 

Fig. from Hebeler, *Phys. Rept.* (2021)

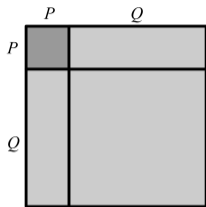
See e.g., Epelbaum et al., *Rev. Mod. Phys.* (2009)

Machleidt et al., *Phys. Rep.* (2011)

Krebs, *Eur. Phys. J. A* (2020)

- A low-energy effective theory of QCD with pions/nucleons (and optionally the  $\Delta$ ) as degrees of freedom, constrained by chiral symmetry and its breaking
- Expansion parameter  $Q/\Lambda_b \simeq 1/3$
- Short-distance (high-energy) physics encoded in low-energy constants (LECs), fitted to NN scattering & few-body observables  ${}^2\text{H}$ ,  ${}^3\text{H}$ ,  $\dots$
- Systematically improvable and allows for uncertainty quantification
- Nuclear currents coupling to external probes (photons, electrons, neutrinos, etc.) can be derived consistently

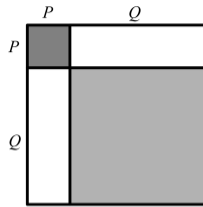
# Valence-space in-medium similarity renormalization group (VS-IMSRG)



$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

$$H = T_{\text{rel}} + \sum_{i<j}^A V_{ij}^{\text{NN}} + \sum_{i<j<k}^A V_{ijk}^{\text{3N}}$$

Unitary transformations  $U(s)$   
 Decouple  $P$  space from  $Q$  space



$$H_{\text{eff}}|\Psi_n^P\rangle = E_n|\Psi_n^P\rangle$$

$$H_{\text{eff}} = [U(s)HU^\dagger(s)]_{s \rightarrow \infty}$$

$$O_{\text{eff}} = [U(s)OU^\dagger(s)]_{s \rightarrow \infty}$$

*Hergert et al., Phys. Rep. (2016)*  
*Stroberg et al., Ann. Rev. Nucl. Part. Sci. (2019)*

- The large model-space eigenvalue problem mapped to a tractable valence-space ( $P$  space) problem
- Particle-hole excitations from  $P$  to  $Q$  encoded in the *effective* Hamiltonian & operators
- Diagonalizing  $H_{\text{eff}} \rightarrow$  energies and wavefunctions  $\rightarrow$  other observables

# Highlights of *ab initio* calculations with VS-IMSRG

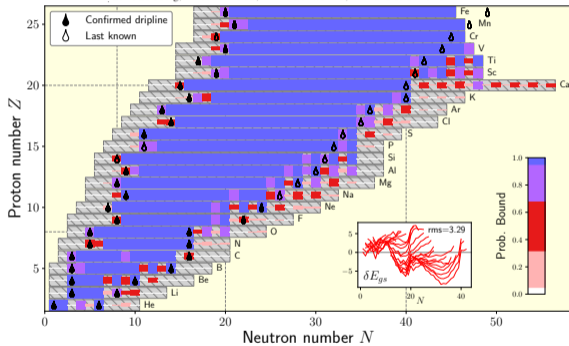
PHYSICAL REVIEW LETTERS 126, 022501 (2021)

Editors' Suggestion

Featured in Physics

## Ab Initio Limits of Atomic Nuclei

S. R. Stroberg,<sup>1,2,\*</sup> J. D. Holt,<sup>2,3,†</sup> A. Schwenk,<sup>4,5,6,‡</sup> and J. Simonis<sup>7,4,5,8</sup>

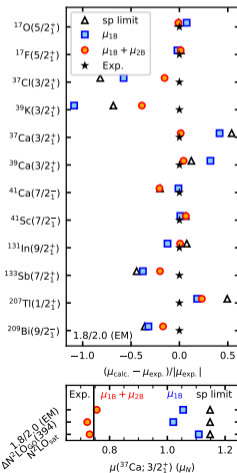


Drip line

PHYSICAL REVIEW LETTERS 132, 232503 (2024)

## Impact of Two-Body Currents on Magnetic Dipole Moments of Nuclei

T. Miyagi,<sup>1,2,3,\*</sup> X. Cao,<sup>4,†</sup> R. Seutin,<sup>3,1,2,‡</sup> S. Bacca,<sup>5,6,8</sup> R. F. Garcia Ruiz,<sup>7,‡</sup> K. Hebeler,<sup>1,2,3,‡</sup> J. D. Holt,<sup>8,9,\*</sup> and A. Schwenk<sup>1,2,3,†</sup>



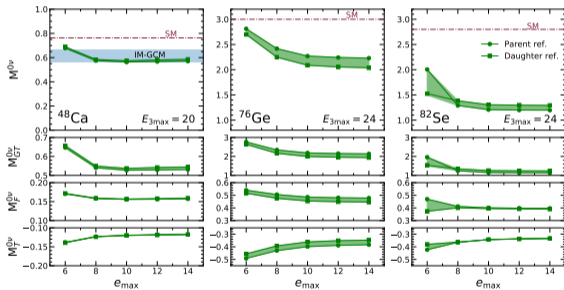
Magnetic dipole moments

# Highlights of *ab initio* calculations with VS-IMSRG

PHYSICAL REVIEW LETTERS **126**, 042502 (2021)

## *Ab Initio* Neutrinoless Double-Beta Decay Matrix Elements for $^{48}\text{Ca}$ , $^{76}\text{Ge}$ , and $^{82}\text{Se}$

A. Belley<sup>1,2,3</sup>, C. G. Payne<sup>1,3,†</sup>, S. R. Stroberg<sup>4</sup>, T. Miyagi<sup>1</sup> and J. D. Holt<sup>1,2,\*</sup>

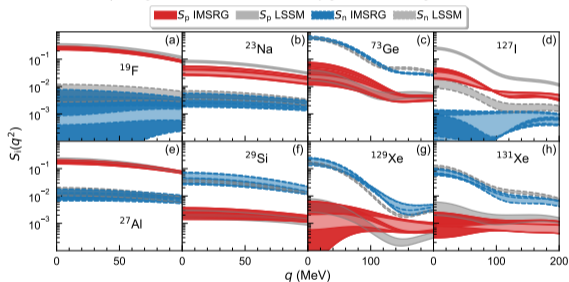


$0\nu\beta\beta$

PHYSICAL REVIEW LETTERS **128**, 072502 (2022)

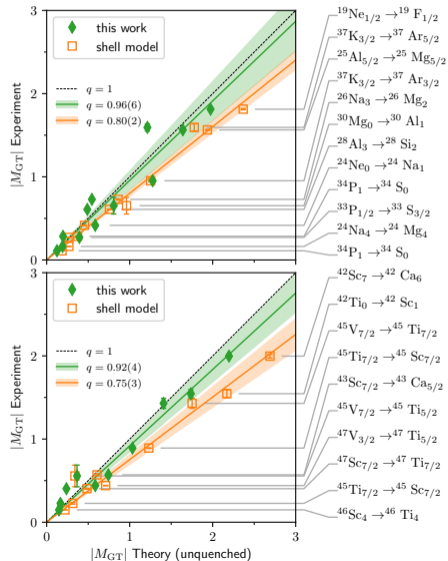
## *Ab Initio* Structure Factors for Spin-Dependent Dark Matter Direct Detection

B. S. Hu<sup>1,\*</sup>, J. Padua-Argüelles<sup>1,2,†</sup>, S. Leutheusser<sup>1,3,‡</sup>, T. Miyagi<sup>1,8</sup>, S. R. Stroberg<sup>4,1,§</sup> and J. D. Holt<sup>1,5,\*\*</sup>



WIMP-nucleus scattering

# Highlights of *ab initio* calculations with VS-IMSRG



LETTERS

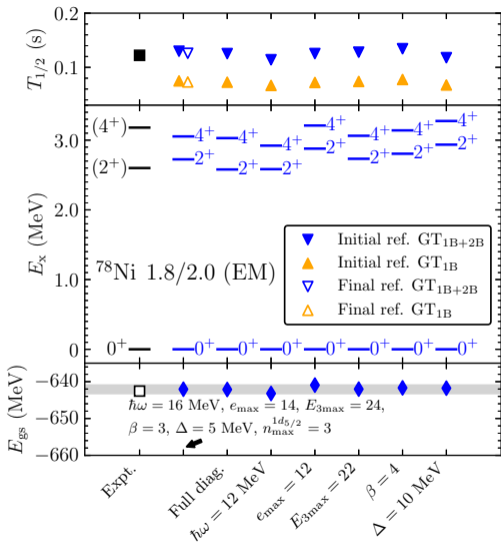
<https://doi.org/10.1038/s41567-019-0450-7>

nature  
physics

## Discrepancy between experimental and theoretical $\beta$ -decay rates resolved from first principles

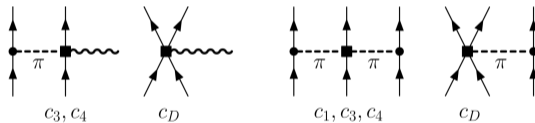
P. Gysbers<sup>1,2</sup>, G. Hagen<sup>3,4\*</sup>, J. D. Holt<sup>5</sup>, G. R. Jansen<sup>3,5</sup>, T. D. Morris<sup>3,4,6</sup>, P. Navrátil<sup>6</sup>, T. Papenbrock<sup>3,4</sup>, S. Quaglioni<sup>7</sup>, A. Schwenk<sup>8,9,10</sup>, S. R. Stroberg<sup>1,11,12</sup> and K. A. Wendt<sup>7</sup>

GT quenching puzzle explained in *ab initio* calculations by taking into account the many-body correlations and two-body currents



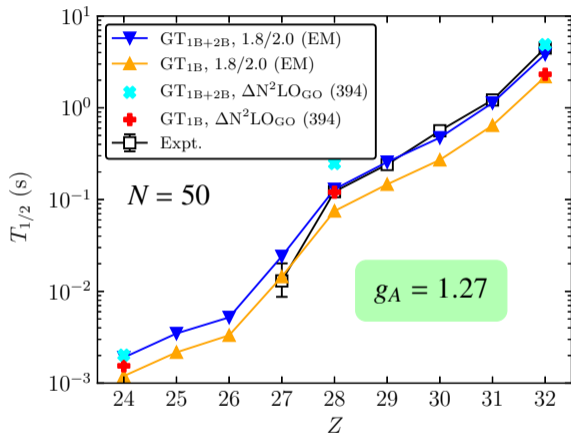
Expt.: Taniuchi et al., *Nature* (2019); Xu et al., *PRL* (2014)

- $^{78}\text{Ni}$  ground-state energy and low-lying spectra are well described using VS-IMSRG with the 1.8/2.0 (EM) interaction *Hebeler et al., PRC (2011)*
- The leading 2BC appears at  $\text{N}^2\text{LO}$ , sharing same LECs as the leading 3NF



*Fig. from Menéndez et al., PRL (2011)*

- GT operators are evolved by VS-IMSRG to include the correlations coupled to the space outside
- 2BC increases the total half-life by reducing the GT transition strength

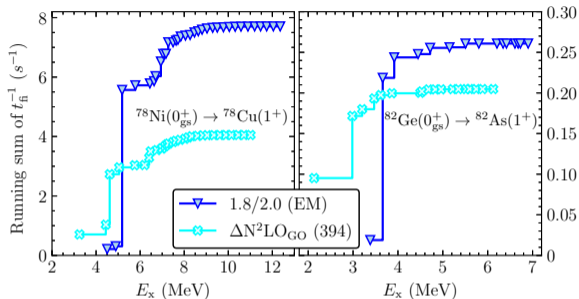
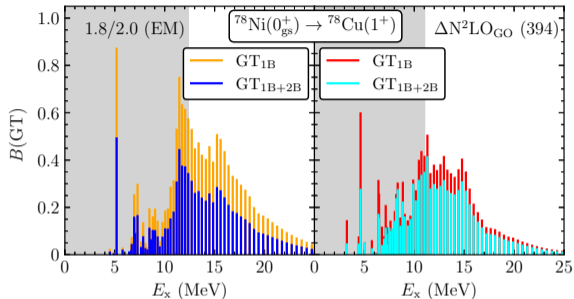


Total Gamow-Teller (dominant) half-lives of  $N = 50$  isotones with VS-IMSRG

- Half-lives of waiting point nuclei ( $N = 50, 82, 126, \dots$  neutron-rich nuclei) are critical inputs for  $r$  process simulations, but less known experimentally
- 2BC increases the total half-life
- Expt. half-lives are well described with the 1.8/2.0 (EM) interaction
- No need to quench  $g_A$  in *ab initio* calculations

1.8/2.0 (EM): Hebel et al., *PRC* (2011)

$\Delta N^2 LO_{GO}$  (394): Jiang et al., *PRC* (2020)



- 2BC reduces  $B(\text{GT})$  strength systematically  $\rightarrow$  increase the total half-life
- Quite different running sums of  $t_{fi}^{-1}$  between 1.8/2.0 (EM) and  $\Delta\text{N}^2\text{LO}_{\text{GO}}$  (394) due to different  $B(\text{GT})$  (related to wavefunctions) and phase space factors (related to energies)

1.8/2.0 (EM): *Hebeler et al., PRC (2011)*

$\Delta\text{N}^2\text{LO}_{\text{GO}}$  (394): *Jiang et al., PRC (2020)*

# Direct detection of WIMP via elastic SD WIMP-nucleus scattering

- Low-momentum-transfer Lagrangian density with axial-vector-axial-vector coupling

$$\mathcal{L}_\chi^{\text{SD}} = -\frac{G_F}{\sqrt{2}} \bar{\chi} \gamma \gamma_5 \chi \cdot \sum_q A_q \bar{q} \gamma \gamma_5 q \quad \text{Engel et al., Int. J. Mod. Phys. E (1992) Jungman et al., RP (1996)}$$

- At one-nucleon level  $\sum_q A_q \bar{q} \gamma \gamma_5 q \rightarrow \sum_{i=1}^A (\mathbf{J}_{i,1b}^0 + \mathbf{J}_{i,1b}^3)$  *Menéndez et al., PRD (2012) Klos et al., PRD (2013)*

$$\mathbf{J}_{i,1b}^0 = \frac{1}{2} a_0 \boldsymbol{\sigma}_i, \quad \mathbf{J}_{i,1b}^3 = \frac{1}{2} a_1 \tau_i^3 \left\{ \left( 1 - \frac{2}{\Lambda_A^2} \mathbf{Q}^2 \right) \boldsymbol{\sigma}_i - \left[ \frac{g_{\pi NN} F_\pi}{(\mathbf{Q}^2 + M_\pi^2) m_N^2 g_A} - \frac{2}{\Lambda_A^2} \right] (\mathbf{Q} \cdot \boldsymbol{\sigma}_i) \mathbf{Q} \right\}$$

- Differential cross section of elastic spin-dependent (SD) WIMP-nucleus scattering

$$\frac{d\sigma^{\text{SD}}}{dQ^2} = \frac{8G_F^2}{(2J+1)v^2} S_A(Q), \quad S_A(Q) = \sum_{\lambda=1,3,5,\dots} \left\{ |\langle J || L_\lambda^5 || J \rangle|^2 + |\langle J || T_\lambda^{\text{el}5} || J \rangle|^2 \right\}$$

- Longitudinal  $L_{\lambda\mu}^5$ , transverse electric  $T_{\lambda\mu}^{\text{el}5}$  and transverse magnetic  $T_{\lambda\mu}^{\text{mag}5}$  (does not contribute to  $S_A$ ) operators from multipole decomposition of nuclear current  $\mathbf{J}$  *Brase et al., PRC (2026)*

$$\mathbf{J}(\mathbf{Q}) = 4\pi \sum_{\lambda\mu} i^{\lambda+1} \left\{ L_{\lambda\mu}^5(Q) \mathbf{Y}_{\lambda\mu}^*(\hat{\mathbf{Q}}) + T_{\lambda\mu}^{\text{el}5}(Q) \boldsymbol{\Psi}_{\lambda\mu}^*(\hat{\mathbf{Q}}) + T_{\lambda\mu}^{\text{mag}5}(Q) [i\boldsymbol{\Phi}_{\lambda\mu}(\hat{\mathbf{Q}})]^* \right\}$$

- $S_A(Q) = a_0^2 S_{00}(Q) + a_0 a_1 S_{01}(Q) + a_1^2 S_{11}(Q)$

# Direct detection of WIMP via elastic SD WIMP-nucleus scattering

- Low-momentum-transfer Lagrangian density with axial-vector-axial-vector coupling

$$\mathcal{L}_\chi^{\text{SD}} = -\frac{G_F}{\sqrt{2}} \bar{\chi} \gamma \gamma_5 \chi \cdot \sum_q A_q \bar{q} \gamma \gamma_5 q \quad \text{Engel et al., Int. J. Mod. Phys. E (1992) Jungman et al., RP (1996)}$$

- At one-nucleon level  $\sum_q A_q \bar{q} \gamma \gamma_5 q \rightarrow \sum_{i=1}^A (\mathbf{J}_{i,1b}^0 + \mathbf{J}_{i,1b}^3)$  *Menéndez et al., PRD (2012) Klos et al., PRD (2013)*

$$\mathbf{J}_{i,1b}^0 = \frac{1}{2} a_0 \boldsymbol{\sigma}_i, \quad \mathbf{J}_{i,1b}^3 = \frac{1}{2} a_1 \tau_i^3 \left\{ \left( 1 - \frac{2}{\Lambda_A^2} \mathbf{Q}^2 \right) \boldsymbol{\sigma}_i - \left[ \frac{g_{\pi NN} F_\pi}{(\mathbf{Q}^2 + M_\pi^2) m_N^2 g_A} - \frac{2}{\Lambda_A^2} \right] (\mathbf{Q} \cdot \boldsymbol{\sigma}_i) \mathbf{Q} \right\}$$

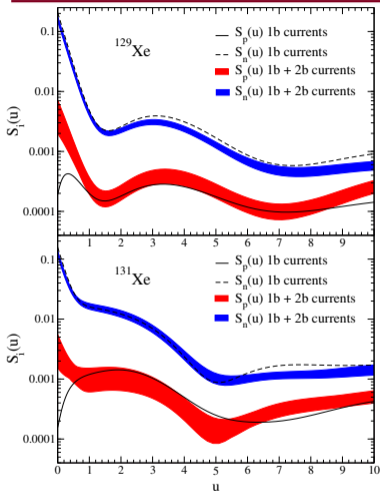
- The isovector  $\mathbf{J}_{i,1b}^3$  is identical to the axial-vector weak neutral current by replacing  $a_1$  by  $g_A$

- 2BC present at N<sup>2</sup>LO in chiral EFT *Krebs, Eur. Phys. J. A (2020) Hoferichter et al., PRD (2020)*

$$\begin{aligned} \mathbf{J}_{2b,12}^{3,1\pi} = & -\frac{a_1}{2F_\pi^2} [\boldsymbol{\tau}_1 \times \boldsymbol{\tau}_2]^3 \left[ c_4 \left( 1 - \frac{\mathbf{Q}\mathbf{Q}\cdot}{\mathbf{Q}^2 + M_\pi^2} \right) (\boldsymbol{\sigma}_1 \times \mathbf{k}_2) + \frac{c_6}{4} (\boldsymbol{\sigma}_1 \times \mathbf{Q}) \right] \frac{\boldsymbol{\sigma}_2 \cdot \mathbf{k}_2}{M_\pi^2 + k_2^2} \\ & - \frac{a_1}{F_\pi^2} \tau_2^3 \left[ c_3 \left( 1 - \frac{\mathbf{Q}\mathbf{Q}\cdot}{\mathbf{Q}^2 + M_\pi^2} \right) \mathbf{k}_2 + 2c_1 M_\pi^2 \frac{\mathbf{Q}}{\mathbf{Q}^2 + M_\pi^2} \right] \frac{\boldsymbol{\sigma}_2 \cdot \mathbf{k}_2}{M_\pi^2 + k_2^2} + (1 \leftrightarrow 2), \end{aligned}$$

$$\mathbf{J}_{2b,12}^{3,\text{ct}} = \frac{a_1}{g_A} \left[ -d_1 \tau_1^3 \left( 1 - \frac{\mathbf{Q}\mathbf{Q}\cdot}{\mathbf{Q}^2 + M_\pi^2} \right) \boldsymbol{\sigma}_1 + (1 \leftrightarrow 2) - d_2 (\boldsymbol{\tau}_1 \times \boldsymbol{\tau}_2)^3 (\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2) \left( 1 - \frac{\mathbf{Q}\mathbf{Q}\cdot}{\mathbf{Q}^2 + M_\pi^2} \right) \right]$$

# Existing calculations of SD structure factors



$$u \equiv Q^2 b^2 / 2$$

Fig. from *Klos et al., PRD (2013)*

$\rho, c_3, c_4 \rightarrow$  uncertainty band

- **Approximate 2BC:** NO1B approx. w/ spin- and isospin-symmetric Fermi gas as the reference state with density  $\rho = 2k_F^3 / (3\pi^2)$

$$\rightarrow \rho\text{-dependent eff. 1BC: } \mathbf{J}_{i,2b}^{\text{eff}}(\rho) = \sum_{\text{occupied } j} (1 - \mathcal{P}_{ij}) \mathbf{J}_{ij}^3$$

- Phenomenological calc.: *Menéndez et al., PRD (2012)*  
*Klos et al., PRD (2013)*    *Pirinen et al., NPA (2019)*  
*Hoferichter et al., PRD (2020)*    *Kasurinen et al., PRC (2025) ...*

- *Ab initio* VS-IMSRG calc.: *Hu et al., PRL (2022)*

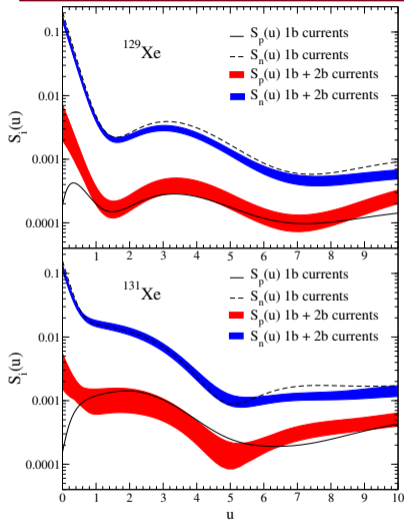
- $S_A(Q=0) = \frac{(J+1)(2J+1)}{4\pi J} \left[ (a_0 + a_1) \langle \hat{S}_p \rangle + (a_0 - a_1) \langle \hat{S}_n \rangle \right]^2$   
 $\langle \hat{S}_{p(n)} \rangle \equiv \langle JM=J | \sum_{i_{p(n)}=1}^{Z(N)} \frac{1}{2} \sigma_{i_{p(n)}} | JM=J \rangle$   
 $^{129,131}\text{Xe: odd } N \rightarrow \langle \hat{S}_n \rangle > \langle \hat{S}_p \rangle$

- Define  $S_p$  with  $a_0 = a_1 = 1$  and  $S_n$  with  $a_0 = -a_1 = 1$ :

$$S_p(Q) = S_{00}(Q) + S_{01}(Q) + S_{11}(Q)$$

$$S_n(Q) = S_{00}(Q) - S_{01}(Q) + S_{11}(Q)$$

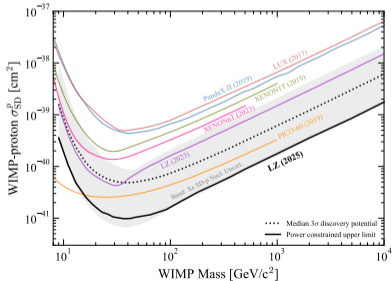
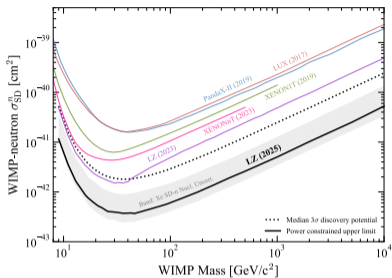
# Existing calculations of SD structure factors



$$u \equiv Q^2 b^2 / 2$$

Fig. from *Klos et al., PRD (2013)*

$\rho, c_3, c_4 \rightarrow$  uncertainty band



- Large uncertainty from  $\rho$  in  $\mathbf{J}_{i,2b}^{\text{eff}}(\rho)$
- Propagate into the WIMP-nucleon cross section calculation

Uncertainty band of *Aalbers et al., PRL (2025)*:

- *Pirinen et al., NPA (2019)*
- *Hoferichter et al., PRD (2020)*
- *Hu et al., PRL (2022)*

all with NO1B 2BC

## Computational setup for $^{19}\text{F}$ , $^{29}\text{Si}$ , $^{129,131}\text{Xe}$ with full leading 2BC

---

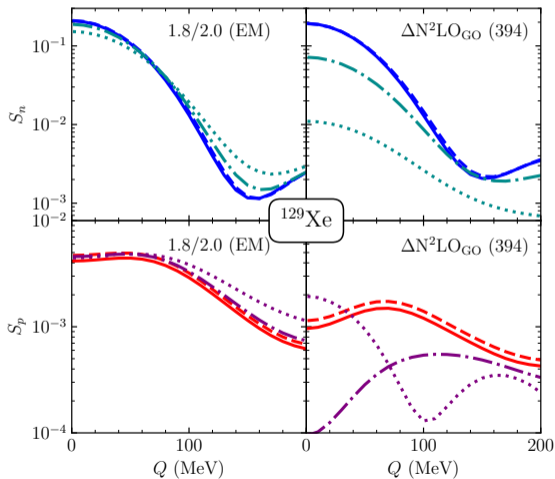
- Multipole decomposition of 2BC using NuHamil by T. Miyagi *Miyagi, EPJA (2023)*
- VS-IMSRG evolution  $\rightarrow H_{\text{eff}}$ ,  $L_{\lambda\mu}^{5,\text{eff}}$ , and  $T_{\lambda\mu}^{\text{el}5,\text{eff}}$  in valence space
- Diagonalize  $H_{\text{eff}}$  in the valence space to get the ground-state wavefunction  $|J\rangle$
- Calculate the nuclear matrix elements  $\langle J||L_{\lambda\mu}^{5,\text{eff}}||J\rangle$  and  $\langle J||T_{\lambda\mu}^{\text{el}5,\text{eff}}||J\rangle$  and therefore the structure factor  $S_{ij}(Q)$  and then  $S_{p,n}(Q)$

# Computational setup for $^{19}\text{F}$ , $^{29}\text{Si}$ , $^{129,131}\text{Xe}$ with full leading 2BC

- NN+3N interactions 1.8/2.0 (EM) and  $\Delta\text{N}^2\text{LO}_{\text{GO}}$  (394) and consistent 2BCs  
*Hebeler et al., PRC (2011) Jiang et al., PRC (2020) Krebs et al., Ann. Phys. (2017) Hoferichter et al., PRD (2020)*
- Basis (build on top of harmonic oscillator basis with  $\hbar\omega = 12$  or 16 MeV):
  - Hartree-Fock (HF): solve HF equation truncated by  $e_{\text{max}}^{\text{HF}} = (2n + l)_{\text{max}}$  *Stroberg et al., PRL (2017)*  
 $e_{\text{max}}^{\text{HF}} = 12$  for  $^{19}\text{F}$ ,  $^{29}\text{Si}$  and  $e_{\text{max}}^{\text{HF}} = 10$  for  $^{129,131}\text{Xe} \rightarrow e_{\text{max}} = e_{\text{max}}^{\text{HF}}$  in VS-IMSRG evolution
  - Natural orbitals (NAT): diagonalize 1B density matrix w/ perturbative corr. *Hoppe et al., PRC (2021)*  
truncated by  $e_{\text{max}}^{\text{NAT}} = 14 \rightarrow e_{\text{max}} = 10$  in VS-IMSRG evolution
- $V_{ijk}^{3\text{N}}$  matrix elements are restricted by  $E_{3\text{max}} = (e_i + e_j + e_k)_{\text{max}} = 24$  *Miyagi et al., PRC (2022)*
- Valence space:
  - $^{19}\text{F}$  and  $^{29}\text{Si}$ : *sd*-shell
  - $^{129,131}\text{Xe}$ :  $\{2s_{1/2}, 1d_{3/2,5/2}, 0g_{7/2}, 0h_{11/2}\}$  (orbitals between the magic numbers 50 and 82)
- Effective Hamiltonian and operators are truncated up to NO2B level *Stroberg et al., PRL (2017)*

# Convergence w.r.t. model-space parameters $\hbar\omega$ and $e_{\max}$ for $^{129,131}\text{Xe}$

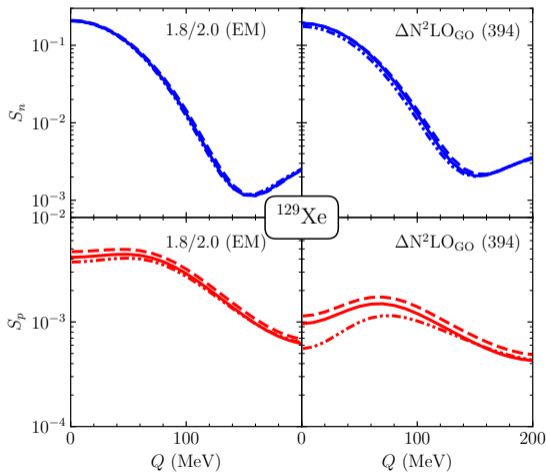
- - - HF,  $\hbar\omega = 12$ ,  $e_{\max} = 8$       ····· HF,  $\hbar\omega = 16$ ,  $e_{\max} = 8$   
 ——— HF,  $\hbar\omega = 12$ ,  $e_{\max} = 10$       - - - HF,  $\hbar\omega = 16$ ,  $e_{\max} = 10$



- **HF basis:**  $e_{\max}^{\text{HF}} = e_{\max}$  in VS-IMSRG evolution
- Faster convergence with  $\hbar\omega = 12$  MeV, especially for  $\Delta N^2\text{LO}_{\text{GO}}$  (394)  
→ **take  $\hbar\omega = 12$  MeV**
- Prohibitively expensive for VS-IMSRG evolution with  $e_{\max} = 12$  in such calculations, since we have to do VS-IMSRG evolution for each momentum  
→ **take  $e_{\max} = 10$  in VS-IMSRG evolution**
- **NAT basis** capture correlations from a larger model space (here  $e_{\max}^{\text{NAT}} = 14$ ) by concentrating their effects into the most important low-lying orbitals, so that a truncated space (here  $e_{\max} = 10$ ) retains more of the relevant physics

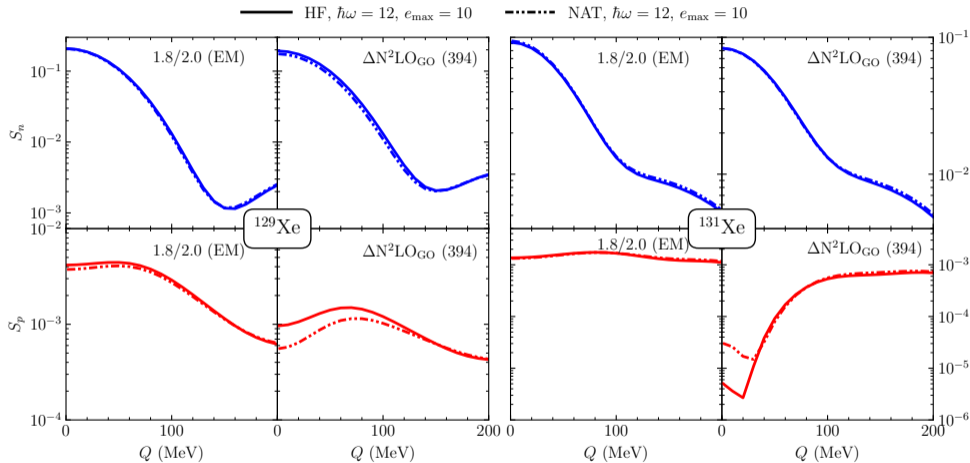
# Convergence w.r.t. model-space parameters $\hbar\omega$ and $e_{\max}$ for $^{129,131}\text{Xe}$

- - - HF,  $\hbar\omega = 12$ ,  $e_{\max} = 8$       - · - · - NAT,  $\hbar\omega = 12$ ,  $e_{\max} = 10$   
 — HF,  $\hbar\omega = 12$ ,  $e_{\max} = 10$



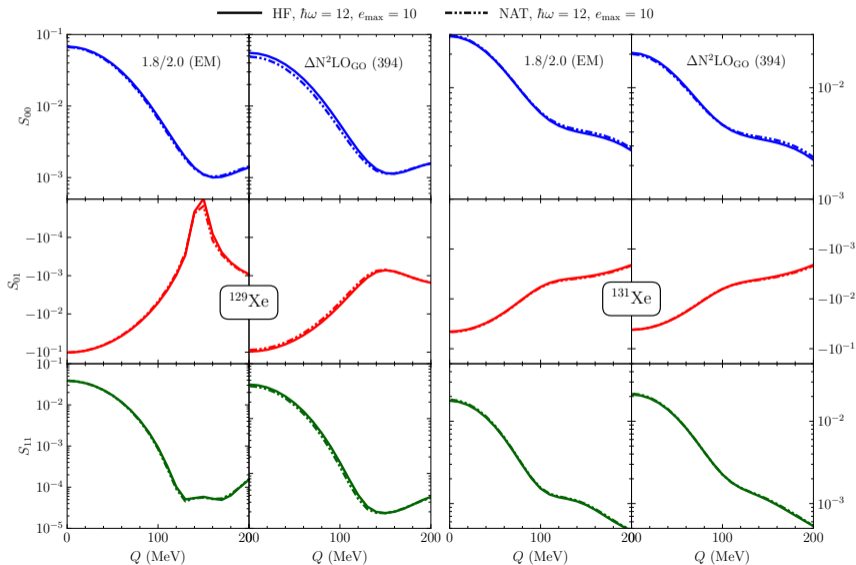
- NAT basis:  $e_{\max}^{\text{NAT}} = 14$   
 →  $e_{\max} = 10$  in VS-IMSRG evolution  
 → captures correlations in the larger model space
- Nice convergence pattern with  $\hbar\omega = 12$  MeV
  - HF basis:  $e_{\max} = 8 \rightarrow e_{\max} = 10$
  - $e_{\max} = 10$ : HF basis → NAT basis
- Slower convergence for  $S_p$  with  $\Delta N^2\text{LO}_{\text{GO}}$  (394)
- Take the spread between HF and NAT basis with  $e_{\max} = 10$  as the uncertainty band

# Convergence w.r.t. model-space parameters $\hbar\omega$ and $e_{\max}$ for $^{129,131}\text{Xe}$



$S_p$  calculated from  $\Delta\text{N}^2\text{LO}_{\text{GO}}$  (394) converges slower

# Convergence w.r.t. model-space parameters $\hbar\omega$ and $e_{\max}$ for $^{129,131}\text{Xe}$



■  $S_{00}$ ,  $S_{01}$ , and  $S_{11}$  are well converged  $\rightarrow$  small uncertainty from model space

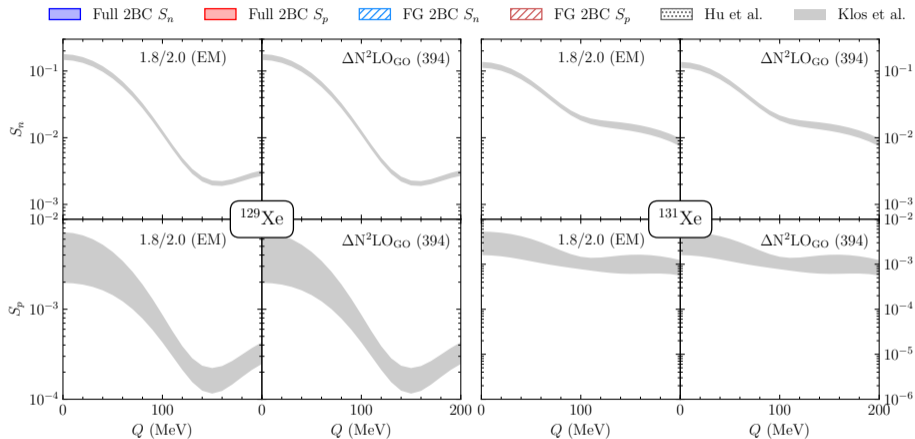
■ The larger uncertainty band for  $S_p$  with  $\Delta N^2 \text{LO}_{\text{GO}}$  (394) is due to the delicate cancellation between positive  $S_{00}(q) + S_{11}(q)$  and negative  $S_{01}(q)$ :

$$S_p(Q) = S_{00}(Q) + S_{11}(Q) + S_{01}(Q)$$

■  $S_n$  is well converged with  $\Delta N^2 \text{LO}_{\text{GO}}$  (394) since

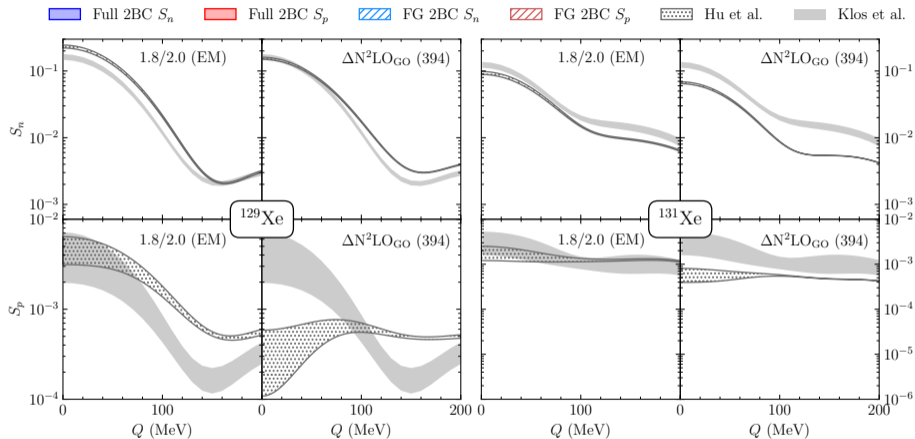
$$S_n(Q) = S_{00}(Q) + S_{11}(Q) - S_{01}(Q)$$

# Structure factors of $^{129}\text{Xe}$ and $^{131}\text{Xe}$ from Klos et al.



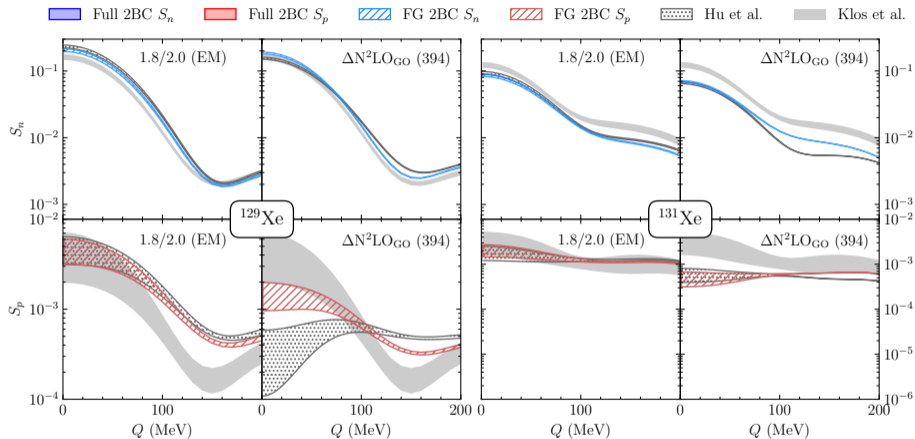
- *Klos et al., PRD (2013)*: phenomenological shell model calculation with NO1B 2BC in FG model

# Structure factors of $^{129}\text{Xe}$ and $^{131}\text{Xe}$ from Klos et al. and Hu et al.



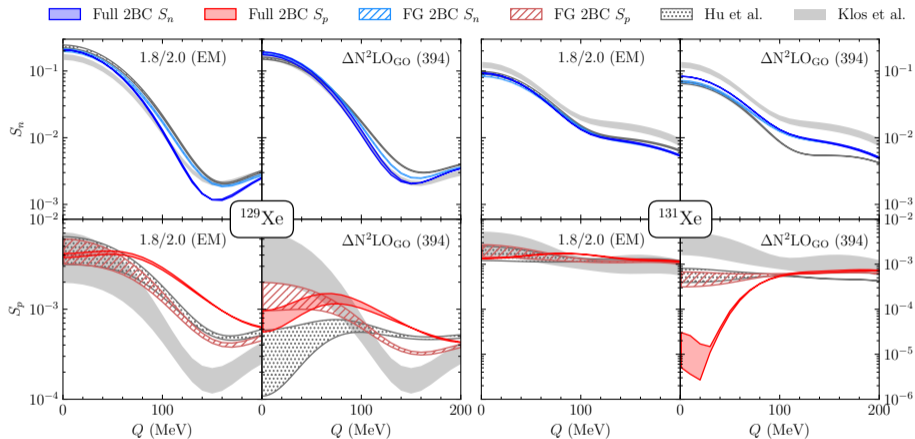
- *Klos et al., PRD (2013)*: phenomenological shell model calculation with NO1B 2BC in FG model
- *Hu et al., PRL (2022)*: *ab initio* calculation using VS-IMSRG with NO1B 2BC in FG model

# Structure factors of $^{129}\text{Xe}$ and $^{131}\text{Xe}$ from NO1B 2BC



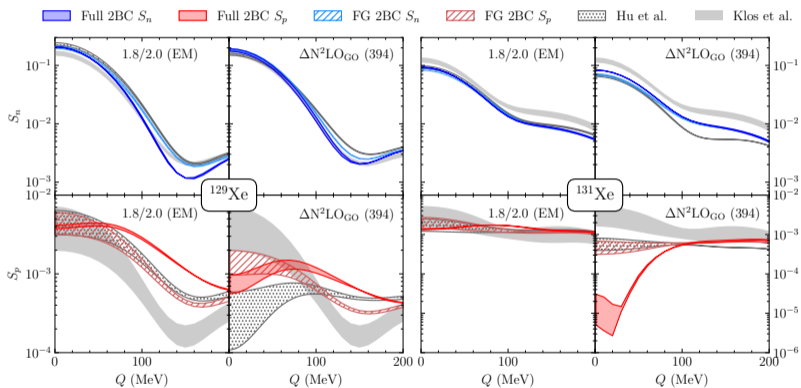
- *Klos et al., PRD (2013)*: phenomenological shell model calculation with NO1B 2BC in FG model
- *Hu et al., PRL (2022)*: *ab initio* calculation using VS-IMSRG with NO1B 2BC in FG model
- FG 2BC  $S_{p,n}$ : Our *ab initio* calculation similar to *Hu et al., PRL (2022)* but with larger model space

# Structure factors of $^{129}\text{Xe}$ and $^{131}\text{Xe}$ from full 2BC



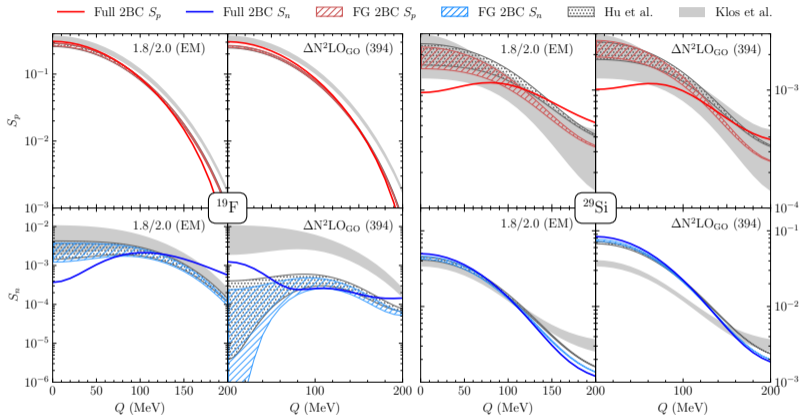
- *Klos et al., PRD (2013)*: phenomenological shell model calculation with NO1B 2BC in FG model
- *Hu et al., PRL (2022)*: *ab initio* calculation using VS-IMSRG with NO1B 2BC in FG model
- FG 2BC  $S_{p,n}$ : Our *ab initio* calculation similar to *Hu et al., PRL (2022)* but with larger model space
- Full 2BC  $S_{p,n}$ : Our *ab initio* calculation using VS-IMSRG with full leading 2BC

# Structure factors of $^{129}\text{Xe}$ and $^{131}\text{Xe}$ from full 2BC



- Xe: even  $Z$  and odd  $N$   
 $\rightarrow$  spin mainly carried by neutrons  
 $\rightarrow S_n > S_p$
- Full leading 2BC  
 $\rightarrow$  no  $\rho$  dependence  
 $\rightarrow$  uncertainty reduction
- The difference between 1.8/2.0 (EM) and  $\Delta N^2\text{LO}_{\text{GO}}$  (394) is much larger than the uncertainty band from the model space  
 $\rightarrow$  UQ for interaction

# Structure factors of $^{19}\text{F}$ and $^{29}\text{Si}$



- Much lighter nuclei, HF basis with  $\hbar\omega = 16$  and  $e_{\text{max}} = 12$  is enough to get converged results
- $^{19}\text{F}$ : odd  $Z \rightarrow S_p > S_n$
- $^{29}\text{Si}$ : odd  $N \rightarrow S_n > S_p$
- Results from 1.8/2.0 (EM) and  $\Delta\text{N}^2\text{LO}_{\text{GO}}$  (394) are quite different  $\rightarrow$  UQ for interaction

# Summary and outlook

---

## Summary

- First *ab initio* calculation of SD nuclear structure factors with full leading 2BC without approximation
- Eliminates the uncertainty associated with  $\rho$  in previous NO1B approximations
- Reduction of uncertainty will propagate into the elastic SD WIMP-nucleon scattering analysis

## Outlook

- Study the impact of the uncertainty reduction of nuclear structure to the limits of elastic SD WIMP-nucleon cross section
- Quantify the uncertainty arising from nuclear interaction and higher-order 2BCs

# Summary and outlook

## Summary

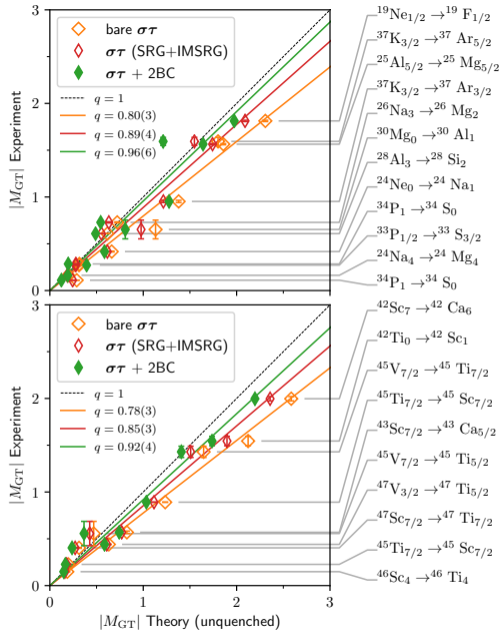
- First *ab initio* calculation of SD nuclear structure factors with full leading 2BC without approximation
- Eliminates the uncertainty associated with  $\rho$  in previous NO1B approximations
- Reduction of uncertainty will propagate into the elastic SD WIMP-nucleon scattering analysis

## Outlook

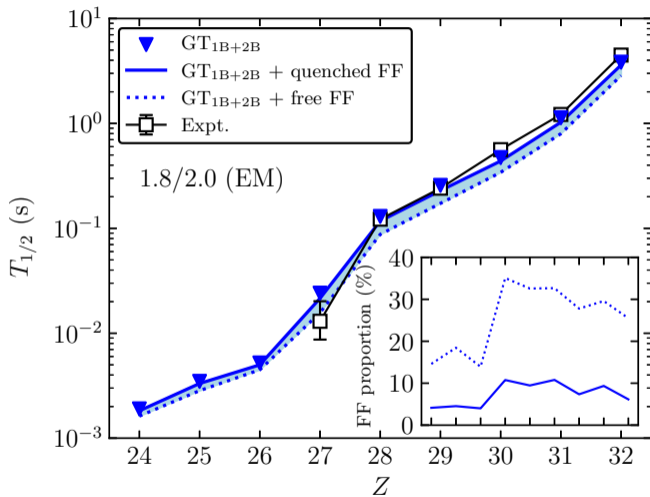
- Study the impact of the uncertainty reduction of nuclear structure to the limits of elastic SD WIMP-nucleon cross section
- Quantify the uncertainty arising from nuclear interaction and higher-order 2BCs

**Thank you for your attention!**

## Backup Slides



# VS-IMSRG calc. of $\beta$ -decay half-lives



# Total half-life $T_{1/2}$ of $\beta$ -decay

- Total  $\beta^-$ -decay half-life from initial ground state:

$$T_{1/2}^{-1} = \sum_f t_{fi}^{-1}$$

$$t_{fi}^{-1} = \frac{1}{\kappa} \int_1^{W_0} C(W) F(Z, W) \sqrt{W^2 - 1} W (W_0 - W)^2 dW$$

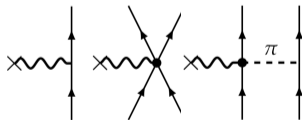
- Gamow-Teller (GT) transition (dominates)

$$C_{GT}(W) = B(GT) = \frac{1}{(2J_i + 1)} |\langle \Psi_f(J_f) || GT || \Psi_i(J_i) \rangle|^2$$

$$t_{fi}^{-1} = \frac{1}{\kappa} B(GT) f_0$$

$$f_0 = \int_1^{W_0} F(Z, W) \sqrt{W^2 - 1} W (W_0 - W)^2 dW$$

$$GT_{1B} = \sum_{k=1}^A g_A \vec{\sigma}_k \tau_k^-, \quad GT_{2B} = \sum_{i < j}^A A_{ij}^-$$



Park et al., PRC 67 (2003) 055206

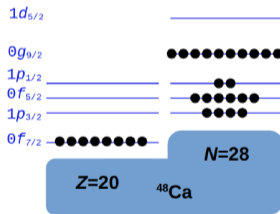
Menéndez, Gazit and Schwenk, PRL 107 (2011) 062501

Krebs, EPJA 56 (2020) 234

# Computational setup for $N = 50$ isotones

- “Magic” 1.8/2.0 (EM) with NN + 3N interactions, consistent 2B currents
- Hartree-Fock basis  $\hbar\omega = 16$  MeV,  $e_{\max} \equiv (2n + l)_{\max} = 14$ ,  
 $E_{3\max} \equiv (e_1 + e_2 + e_3)_{\max} = 24$
- VS-IMSRG(2), NO2B approximation with ensemble reference
- $\mathbb{P}$ : core  $^{48}\text{Ca}$  + valence space  $\{0f_{7/2,5/2}^p, 1p_{3/2,1/2}^p, 0f_{5/2}^n, 1p_{3/2,1/2}^n, 0g_{9/2}^n, 1d_{5/2}^n\}$

- Arctangent (White) generator with  $\Delta = 5$  MeV



- $H' = H + \beta H_{\text{cm}}$ ,  $\beta = 3$

- Effective Hamiltonian  $H_{\text{eff}} = [U(s)H'U^\dagger(s)]_{s \rightarrow \infty}$

- Reference state from initial nucleus to evolve GT operator  $\text{GT}_{\text{eff}} = [U(s)\text{GT}U^\dagger(s)]_{s \rightarrow \infty}$

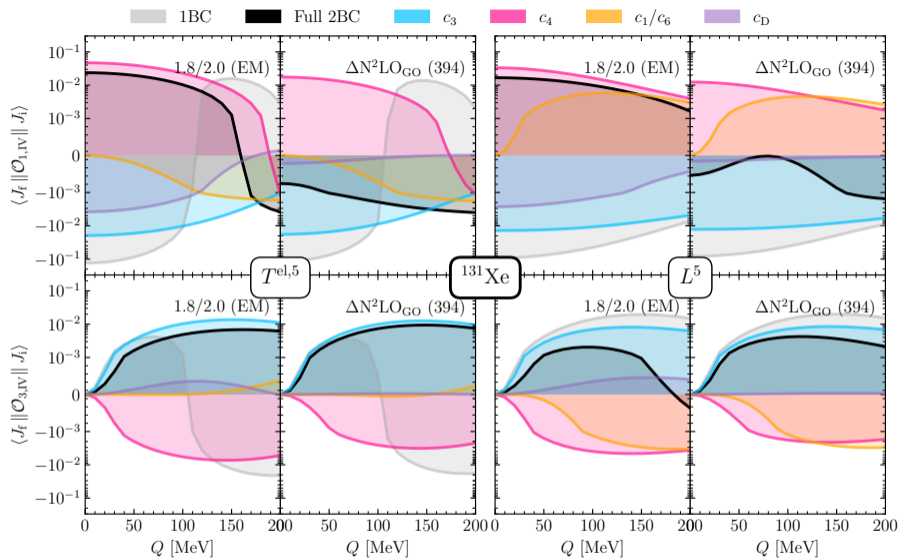
- Lanczos strength function method in the calculation of total GT transition probability

1.8/2.0 (EM): Hebeler et al., PRC 83 (2011) 031301

VS-IMSRG(2): Stroberg et al., PRL 118 (2017) 032502

Multi-shell valence space: Miyagi et al., PRC 102 (2020) 034320

Lanczos strength function: Haxton et al., PRC 72 (2005) 065501



$c_3$  and  $c_4$  terms dominate



# Ground-state energies and spectra for $^{129}\text{Xe}$ and $^{131}\text{Xe}$

