Electroweak reactions with QMC methods

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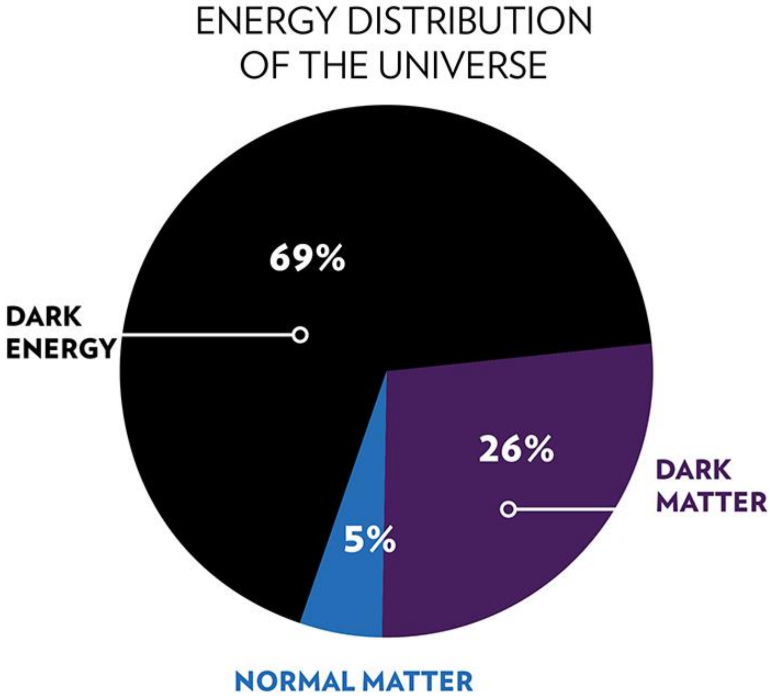
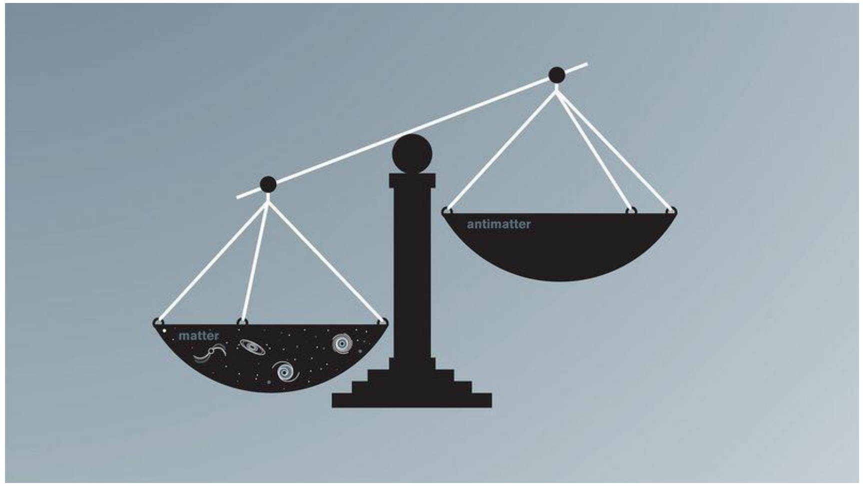
Motivation

Fermi Lab / Sandbox Studio, Chicago



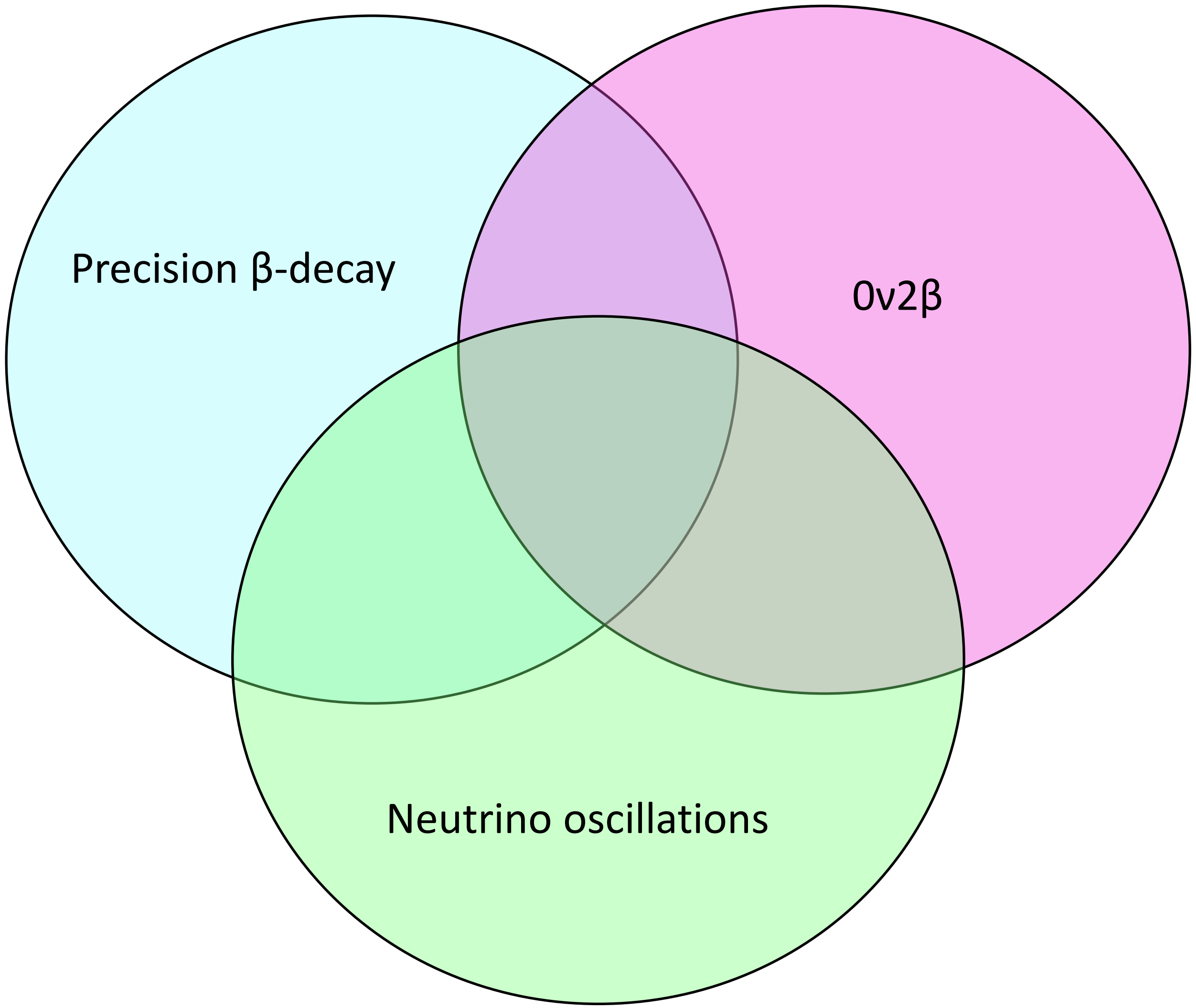
NASA / Chandra X-ray Center/ K. Divona



Symmetry Magazine / Sandbox Studio, Chicago

Nuclei for new physics

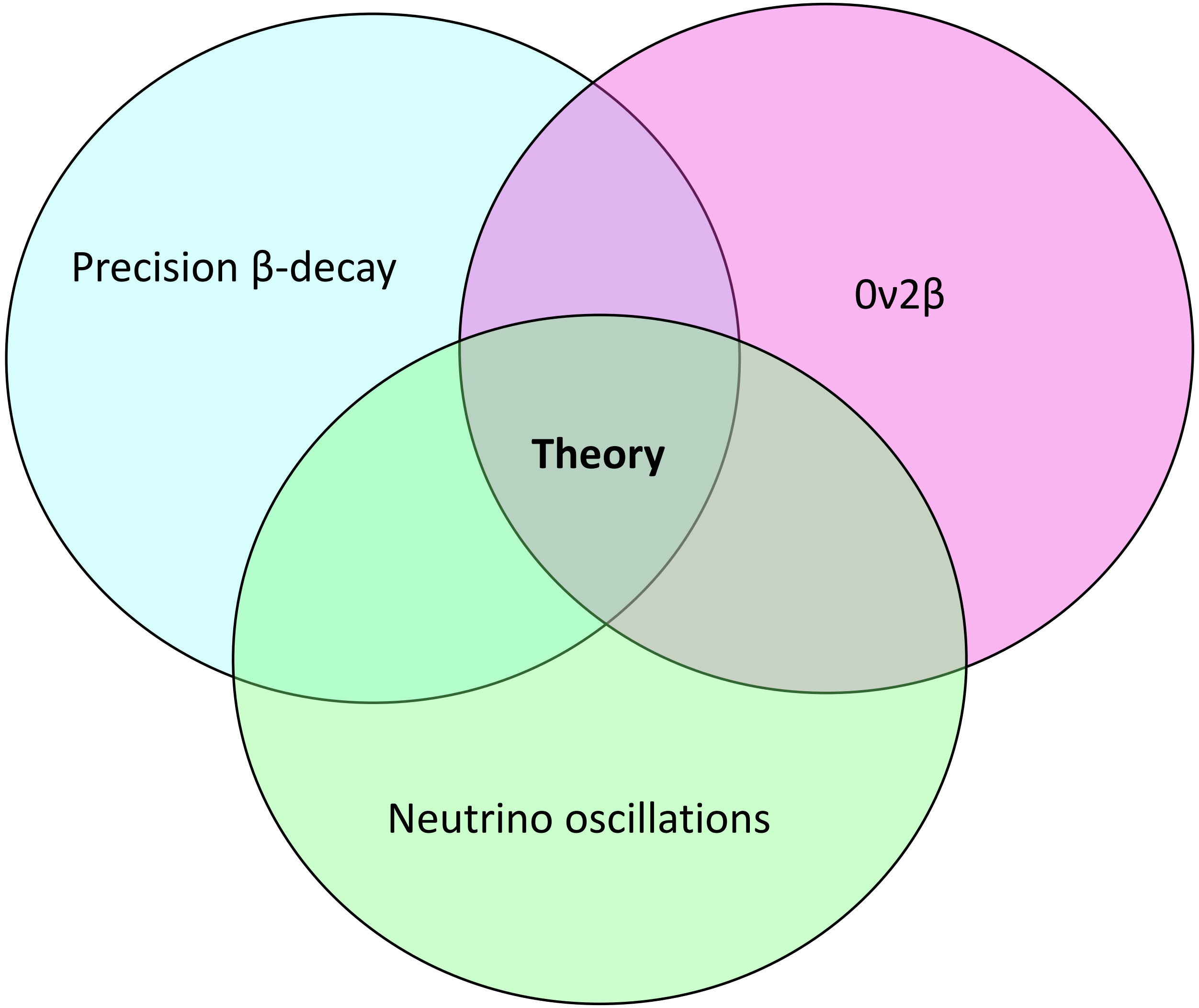
On-going effort to measure **Standard Model (SM) allowed**, **SM forbidden**, and **known beyond SM** phenomena to better understand new physics



Nuclei for new physics

On-going effort to measure Standard Model (SM) allowed, SM forbidden, and known beyond SM phenomena to better understand new physics

Nuclear theory needed to aid in the interpretation of new physics

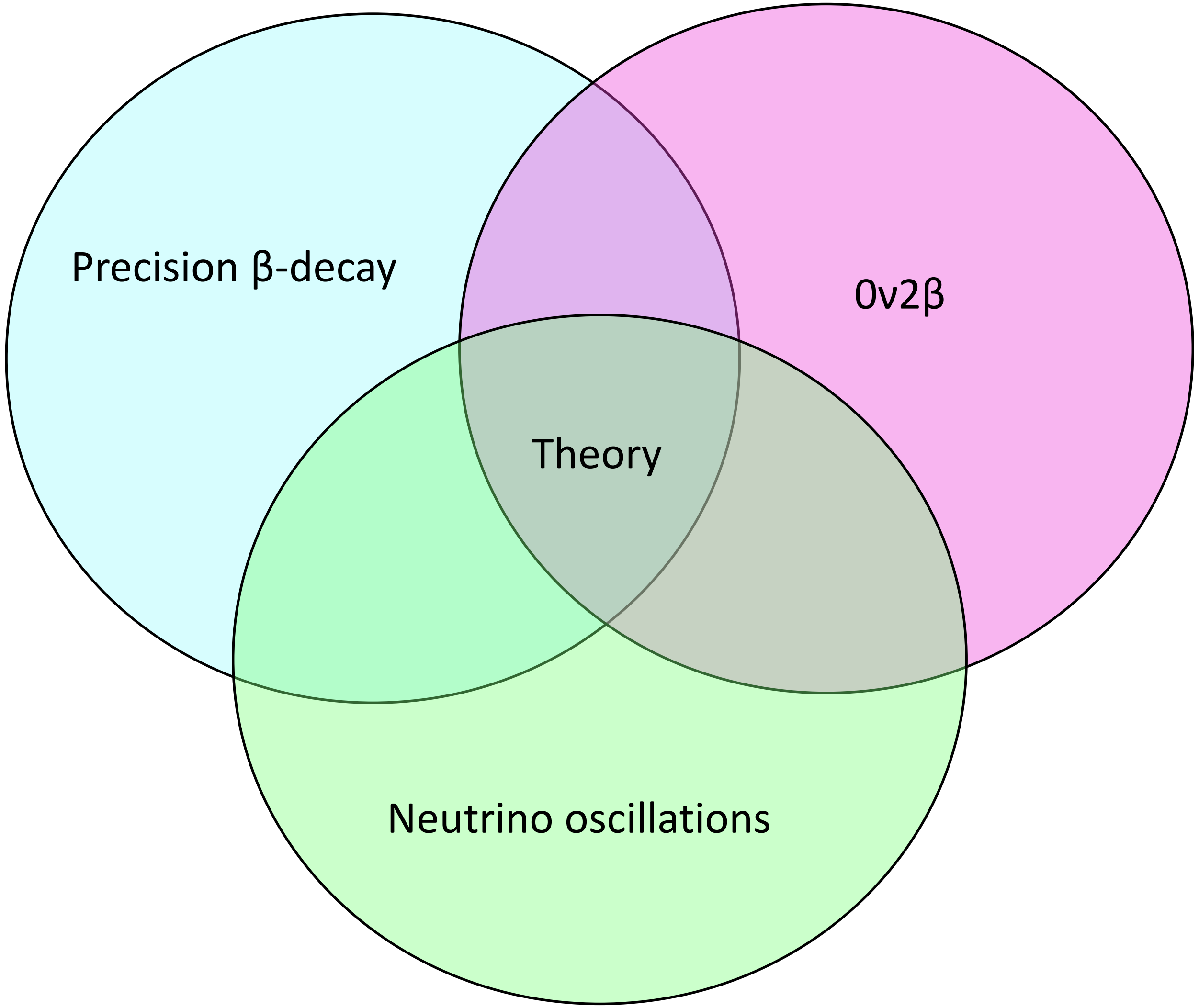


Nuclei for new physics

On-going effort to measure **Standard Model (SM) allowed**, **SM forbidden**, and **known beyond SM** phenomena to better understand new physics

Nuclear theory needed to aid in the interpretation of new physics

Need an accurate and predictable model of nuclear physics at all relevant kinematics



Outline

- Microscopic description of nuclei
  - The many-body problem
  - Quantum Monte Carlo methods
  - The NV2+3 nuclear model
- Model validation
  - β-decay matrix elements
  - Magnetic structure (moments, form factors)
  - Muon capture rates
- Prediction of the ^{6}He β-decay spectrum

Recent review:

King and Pastore, arXiv:2402.06602 (*accepted Ann. Rev. Nucl. Part. Sci.)*

Microscopic description of nuclei

Comprehensive theory that describes quantitatively and predictably nuclear structure and reactions in terms of nucleon degrees of freedom

Requirements:

- A **computational method** to solve the nuclear many-body problem and compute observables
- An accurate understanding of the interactions/correlations between nucleons in pairs, triplets, … **(two- and three-nucleon forces)**
- An accurate understanding of the electroweak interactions of external probes (electrons, neutrinos, photons) with nucleons, correlated pairs of nucleons, … **(one- and two-body electroweak charges and currents)**

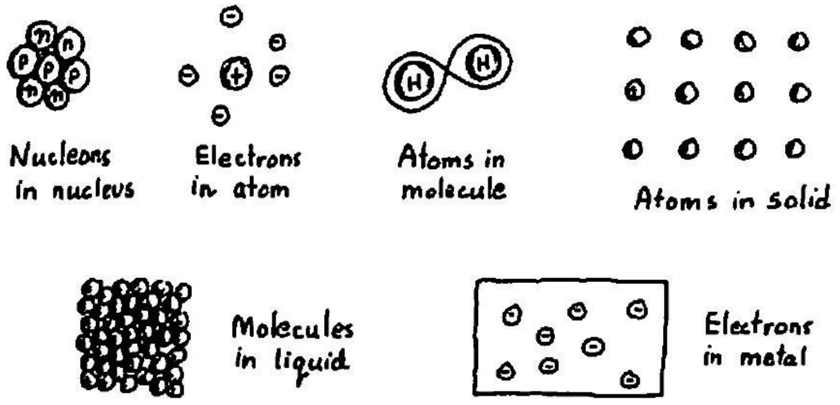
Quantum many-body problem

Modeling physical phenomena in a system with many bodies interacting amongst themselves

$$H = \sum_i T_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \dots$$

Interaction generates *correlations* in solution of the Schrödinger equation

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



Mattuck, “A Guide to Feynman Diagrams in the Many-Body Problem”, McGraw-Hill

Several approaches in nuclear physics:

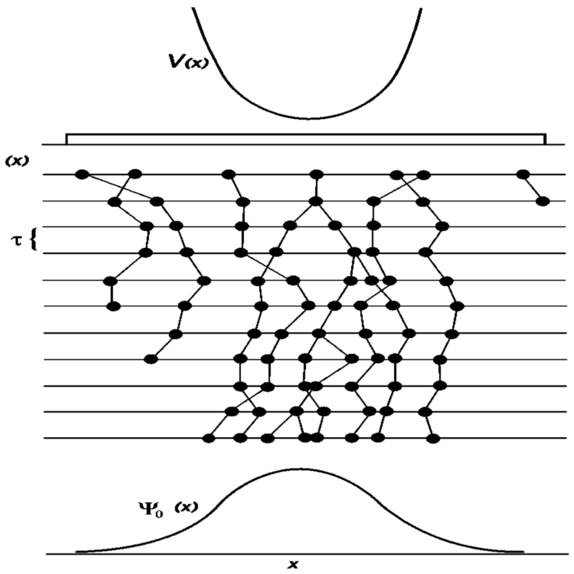
Quantum Monte Carlo, No-core shell model (NCSM), couple cluster, …

Quantum Monte Carlo (QMC)

Solving the many-body problem by stochastically solving the Schrödinger equation

Variational MC wave function $|\Psi_T\rangle = \mathcal{F}|\Phi\rangle$ contains model wave function and many-body correlations optimized by minimizing:

$$E_V = \min\left\{\frac{\langle\Psi_T|H|\Psi_T\rangle}{\langle\Psi_T|\Psi_T\rangle}\right\} \geq E_0$$



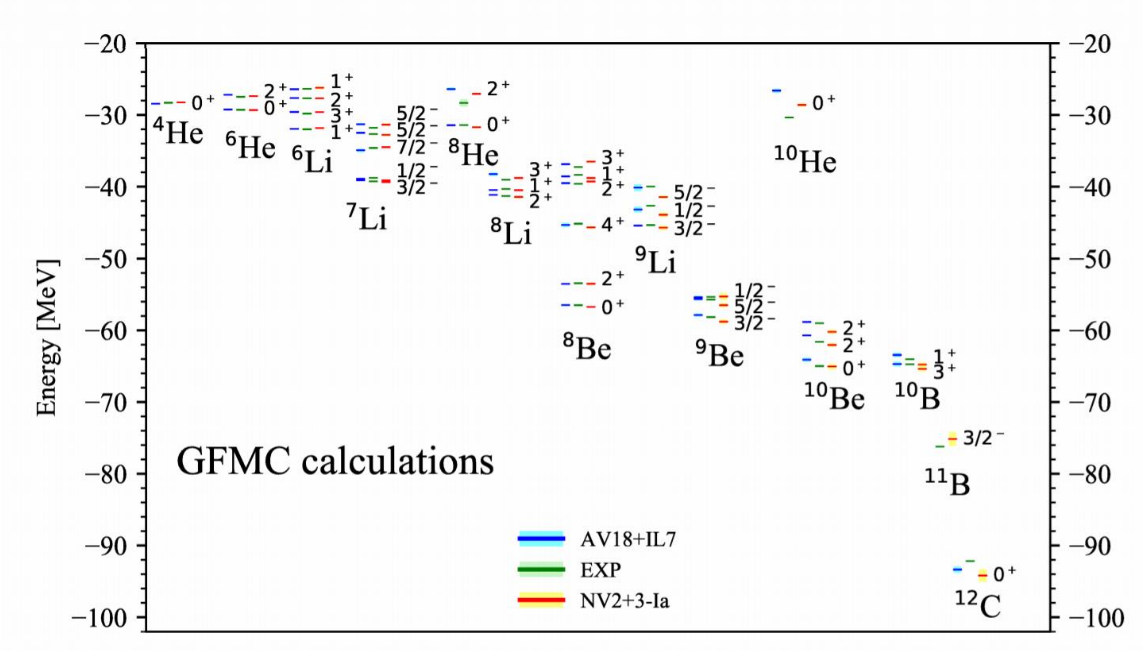
Green's function MC improves by ***removing excited state contamination*** ***and gives the exact ground state***

$$\lim_{\tau\to\infty} e^{-(H-E_0)\tau}\Psi_V = \lim_{\tau\to\infty} e^{-(H-E_0)\tau}\left(c_0\psi_0 + \sum_{i=1}^{N} c_i\psi_i\right) \to c_0\psi_0$$

Foulkes et al. Rev. Mod. Phys. 73, 33 (2001)

The Norfolk (NV2+3) interaction

$$H = \sum_i K_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$



Model derived from χEFT with pion, nucleon, and delta degrees of freedom

NV2 contains 26 unknown LECs in contacts, two more from the NV3

Eight model classes arrived at from different procedures to constrain the unknown LECs

Piarulli et al. PRL 120, 052503 (2018)

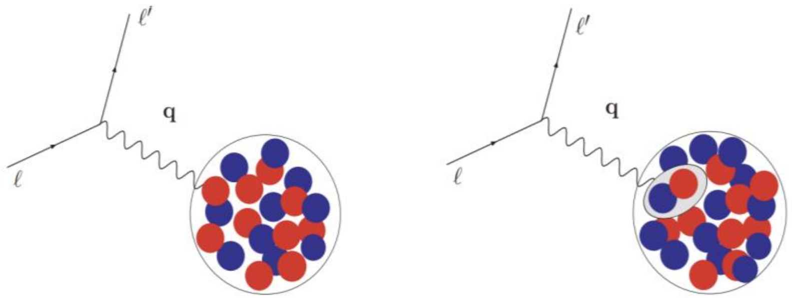
Electroweak charge and currents

Need nuclear electroweak charge and current operators as well

Schematically:

$$\rho = \sum_{i=1}^{A} \rho_i + \sum_{i<j} \rho_{ij} + \ldots$$
$$\mathbf{j} = \sum_{i=1}^{A} \mathbf{j}_i + \sum_{i<j} \mathbf{j}_{ij} + \ldots$$

External field interacts with single nucleons and correlated pairs of nucleons



Pastore et al. PRC 80, 034004 (2009), Pastore et al. PRC 84, 024001 (2011), Piarulli et al. PRC 87, 014006 (2013), Schiavilla et al. PRC 99, 034005 (2019), Baroni et al. PRC 93, 049902 (2016), …

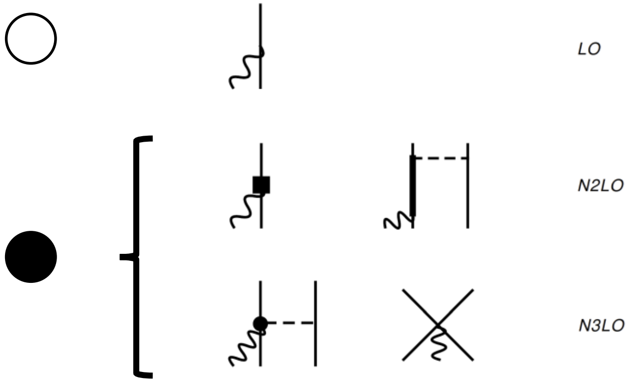
Model Validation

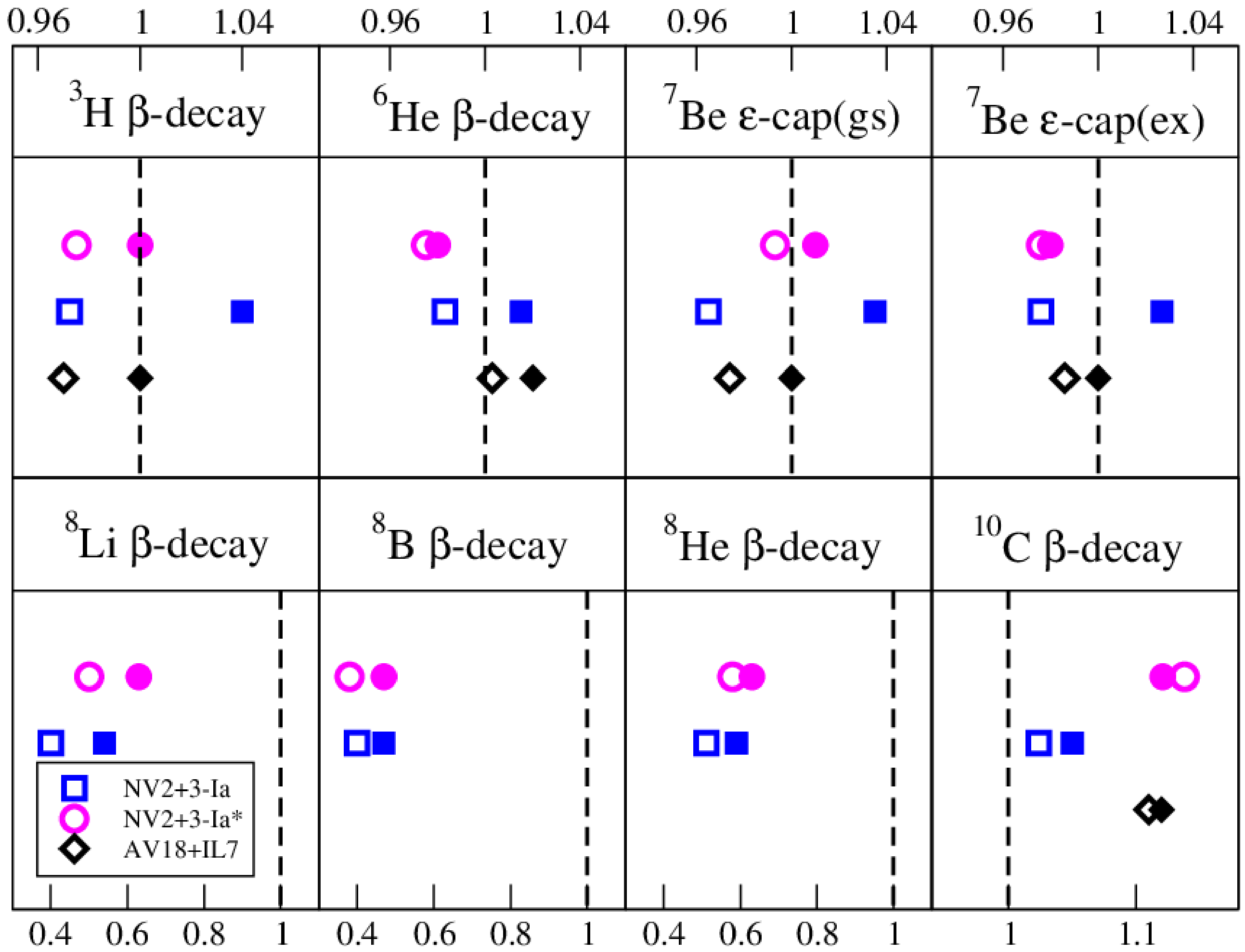
Beta-decay: Gamow-Teller matrix elements

Calculations with NV2+3-Ia* and NV2+3-Ia compared to AV18+IL7 (◊) and exp (dashes)

Correlations provide bulk of quenching

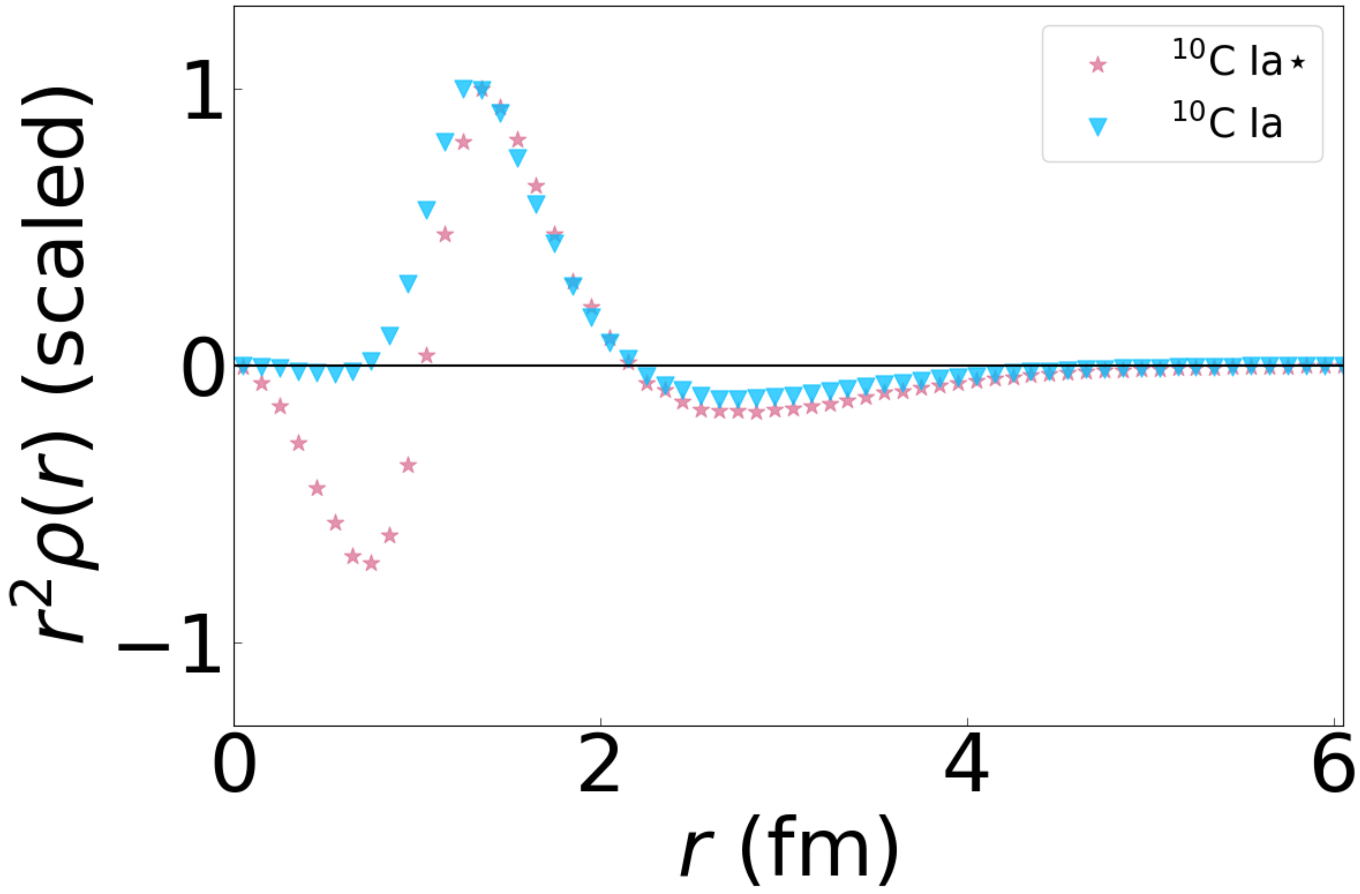
Two-body almost always enhances





King et al. PRC 121, 025501 (2020)

Beta-decay: two-body densities



Different approaches to fitting the NV2+3 can result in different short-range behavior

This alters the total two-body contribution depending on the model

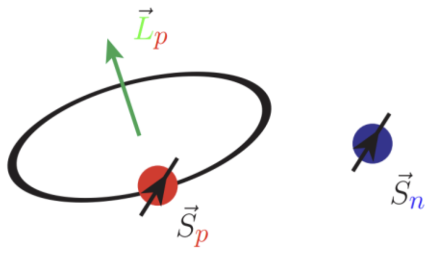
$$M_{\mathrm{GT}}^{\mathrm{2b}} = \int dr_{ij} 4\pi r_{ij}^2 \rho_{\mathrm{GT}}^{\mathrm{2b}}(r_{ij})$$

King et al. PRC 121, 025501 (2020)

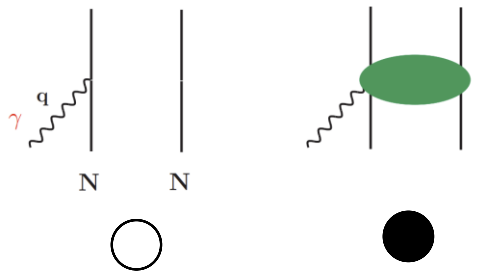
Magnetic structure: two-body currents

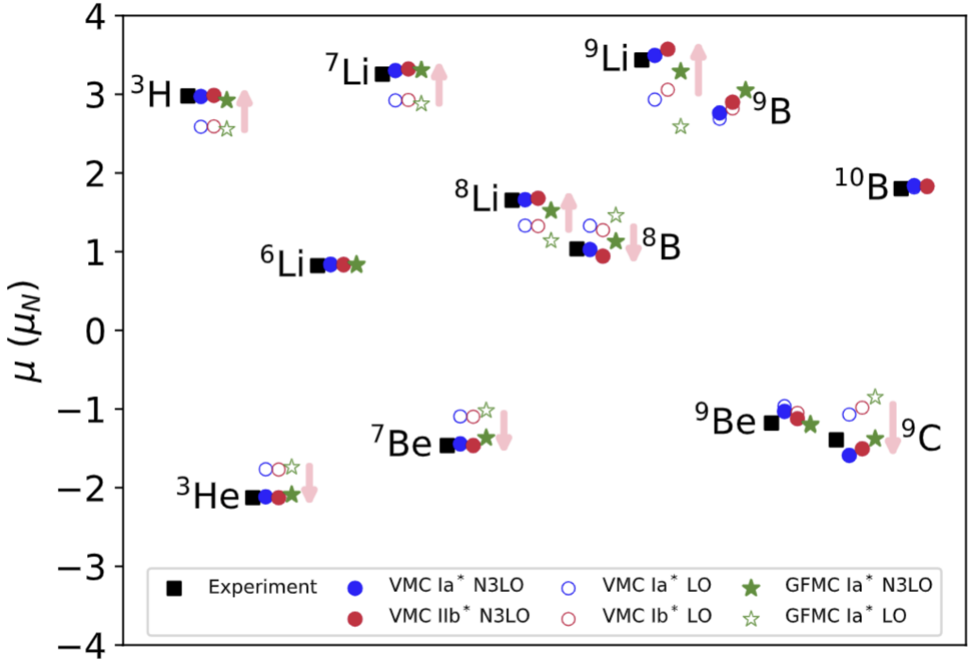
One-body picture:

$$\mu^{LO} = \sum_i \left(L_{i,z} + g_p S_{i,z}\right) \frac{1+\tau_{3,i}}{2} + g_n S_{i,z} \frac{1-\tau_{3,i}}{2}$$



Two-body currents can play a large role (up to ~33%) in describing magnetic dipole moments





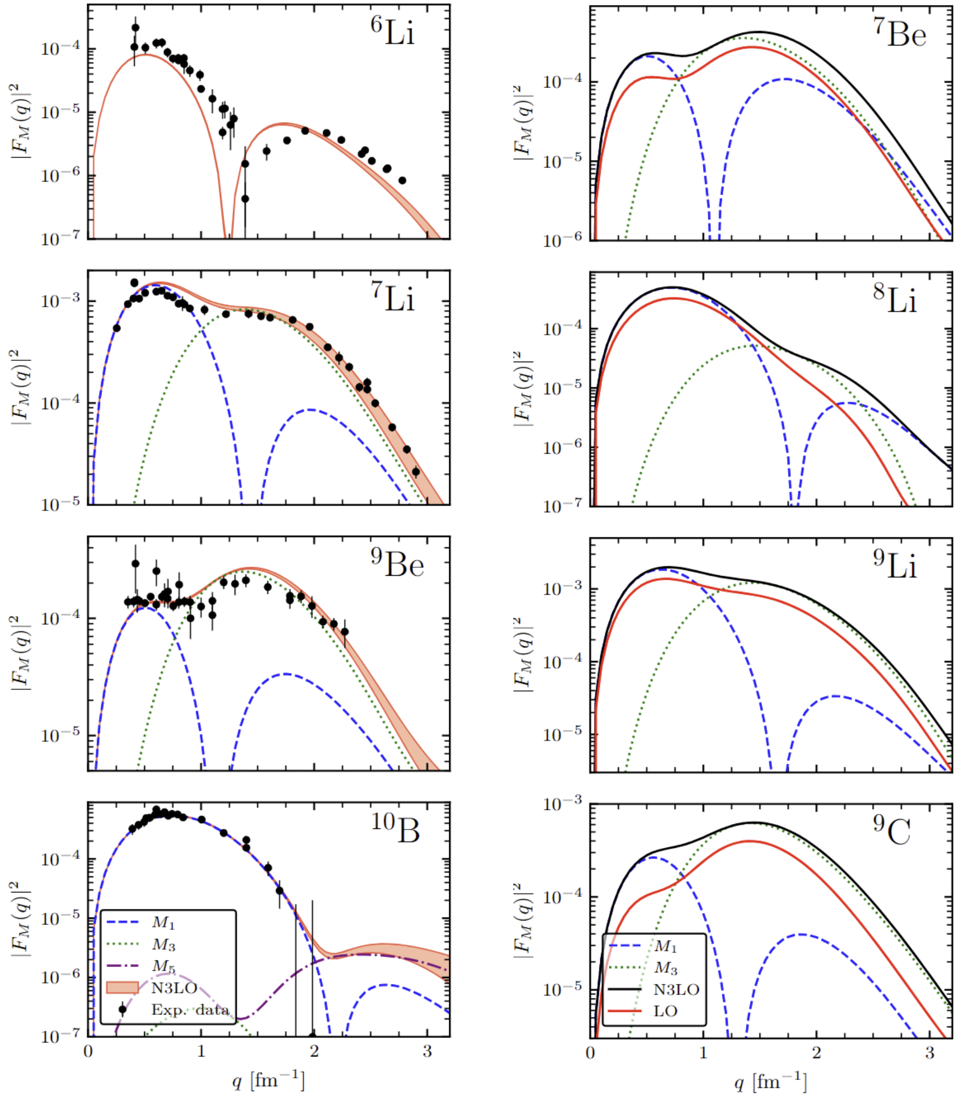
Chambers-Wall, Gnech, King et al. arXiv:2407.03487, arXiv:2407. …

Magnetic structure: form factors

NV2+3-IIb* is able to capture the shape of magnetic form factor

In some cases, good quantitative agreement at large momentum transfer

Two-body effects ~20% to 50% at large momentum transfer in various radioisotopes



Chambers-Wall, Gnech, King et al.
arXiv:2407.03487, arXiv:2407. …

Prediction: ^{6}He β-decay spectrum

^{6}He beta decay spectrum: Overview

Differential rate:

$$d\Gamma_\beta = |M_\beta(q)|^2 \times (\text{kinematic factors})$$

In the $q \to 0$ limit:

$$\frac{d\Gamma_\beta}{dE_e} = \frac{d\Gamma_0}{dE_e}\left[1 + b\frac{m_e}{E_e}\right]$$

SM ($q \to 0$):

$$b = 0$$

Vector
Scalar → **Fermi**

Axial
Tensor
Pseudoscalar → **GT**

^{6}He beta decay spectrum: Overview

Differential rate: $$d\Gamma_\beta = |M_\beta(q)|^2 \times (\text{kinematic factors})$$

In the $q \to 0$ limit: $$\frac{d\Gamma_\beta}{dE_e} = \frac{d\Gamma_0}{dE_e}\left[1 + b\frac{m_e}{E_e}\right]$$

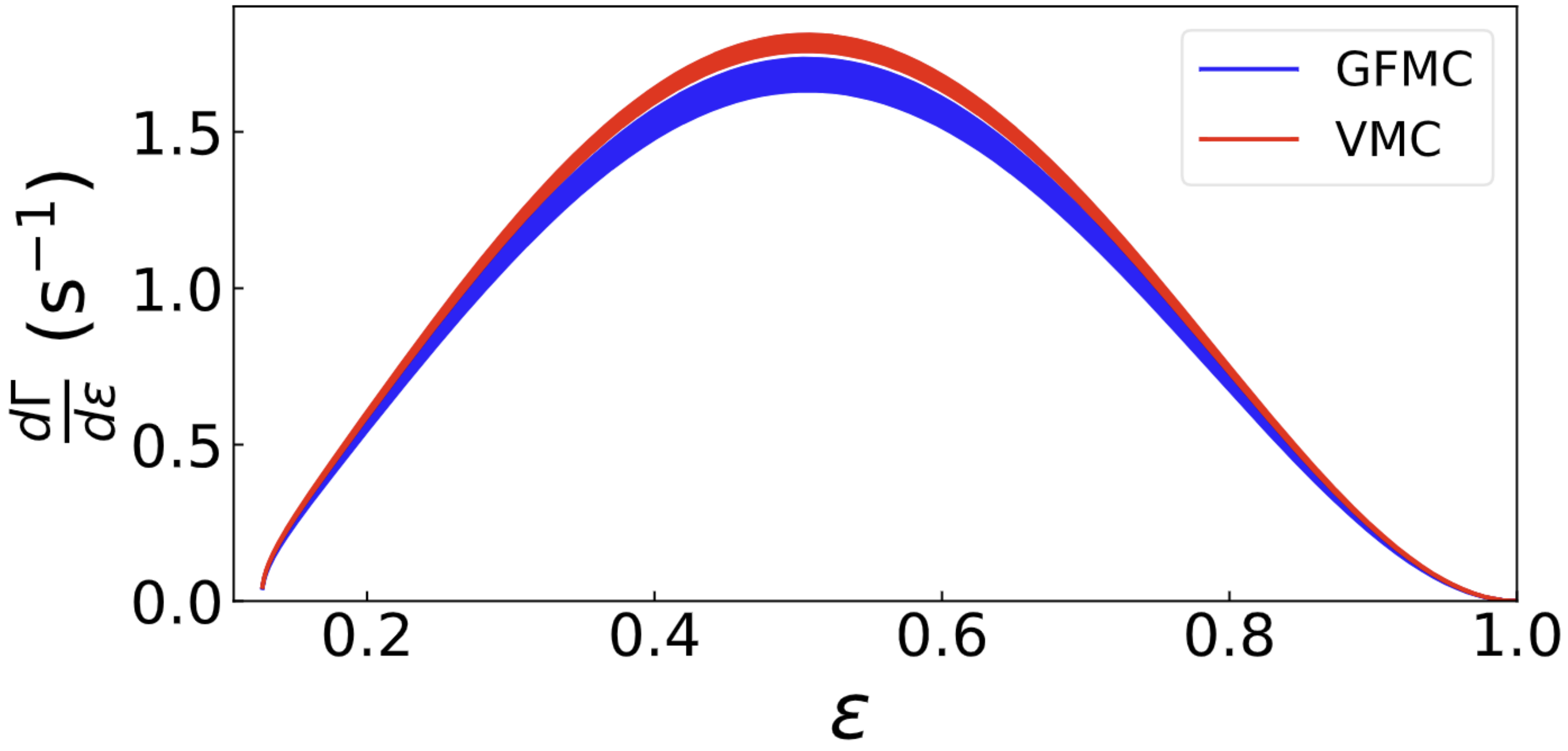
SM ($q \to 0$): $$b = 0$$

SM (with recoil): $$b = 0 + \Delta b$$

Vector
Scalar
→ **Fermi**

Axial
Tensor
Pseudoscalar
→ **GT**

^{6}He beta decay spectrum: SM results



τ_{VMC} = 762 +/- 11 ms

τ_{GFMC} = 808 +/- 24 ms

$\tau_{Expt.}$ = 807.25 +/- 0.16 +/- 0.11 ms

[Kanafani et al. PRC 106, 045502 (2022)]

$$\varepsilon = \frac{E_e}{W_0}$$

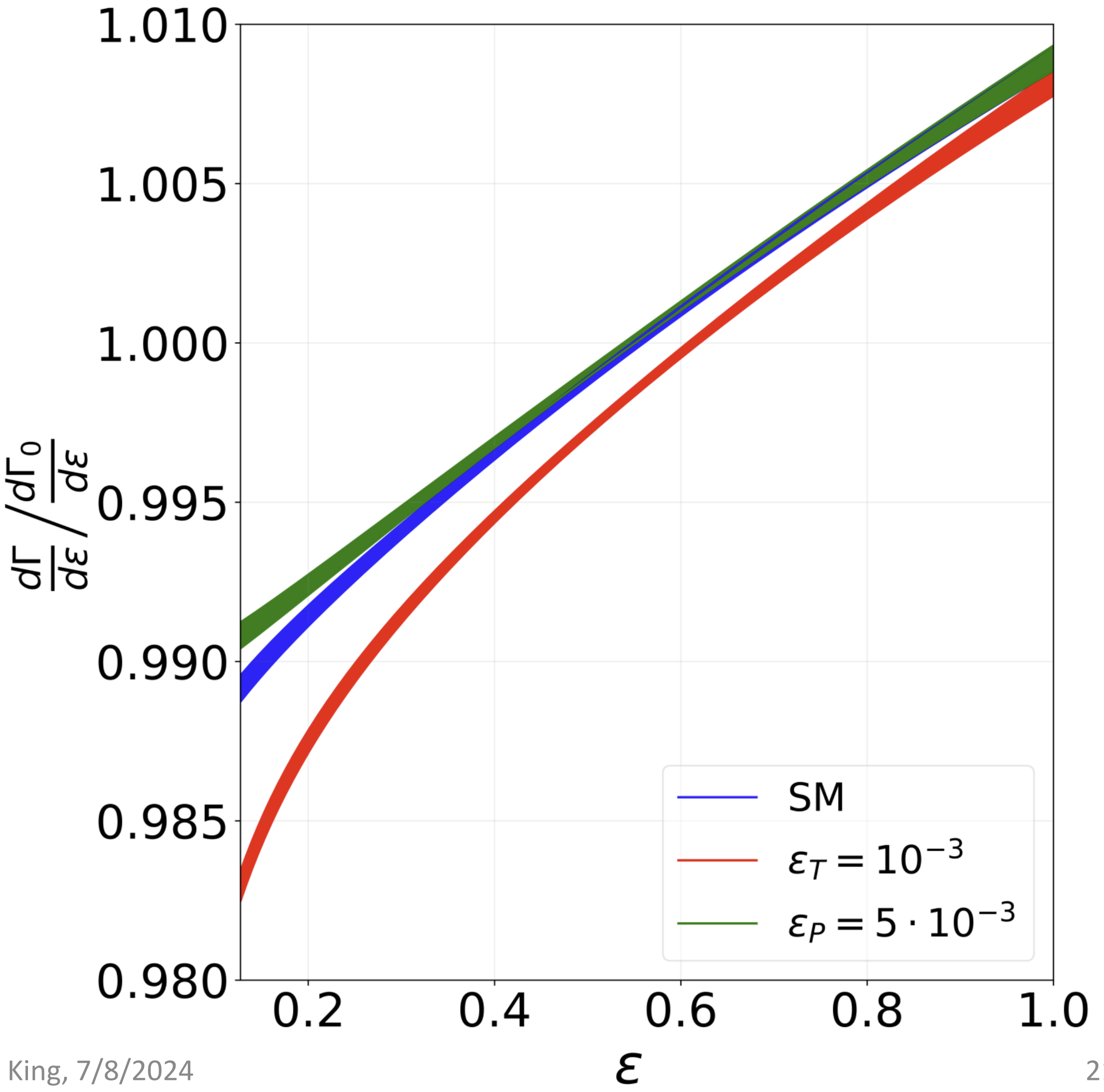
King et al. PRC 107, 015503 (2023)

^{6}He beta decay spectrum: BSM connections

Include new physics with strengths ϵ_i allowed from current analyses

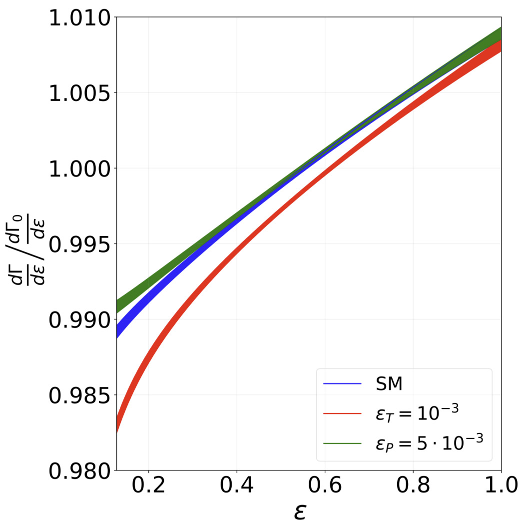
With permille precision, it will be possible to further constrain new physics

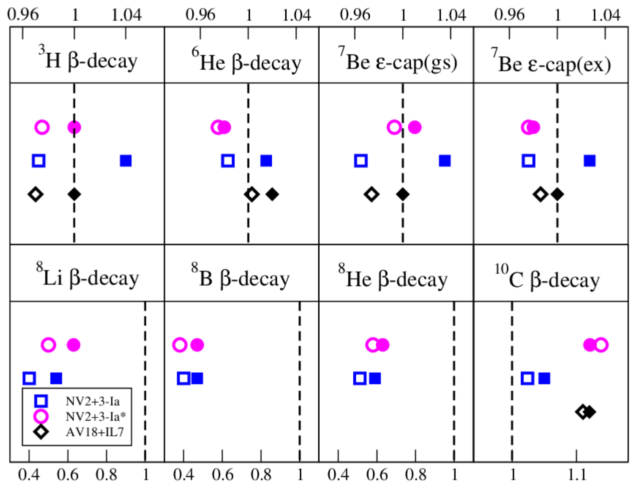
$$\Lambda_{\text{BSM}} \sim \frac{\Lambda_{\text{EW}}}{\sqrt{\epsilon_i}} \sim 1\text{–}10\ \text{TeV}$$

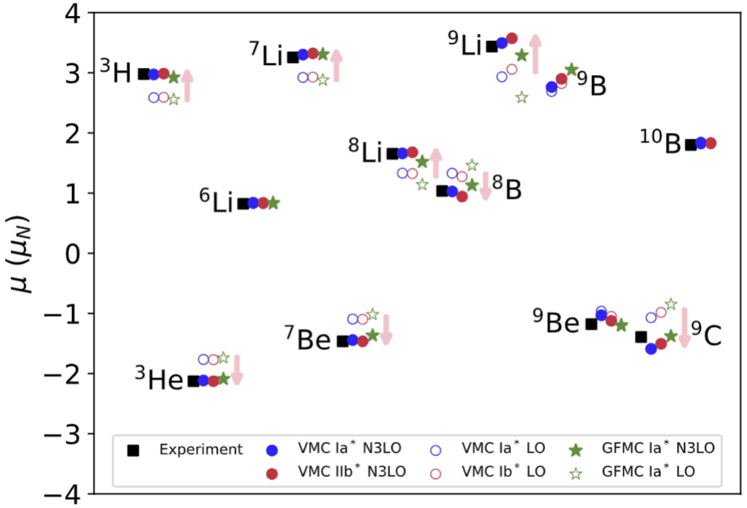


King et al. PRC 107, 015503 (2023)

Conclusions







Many-body plus χEFT is a powerful to understand the impact of the nuclear dynamics on electroweak structure

Impact of different approaches to fitting potential, currents on observables

Ad-hoc uncertainty estimations have been performed for the model, but more robust UQ increasingly important (see Maria's talk Thu)

Future: neutrino-nucleus scattering, radiative corrections to beta decay

Acknowledgements

WU NS: Bub (GS), Chambers-Wall (GS), Andreoli (former), Flores (PD), McCoy (former), Novario (PD), Pastore (PI), Piarulli (PI)

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LANL: Carlson, Gandolfi, Mereghetti

LPC Caen: Hayen

ORNL: Baroni

UW: Cirigliano

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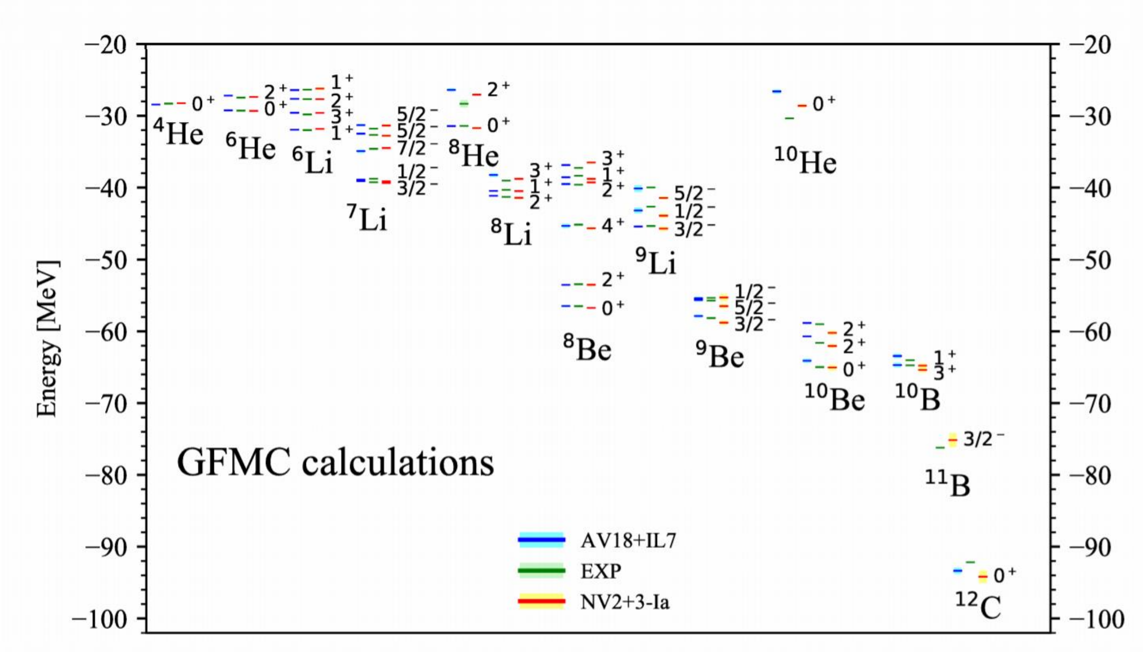
STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

Additional Slides

The Norfolk (NV2+3) Interaction

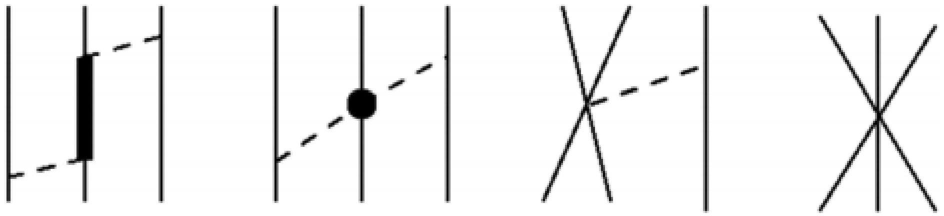
$$H = \sum_i K_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$



Piarulli et al. PRL 120, 052503 (2018)

Eight different Model classes:

- I [II]: NN scattering to fit two-body interaction from 0 to 125 [200] MeV
- a [b]: Long- and short-range regulators (R_L,R_S) = (1.2 fm, 0.8 fm) [(1.0 fm, 0.7 fm)]
- Unstarred: Three-body term constrained with strong data only
- Star: Three-body term constrained with strong and weak data



Variational Monte Carlo (VMC)

$$|\Psi_T\rangle = \left[\mathcal{S}\prod_{i<j}(1 + U_{ij} + \sum_{k\neq i,j} U_{ijk})\right]\left[\sum_{i<j} f_c(r_{ij})\right]|\Phi_A(JMTT_z)\rangle$$

Slater determinant of nucleons in s- and p-shell coupled to the appropriate quantum numbers

Pair correlation operator encoding appropriate cluster structure

Two- and three-body correlation operator to reflect impact of nuclear interaction at short distances

Omptimize when you minimize:

$$E_V = \frac{\langle\Psi_V|H|\Psi_V\rangle}{\langle\Psi_V|\Psi_V\rangle} \geq E_0$$

Carlson et al. Rev. Mod. Phys. 87, 1607 (2015)

Green's Function Monte Carlo (GFMC)

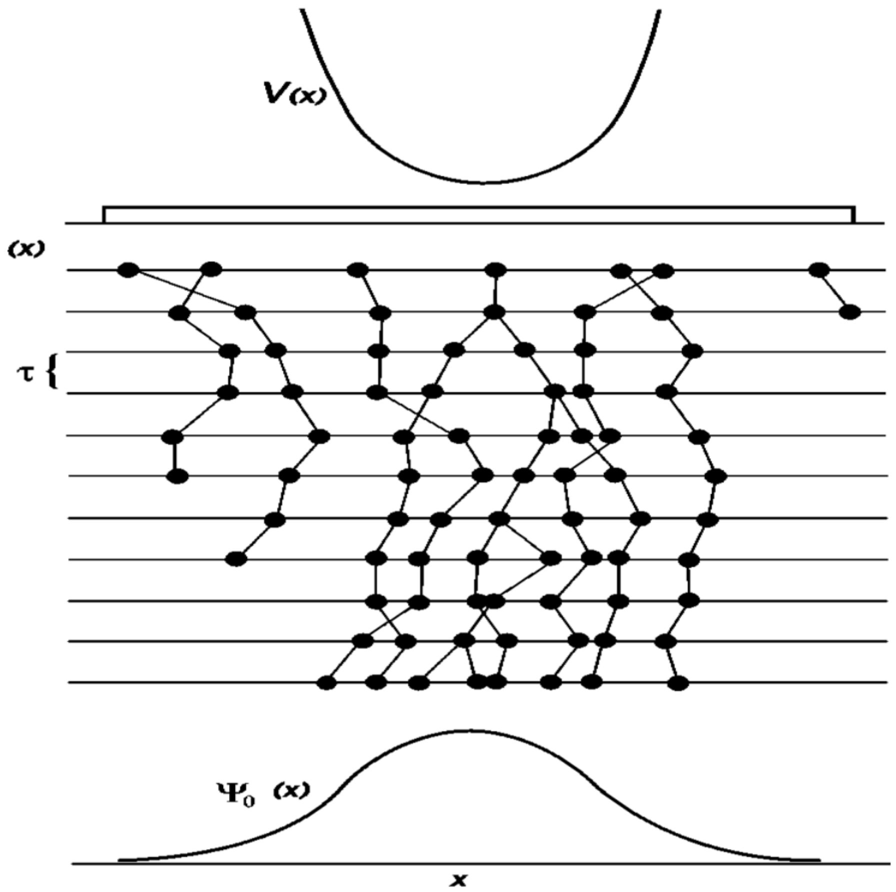
Can expand in exact states *H:* $|\Psi_V\rangle = c_0\psi_0 + \sum_{i=1}^{n} c_n|\psi_n\rangle$

Imaginary time propagation***:***

$$\Psi(\tau) = e^{-(H-E_0)\tau}\Psi_V = \left[e^{-(H-E_0)\Delta\tau}\right]^n \Psi_V$$

Removes excited state contamination and gives the exact ground state

$$\lim_{\tau\to\infty} e^{-(H-E_0)\tau}\Psi_V \to c_0\psi_0$$

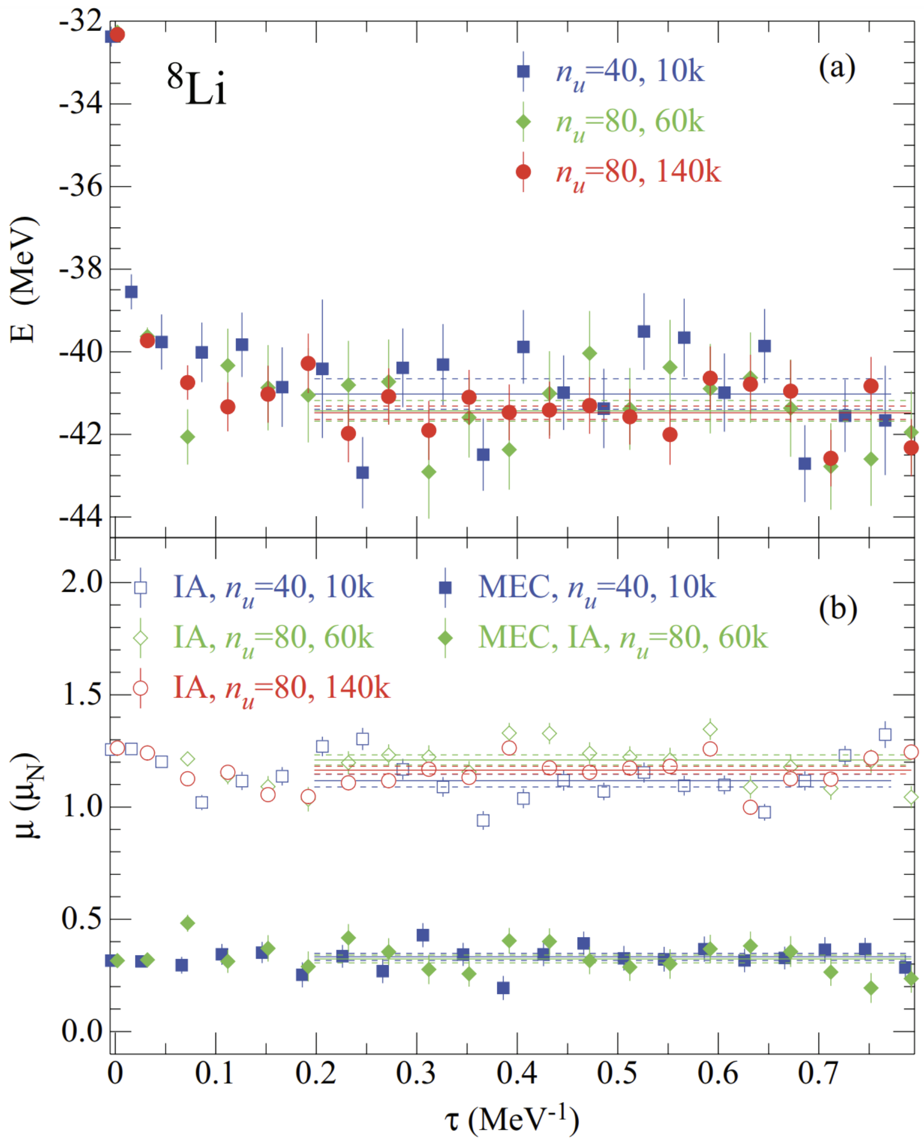


Foulkes et al. Rev. Mod. Phys. 73, 33 (2001)

Carlson et al. Rev. Mod. Phys. 87, 1607 (2015)

Mixed estimate

Pastore et al. PRC 87, 035503



Assume small correction to VMC:

$$\Psi(\tau) = \Psi_V + \delta\Psi$$

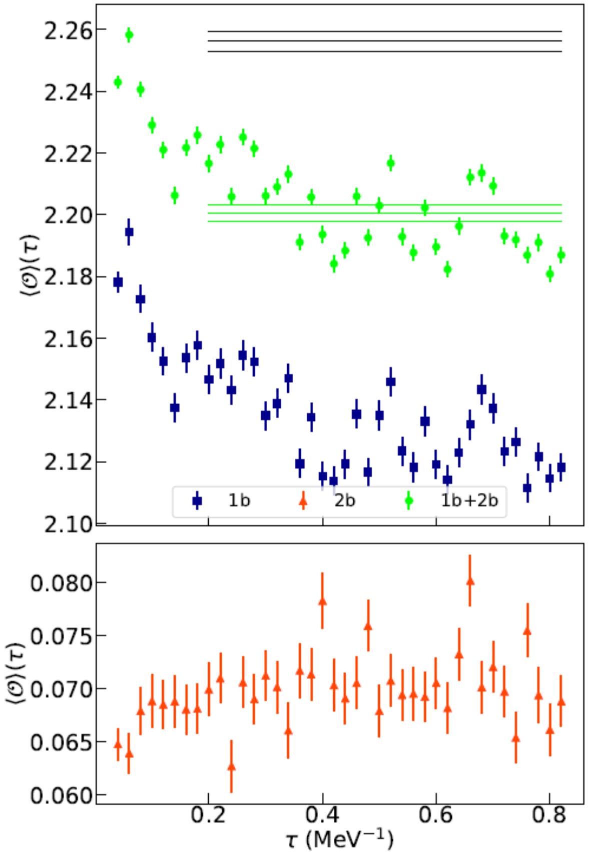
To first order in the correction:

$$\langle\Psi(\tau)|\mathcal{O}|\Psi(\tau)\rangle = 2\frac{\langle\Psi(\tau)|\mathcal{O}|\Psi_V\rangle}{\langle\Psi(\tau)|\Psi_V\rangle} - \langle\mathcal{O}\rangle_{\mathrm{VMC}}$$

Carlson et al. Rev. Mod. Phys. 87, 1607 (2015)

Off-diagonal mixed estimate

^{6}He → ^{6}Li GT RME extrapolation



Mixed estimate for off-diagonal transitions:

$$\langle \mathcal{O}(\tau)\rangle = \frac{\langle \Psi^f(\tau)|\mathcal{O}|\Psi^i(\tau)\rangle}{\sqrt{\langle \Psi^f(\tau)|\Psi^f(\tau)\rangle}\sqrt{\langle \Psi^i(\tau)|\Psi^i(\tau)\rangle}}$$

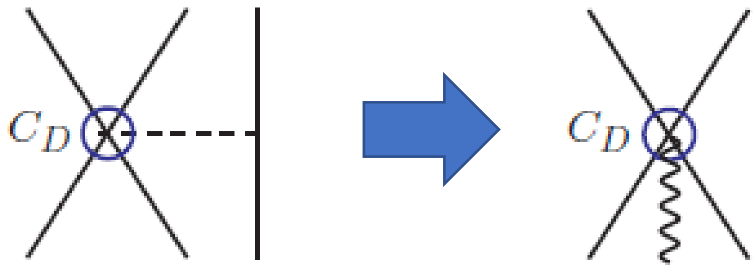
$$\simeq \langle \mathcal{O}(\tau)\rangle_{M_f} + \langle \mathcal{O}(\tau)\rangle_{M_i} - \langle \mathcal{O}\rangle_{\mathrm{VMC}}$$

where

$$\langle \mathcal{O}(\tau)\rangle_{M_f} = \frac{\langle \Psi^f(\tau)|\mathcal{O}|\Psi^i_V\rangle}{\langle \Psi^f(\tau)|\Psi^i_V\rangle}\frac{\sqrt{\langle \Psi^f_V|\Psi^f_V\rangle}}{\sqrt{\langle \Psi^i_V|\Psi^i_V\rangle}}$$

Pervin, Pieper, and Wiringa PRC 76, 064319 (2007)

Three-body LECs and N3LO-CT



$$\mathbf{j}^{\mathrm{N3LO}}_{5,a}(\mathbf{q};\mathrm{CT}) = z_0 \mathcal{O}_{ij}(\mathbf{q})$$

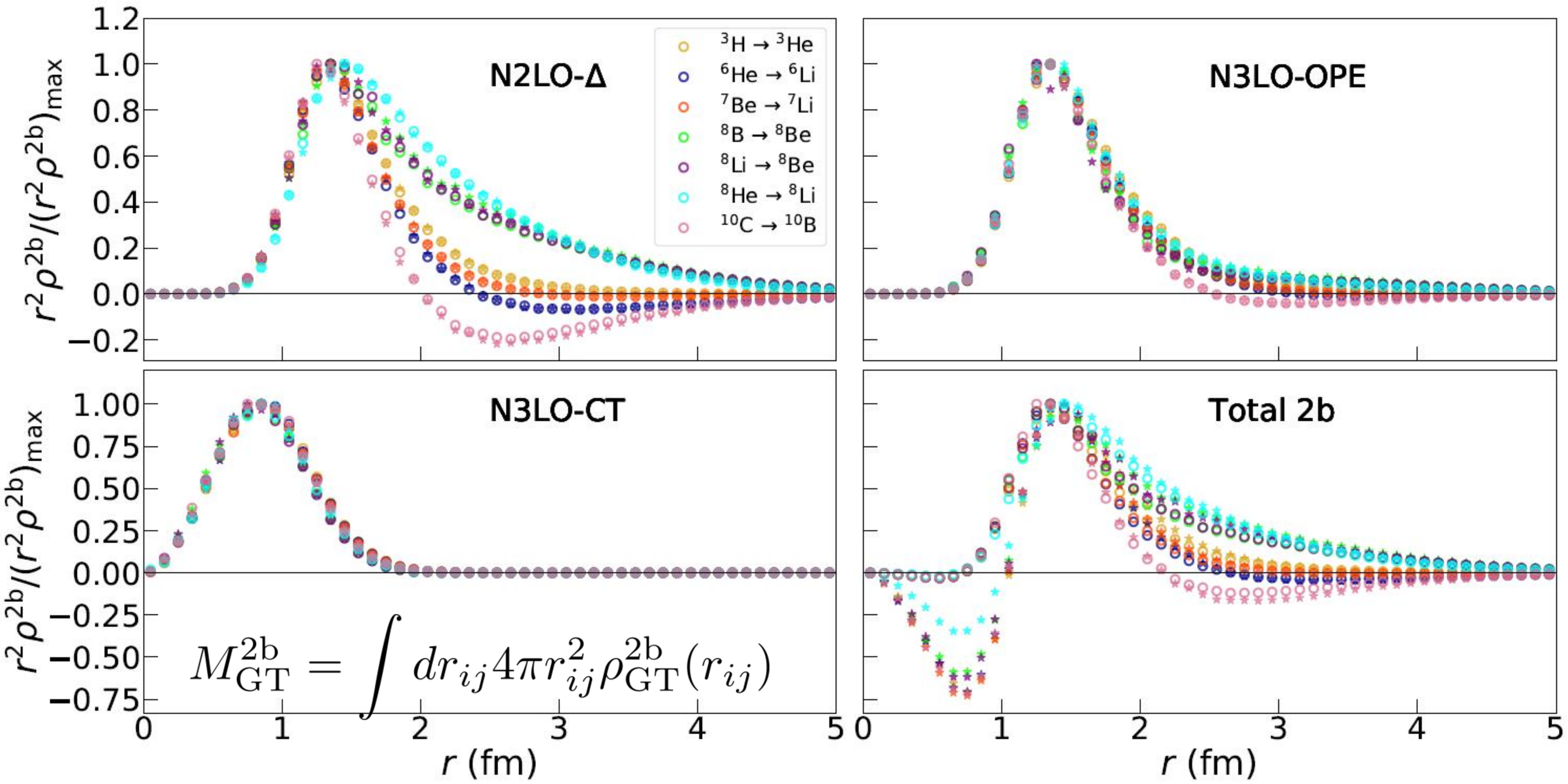
$$z_0 \propto (c_D + \text{ known LECs})$$

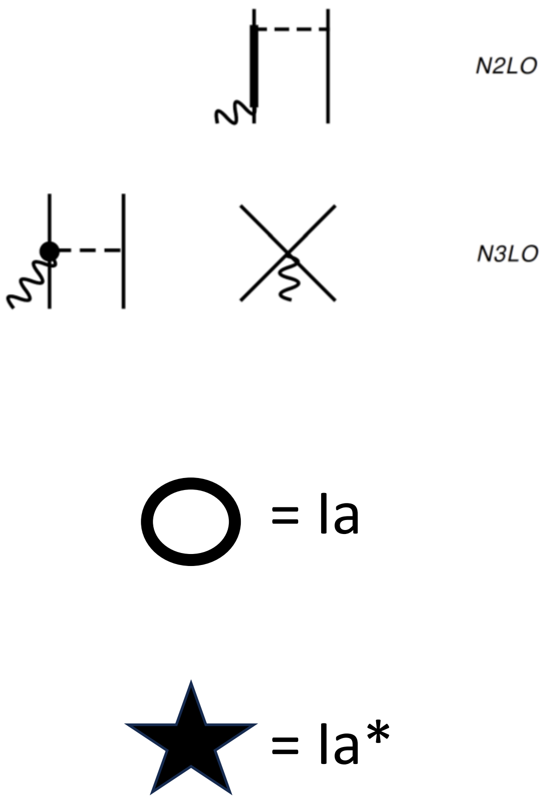
The NV2+3-Ia model fits c_D using *strong interaction data only*

The NV2+3-Ia* model fits c_D with *strong and weak interaction data*

Gardestig and Phillips PRL 96, 232301 (2006)

Scaled two-body transition densities



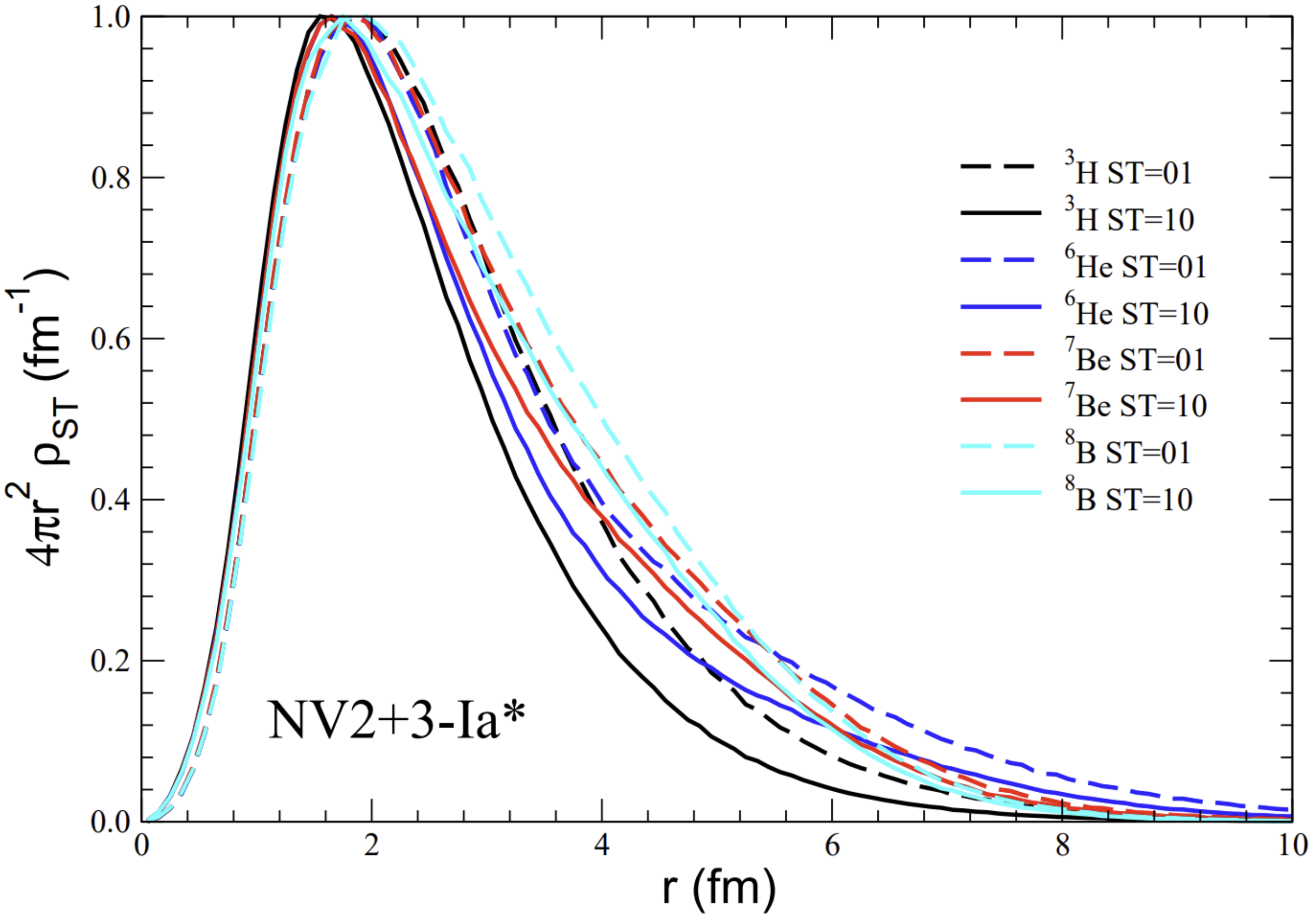


King et al. PRC 121, 025501 (2020)

Explanation of universal scaling behaviors

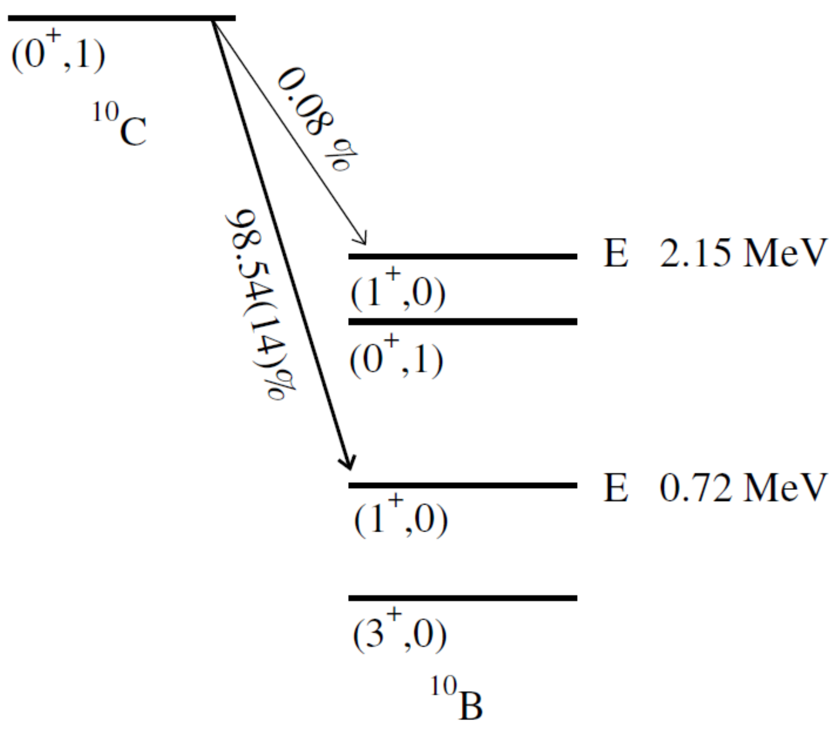
ST=01 and 10 pairs dominate short distances due to suppression of P-waves

$$N_{ST} = \int dr_{ij} 4\pi r_{ij}^2 \rho_M^{2b}(r_{ij})$$



King et al. PRC 121, 025501 (2020)

^{10}C to ^{10}B GT beta decay



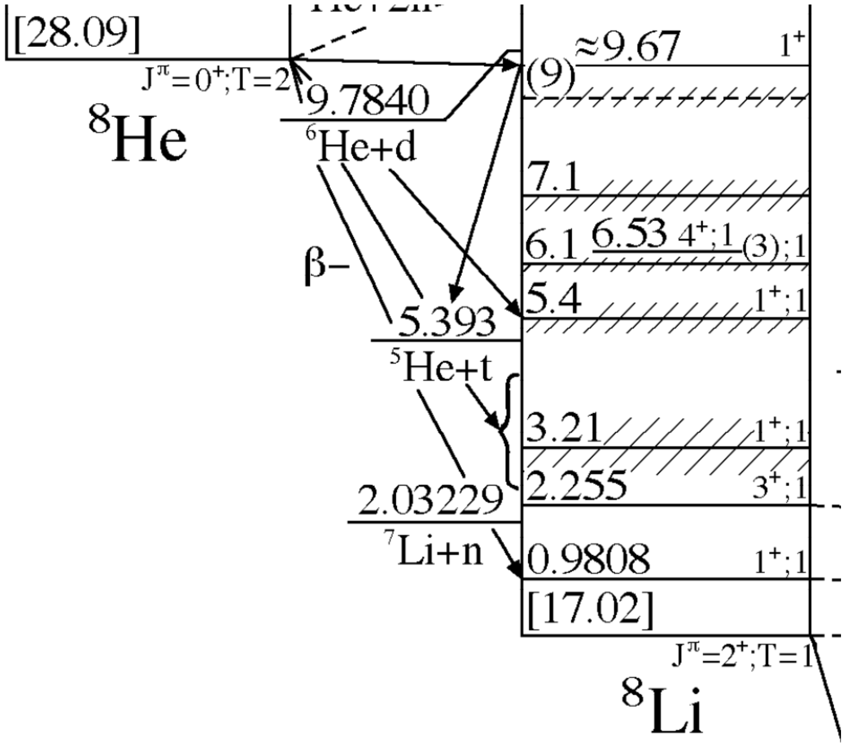
https://nucldata.tunl.duke.edu/

Two states of the same quantum numbers nearby

The result depends strongly on the *LS* mixing of the *p*-shell

Particularly sensitive to the $^3S_1$ and $^3D_1$ mixing because *S* to *S* produces a larger m.e. and ^{10}C is predominantly *S* wave

^{8}He to ^{8}LI GT beta decay



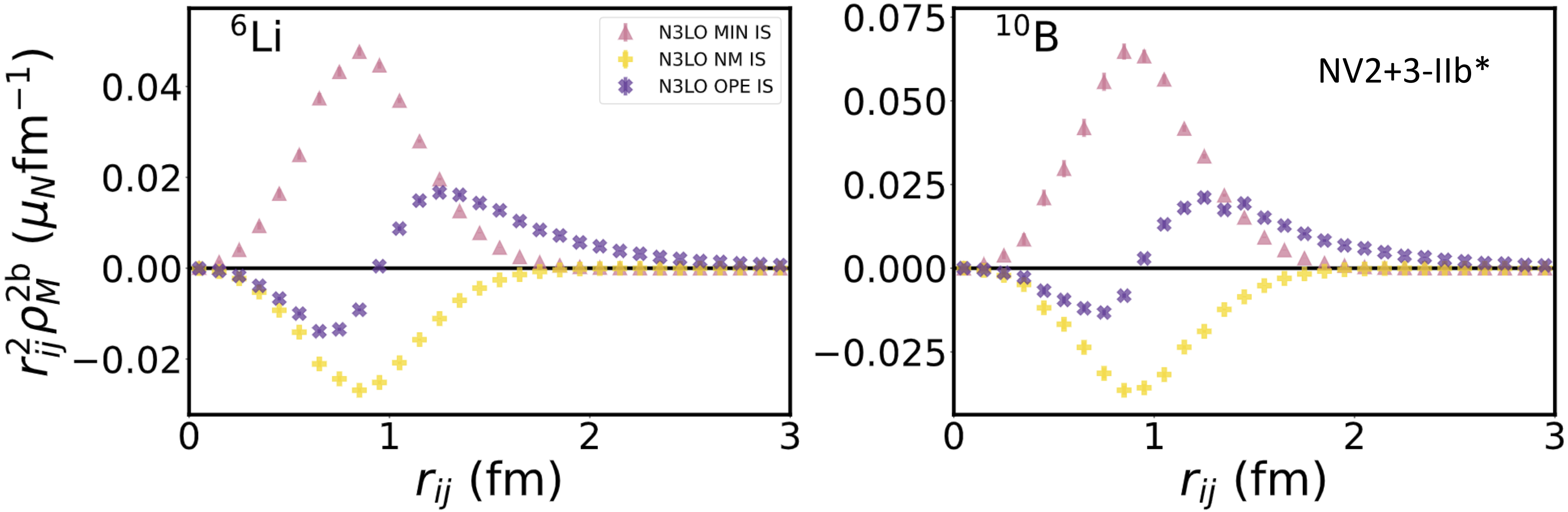
https://nucldata.tunl.duke.edu/

Three (1$^+$;1) states within a few MeV

Different dominant spatial symmetries → sensitivity to the precise mixing of small components in the wave function

Improving the mixing of the small components in the (1$^+$;1) states is crucial to getting an improved m.e.

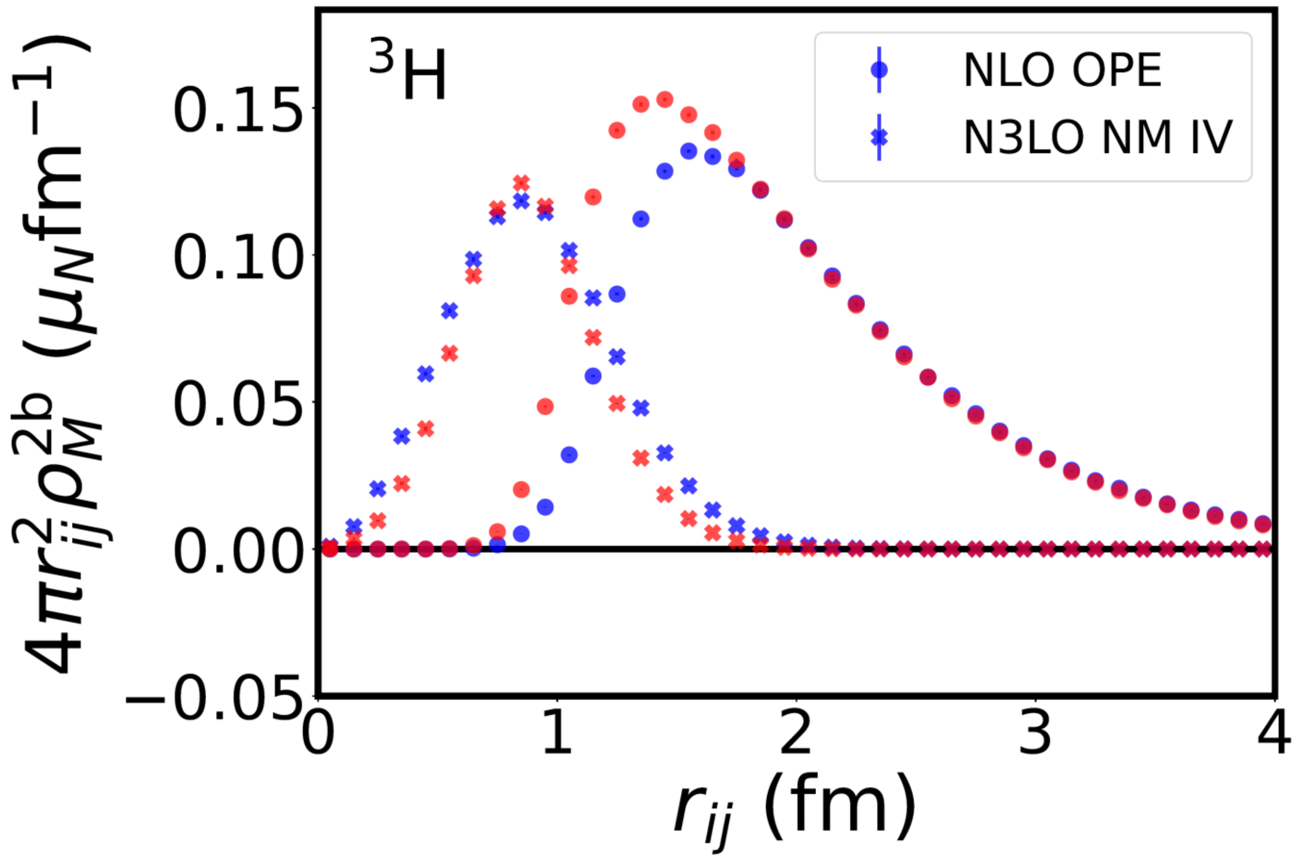
Isoscalar (IS) two-body magnetic densities



$$\mu^{2b} = \int dr_{ij} 4\pi r_{ij}^2 \rho_M^{2b}(r_{ij})$$

Chambers-Wall, King, et al. ***in preparation***

Cutoff dependence: magnetic currents



Regulator choice between model Ia* and IIb* strongly influences the short-range dynamics

Chambers-Wall, King, et al. in preparation

Partial Muon Capture Rates with QMC

Assuming a muon at rest in a Hydrogen-like 1s orbital:

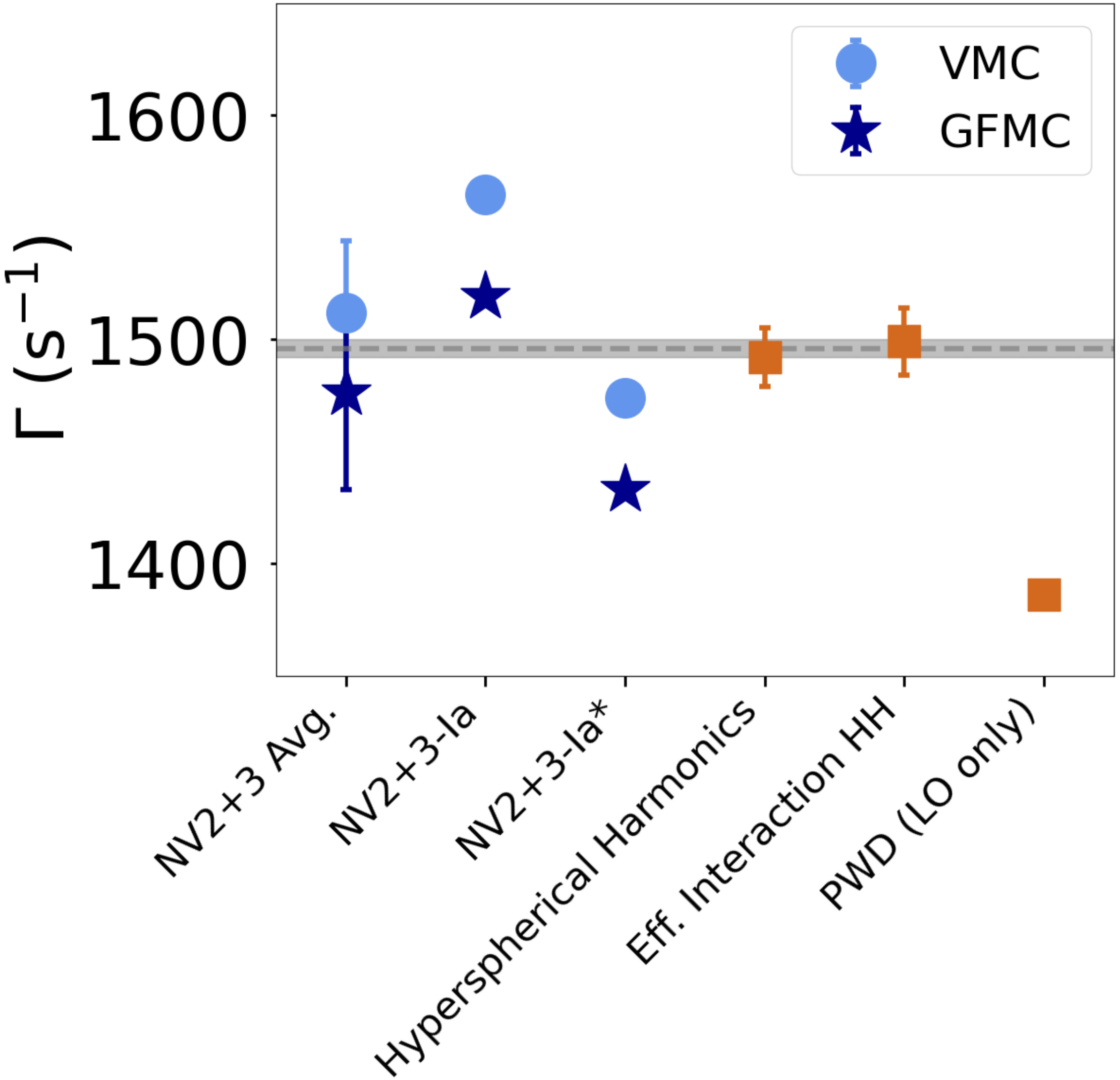
$$\Gamma = \frac{G_V^2}{2\pi} \frac{|\psi_{1s}^{\rm av}|^2}{(2J_i+1)} \frac{E_\nu^{*2}}{\rm recoil} \sum_{M_f, M_i} |\langle J_f, M_f|\rho(E_\nu^*\hat{\mathbf{z}})|J_i, M_i\rangle|^2 + |\langle J_f, M_f|\mathbf{j}_z(E_\nu^*\hat{\mathbf{z}})|J_i, M_i\rangle|^2$$

$$+ 2\,{\rm Re}\left[\langle J_f, M_f|\rho(E_\nu^*\hat{\mathbf{z}})|J_i, M_i\rangle \langle J_f, M_f|\mathbf{j}_z(E_\nu^*\hat{\mathbf{z}})|J_i, M_i\rangle^*\right] + |\langle J_f, M_f|\mathbf{j}_x(E_\nu^*\hat{\mathbf{z}})|J_i, M_i\rangle|^2$$

$$+ |\langle J_f, M_f|\mathbf{j}_y(E_\nu^*\hat{\mathbf{z}})|J_i, M_i\rangle|^2 - 2\,{\rm Im}\left[\langle J_f, M_f|\mathbf{j}_x(E_\nu^*\hat{\mathbf{z}})|J_i, M_i\rangle \langle J_f, M_f|\mathbf{j}_y(E_\nu^*\hat{\mathbf{z}})|J_i, M_i\rangle^*\right]$$

King et al. PRC 105, L042501 (2022)

Partial muon capture rates with QMC



$^3He(1/2^+;1/2) \rightarrow {^3H}(1/2^+;1/2)$ agrees with datum of **Ackerbauer et al. Phys. Lett. B 417 (1998)**

Most sensitive to the 3N force

Two-body provide ~9%-16% of the rate for different models

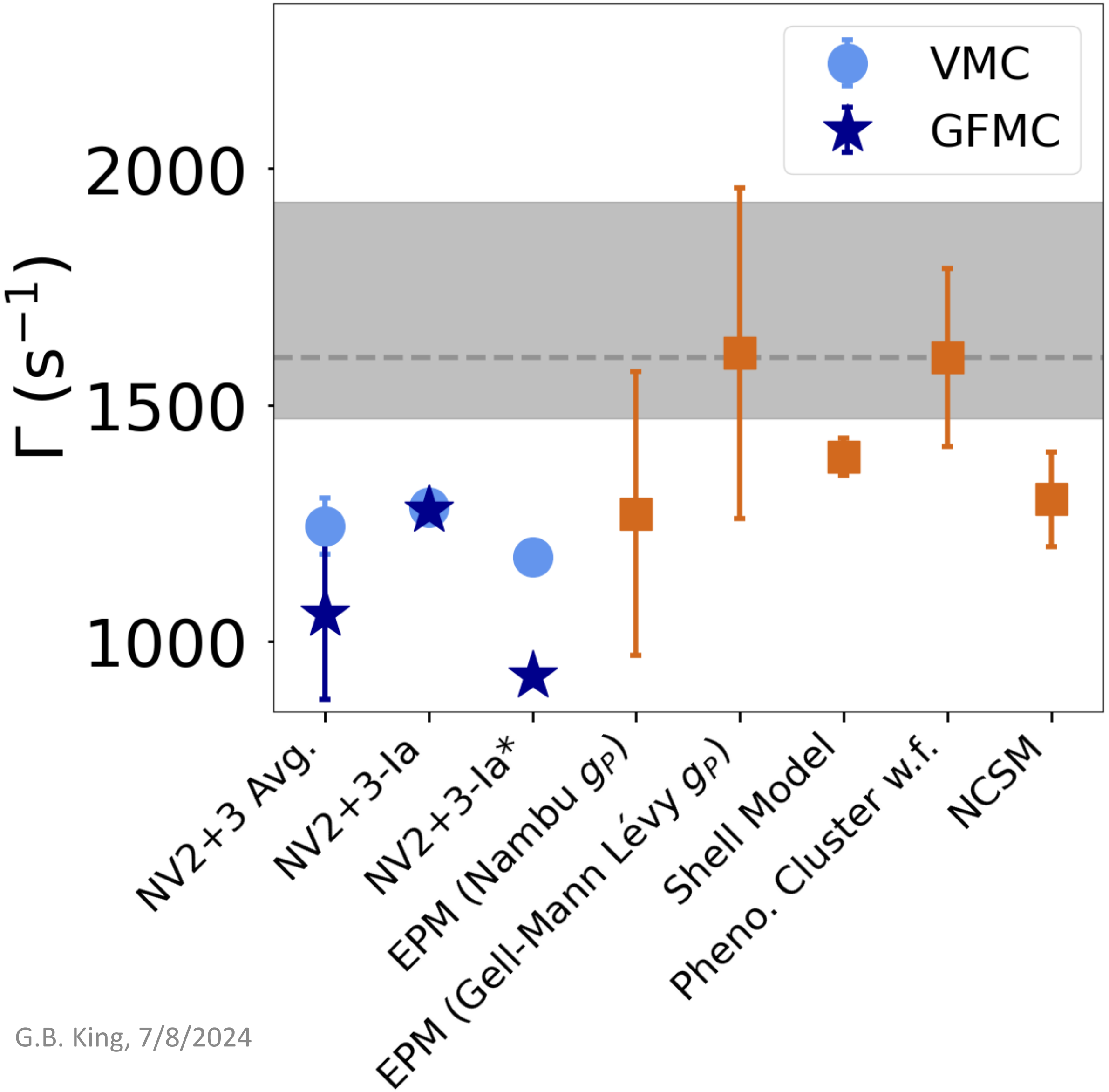
King et al. PRC 105, L042501 (2022)

Partial muon capture rates with QMC

$^{6}Li(g.s.) \rightarrow {}^{6}He(g.s.)$ disagrees with datum from **Deutsch et al. Phys. Lett. B26, 315 (1968)**

Subsequent NCSM evaluation agrees with QMC results

Could merit further attention



King et al. PRC 105, L042501 (2022)

^{6}He Beta Decay Spectrum: Multipoles

The (standard model) matrix element may be decomposed into reduced matrix elements of four multipoles operators:

$$\sum_{M_i}\sum_{M_f}|\langle f|H_W|i\rangle|^2 \propto \sum_{J=0}^{\infty}\left[(1+\hat{\boldsymbol{\nu}}\cdot\boldsymbol{\beta})|C_J(q)|^2 + (1-\hat{\boldsymbol{\nu}}\cdot\boldsymbol{\beta}+2(\hat{\boldsymbol{\nu}}\cdot\hat{\mathbf{q}})(\hat{\mathbf{q}}\cdot\boldsymbol{\beta}))|L_J(q)|^2 - \hat{\mathbf{q}}\cdot(\hat{\boldsymbol{\nu}}+\boldsymbol{\beta})2\mathrm{Re}(L_J(q)M_J^*(q))\right]$$

$$+\sum_{J=1}^{\infty}\left[(1-(\hat{\boldsymbol{\nu}}\cdot\hat{\mathbf{q}})(\hat{\mathbf{q}}\cdot\boldsymbol{\beta}))(|M_J(q)|^2+|E_J(q)|^2)+\hat{\mathbf{q}}\cdot(\hat{\boldsymbol{\nu}}-\boldsymbol{\beta})2\mathrm{Re}(M_J(q)E_J^*(q))\right]$$

With the standard operator definitions as **[Walecka 1975, Oxford University Press]**:

$$C_{JM}(q) = \int d^3x[j_J(qx)Y_{JM}(\Omega_x)](\rho(\mathbf{x};V)+\rho(\mathbf{x};J))$$

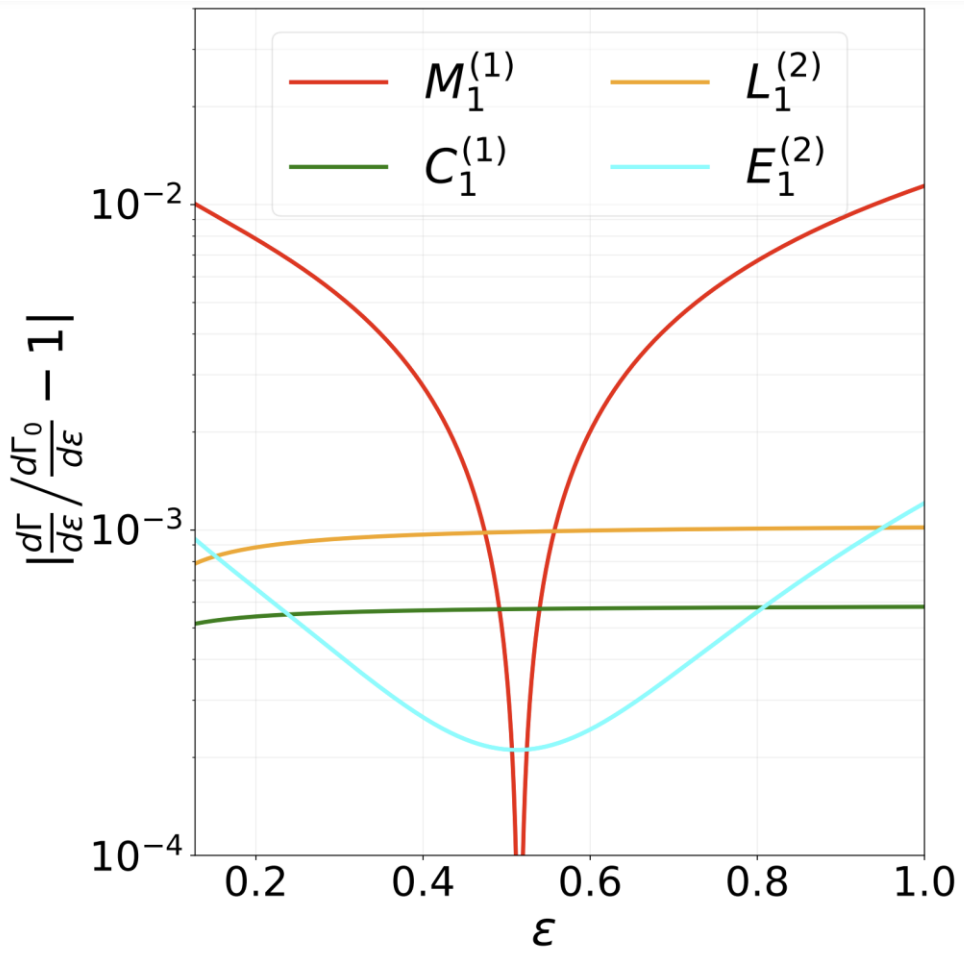
$$L_{JM}(q) = \frac{i}{q}\int d^3x\{\nabla[j_J(qx)Y_{JM}(\Omega_x)]\}\cdot(\mathbf{j}(\mathbf{x};V)+\mathbf{j}(\mathbf{x};A))$$

$$E_{JM}(q) = \frac{1}{q}\int d^3x[\nabla\times j_J(qx)\boldsymbol{\mathcal{Y}}^M_{JJ1}(\Omega_x)]\cdot(\mathbf{j}(\mathbf{x};V)+\mathbf{j}(\mathbf{x};A))$$

$$M_{JM}(q) = \int d^3x[j_j(qx)\boldsymbol{\mathcal{Y}}^M_{JJ1}(\Omega_x)\cdot(\mathbf{j}(\mathbf{x};V)+\mathbf{j}(\mathbf{x};A))$$

Parity and angular momentum selection rules preserve only the four *J*=1, positive parity multipoles for ^{6}He beta-decay

^{6}He beta decay spectrum: SM results

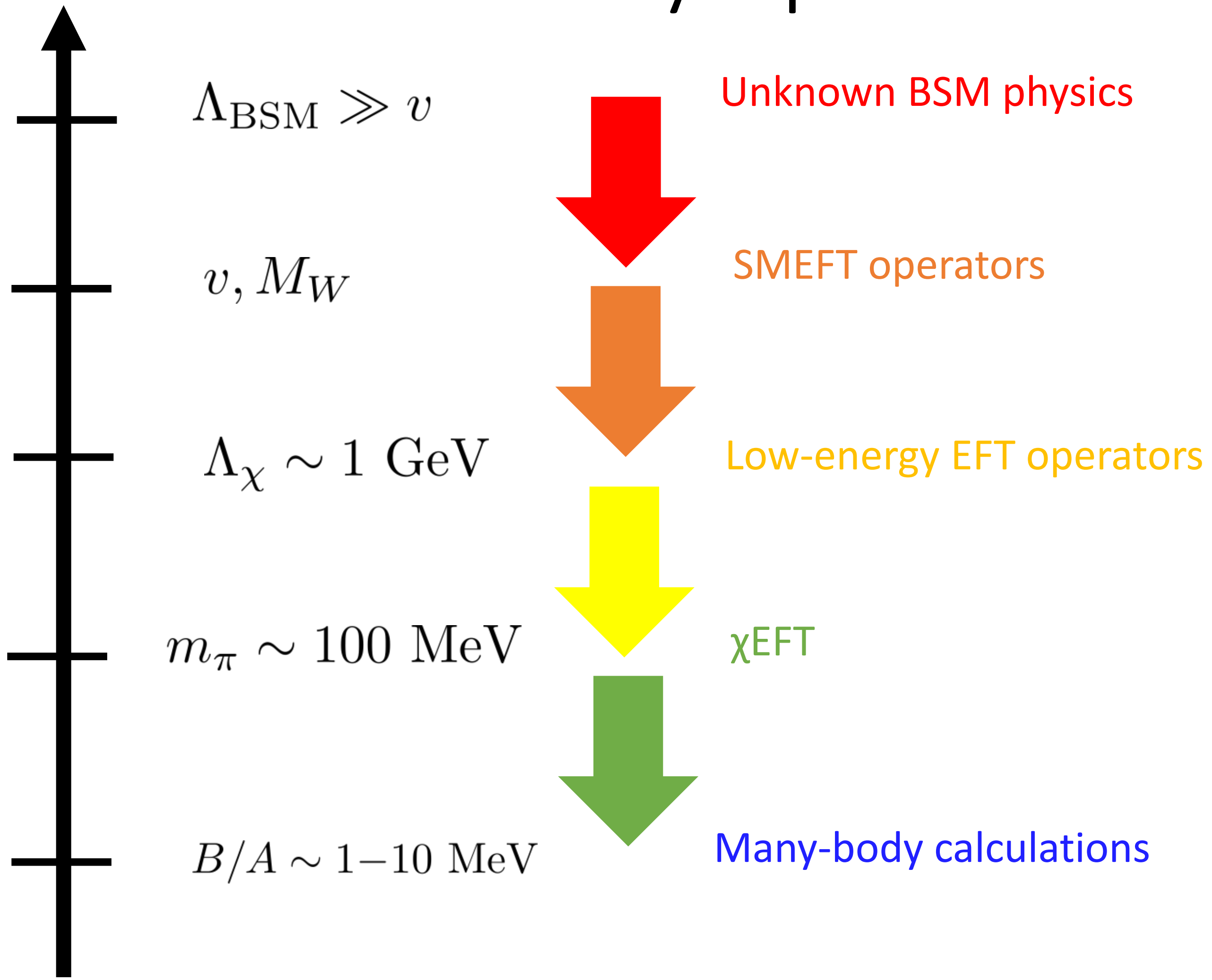


τ_{VMC} = 762 +/- 11 ms
τ_{GFMC} = 808 +/- 24 ms
$\tau_{Expt.}$ = 807.25 +/- 0.16 +/- 0.11 ms
[Kanafani et al. PRC 106, 045502 (2022)]

$$\varepsilon = \frac{E_e}{\omega}$$

King et al. PRC 107, 015503 (2023)

^{6}He Beta Decay Spectrum: BSM Connections



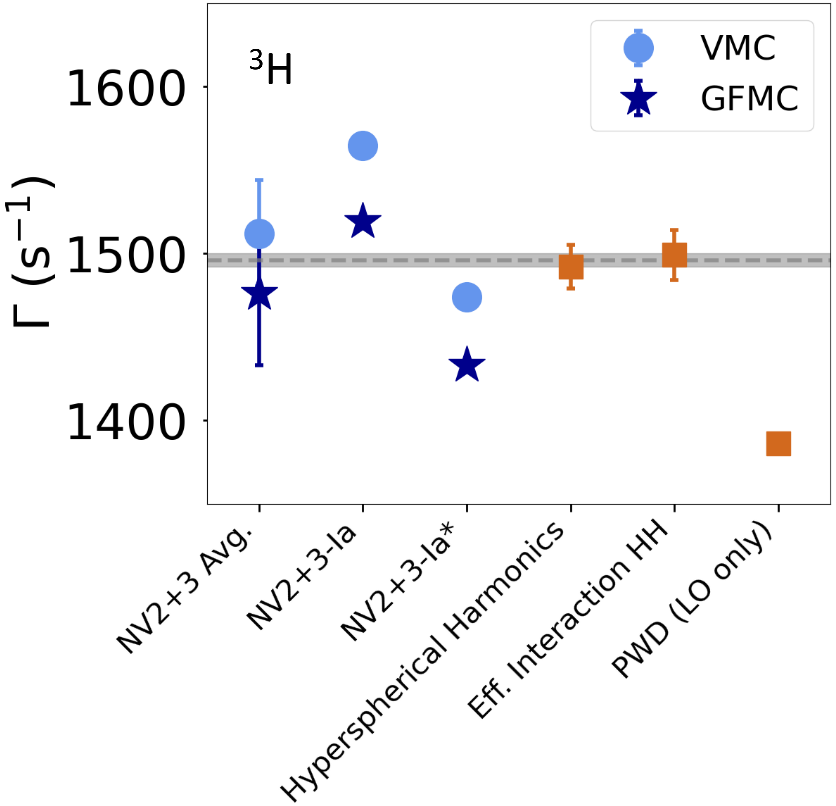
Standard Model Effective Field Theory (SMEFT) gives most general set of gauge-invariant operators complimenting the SM

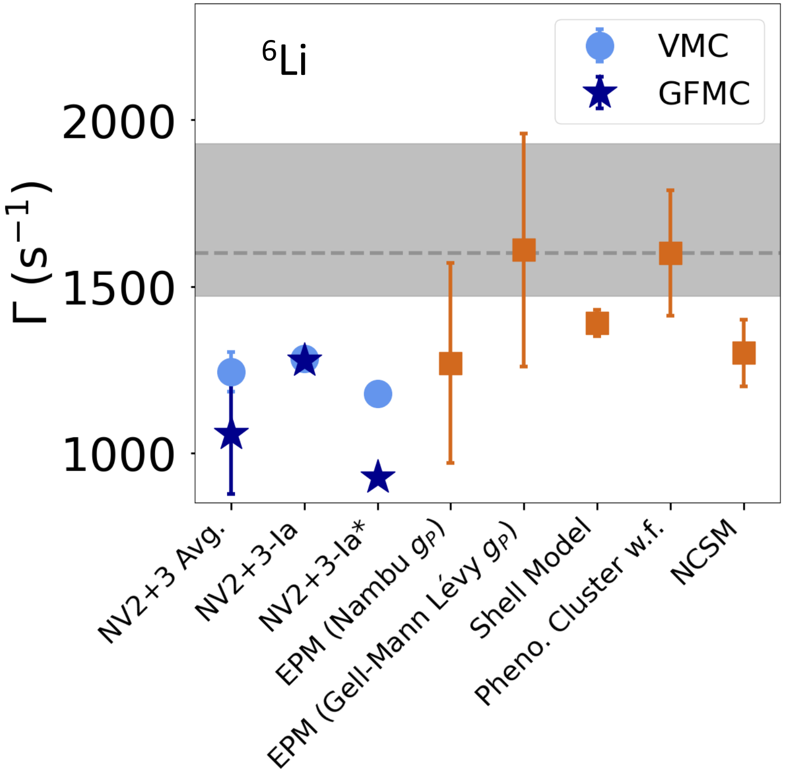
Tensor and pseudoscalar charged current interactions introduced at dimension-6

Matching the SMEFT to low-energy theory, one can investigate impact of BSM physics on the ^{6}He beta-decay spectrum **(effort led by Mereghetti+)**

King et al. PRC 107, 015503 (2023)

Muon capture: non-zero momentum transfer





$$\Gamma \propto \sum_{\alpha\beta} |M_{\alpha\beta}|^2$$

Momentum transfer ~ 100 MeV/c

Two-body currents play a ~9%-16% role for A=3, ~3%-7% for A=6

Many-body calculations with χEFT based models not presently capturing the data

King et al. PRC 105, L042501 (2022)

^{6}He beta decay spectrum: SM results

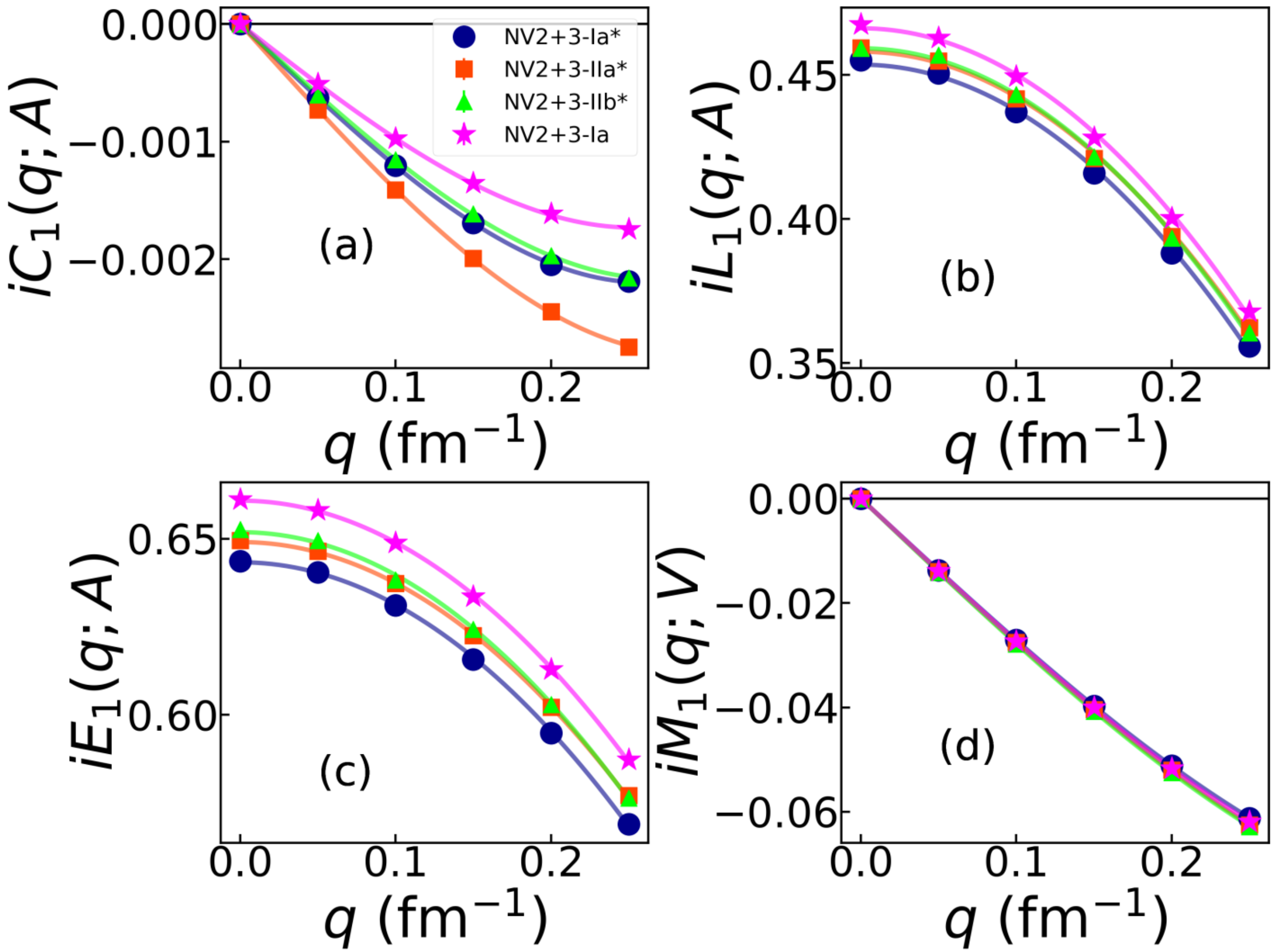
Fully retain two-body physics by leveraging low-q behavior

$$C_1(q;A) = \frac{i}{\sqrt{4\pi}}\langle {}^6\mathrm{Li},10|\rho_+^\dagger(q\hat{\mathbf{z}};A)|{}^6\mathrm{He},00\rangle$$

$$L_1(q;A) = \frac{i}{\sqrt{4\pi}}\langle {}^6\mathrm{Li},10|\hat{\mathbf{z}}\cdot\mathbf{j}_+^\dagger(q\hat{\mathbf{z}};A)|{}^6\mathrm{He},00\rangle$$

$$E_1(q;A) = \frac{i}{\sqrt{2\pi}}\langle {}^6\mathrm{Li},10|\hat{\mathbf{z}}\cdot\mathbf{j}_+^\dagger(q\hat{\mathbf{x}};A)|{}^6\mathrm{He},00\rangle$$

$$M_1(q;V) = -\frac{1}{\sqrt{2\pi}}\langle {}^6\mathrm{Li},10|\hat{\mathbf{y}}\cdot\mathbf{j}_+^\dagger(q\hat{\mathbf{x}};V)|{}^6\mathrm{He},00\rangle$$



VMC multipoles

King et al. PRC 107, 015503 (2023)