



Electroweak reactions with QMC methods

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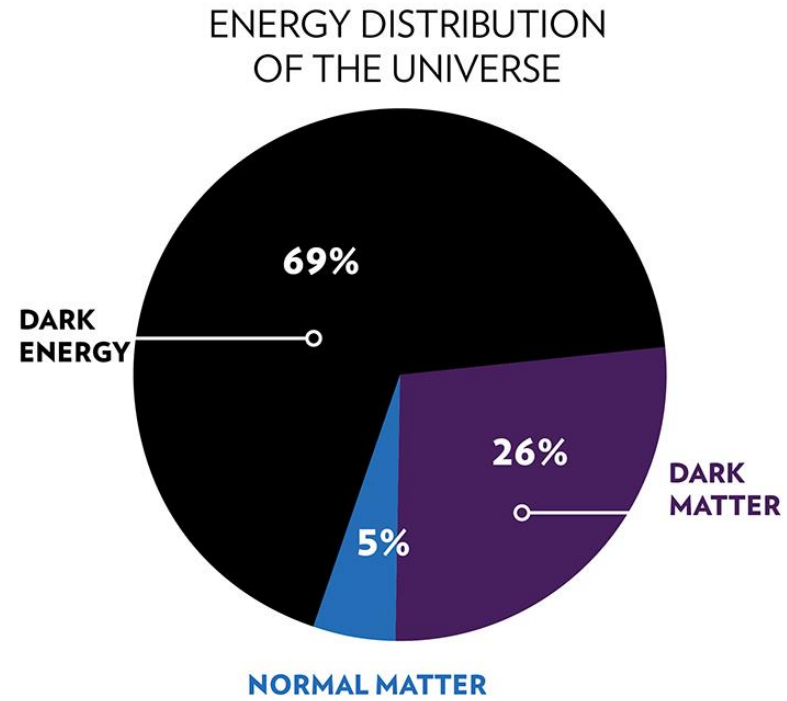
Collaborators: Andreoli, Baroni, Brown, Carlson, Cirigliano, Chambers-Wall, Gandolfi, Gnech, Hayen, Mereghetti, Schiavilla, Wiringa



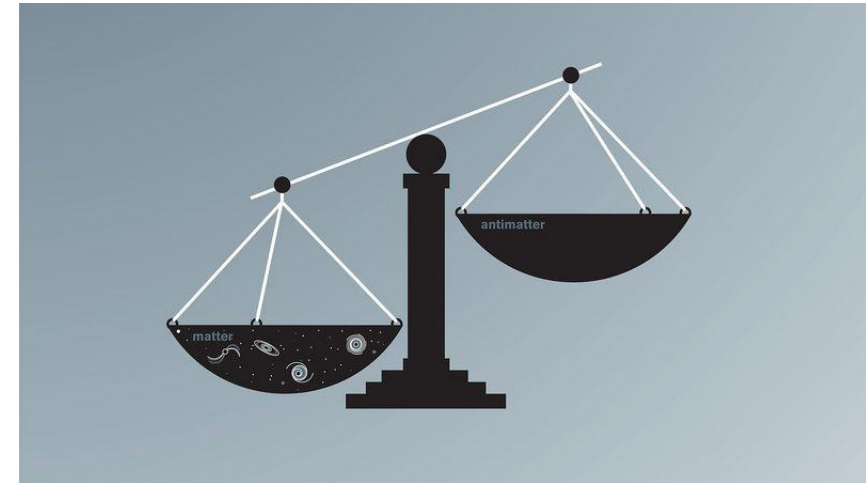
Motivation



Fermi Lab / Sandbox Studio, Chicago



NASA / Chandra X-ray Center/ K. Divona

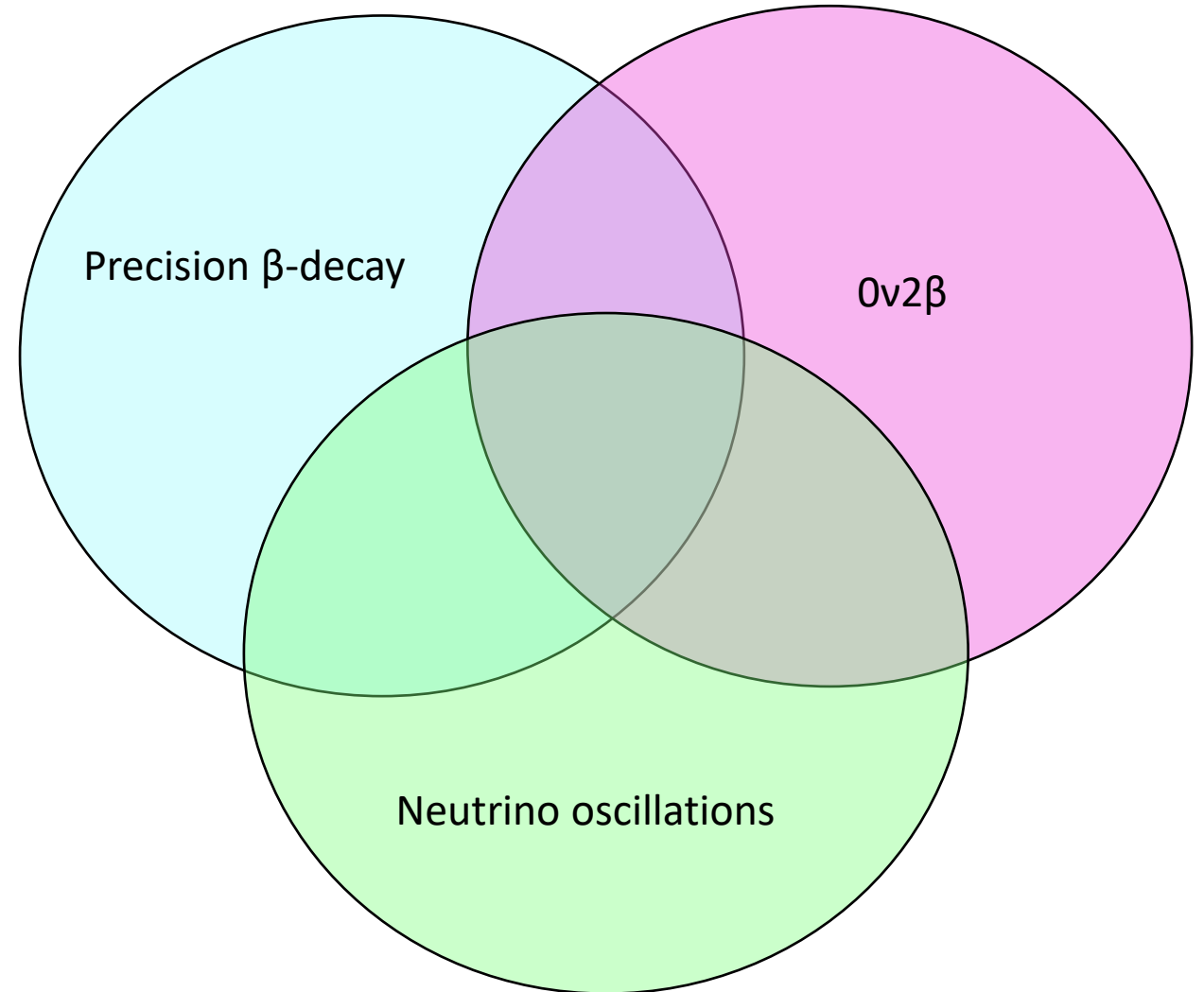


Symmetry Magazine / Sandbox Studio, Chicago



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

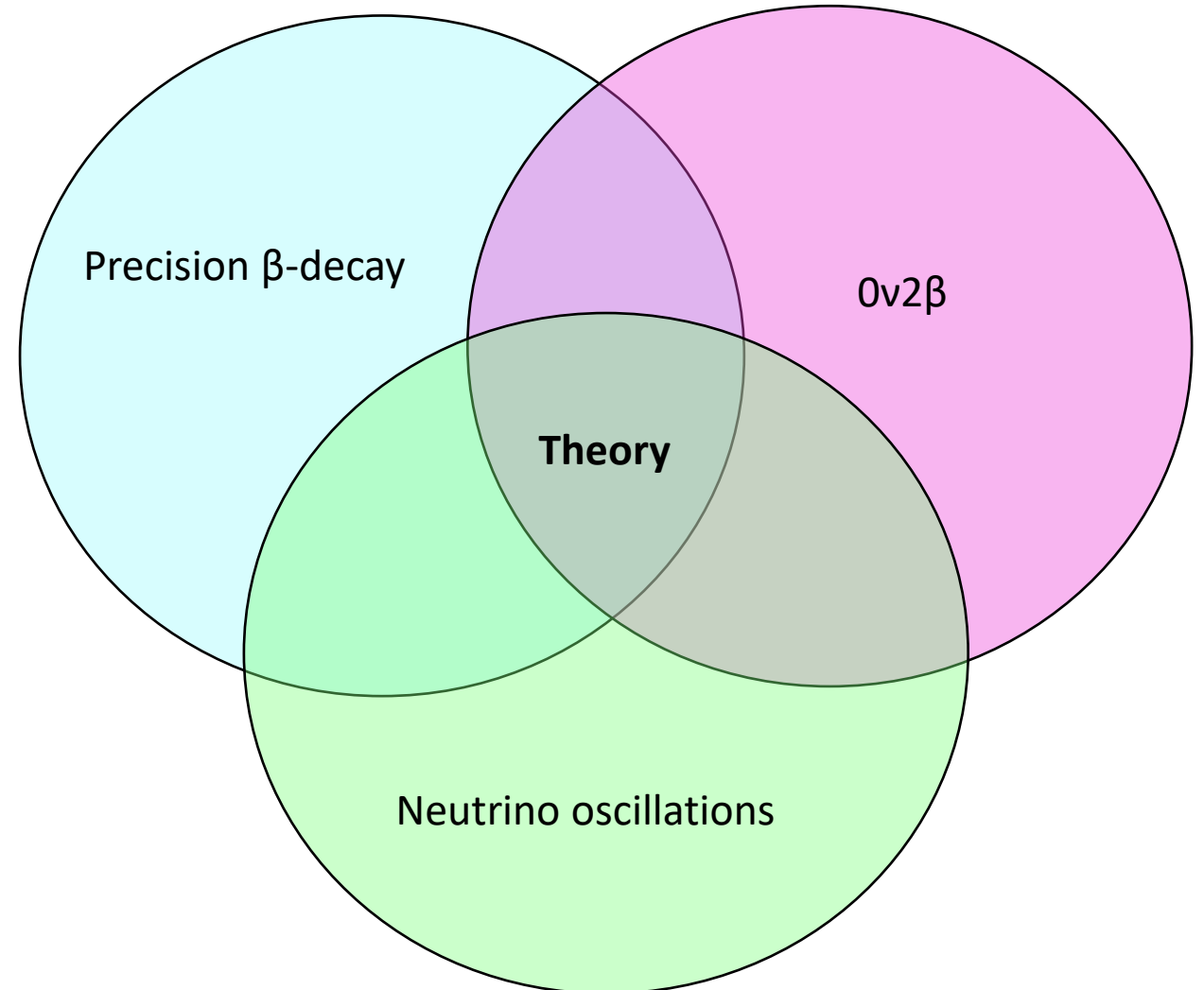




Nuclei for new physics

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



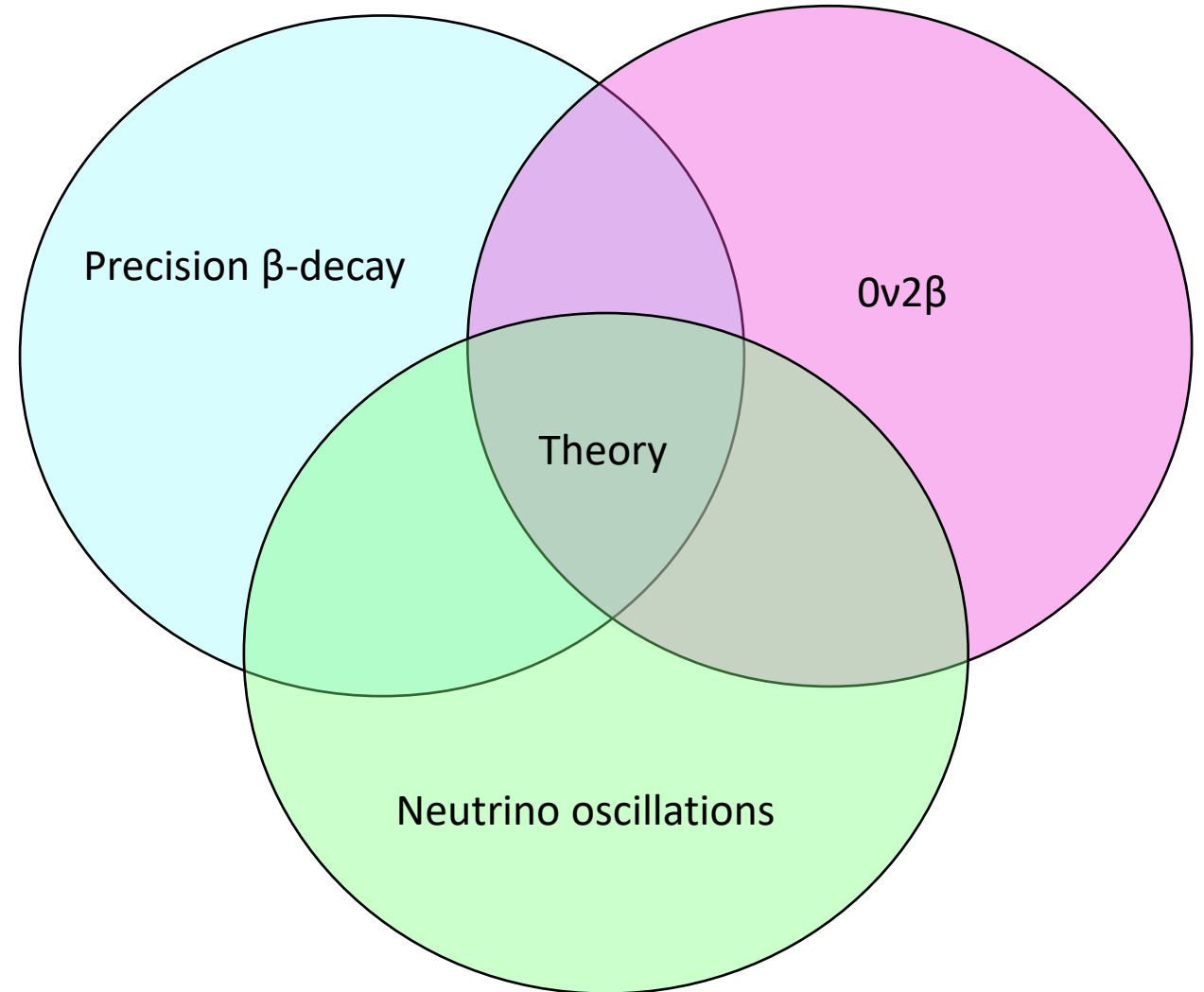


Nuclei for new physics

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





Developing a reliable model

Validate on available data



Predict relevant quantities



Developing a reliable model

Validate on available data



Predict relevant quantities

Decay rates, magnetic moments



Precision decays, moments

Electron scattering



Neutrino scattering



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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 ${}^6\text{He}$ 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**)



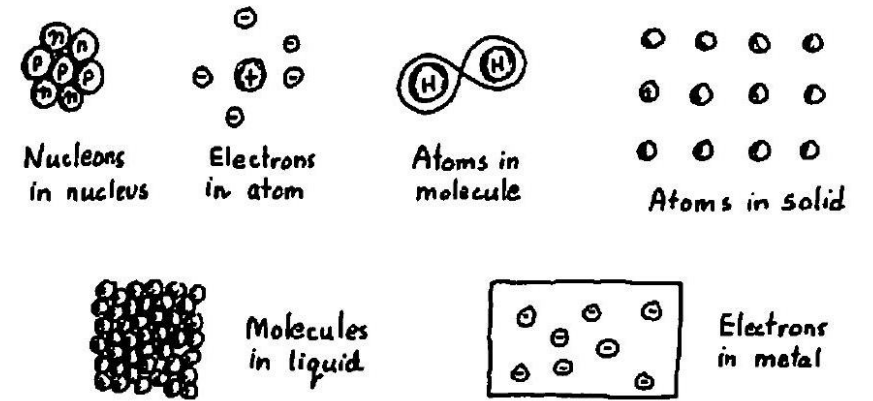
Quantum many-body problem

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, ...

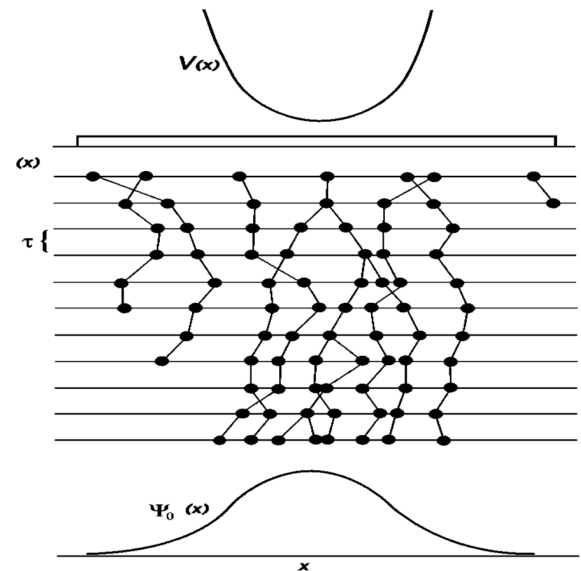


Quantum Monte Carlo (QMC)

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:

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

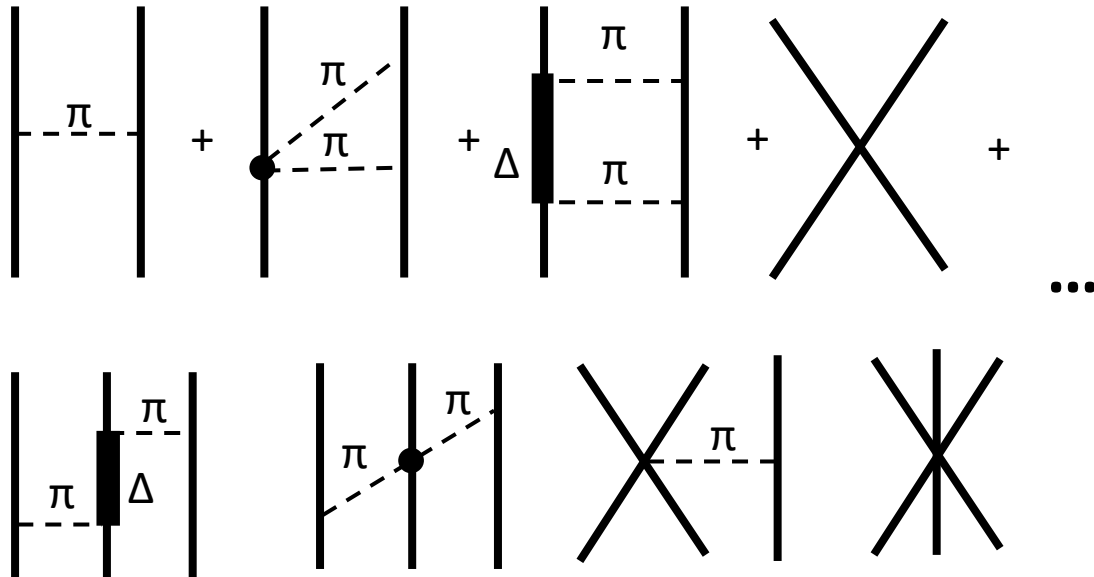


Green's function MC improves by **removing excited state contamination** and **gives the exact ground state**

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



Chiral Effective Field Theory (χ EFT)



Procedure to obtain NN interaction rooted in the underlying symmetry of Quantum Chromodynamics

Separation of scales: Nucleon momentum $Q \sim m_\pi \sim m_N - m_\Delta$ vs. heavier mesons at the scale $\Lambda \sim 1 \text{ GeV}$

Heavy degrees of freedom integrated out

Low-energy constants (LECs) subsume the underlying QCD

Weinberg, van Kolck, Ordóñez, Epelbaum, Hammer, Meißner, Entem, Machleidt, Piarulli, ...

Piarulli and Tews, *Front. Phys.* 30 (2020)

Entem and Machleidt, *J. Phys. Rep* 503(1) (2011)



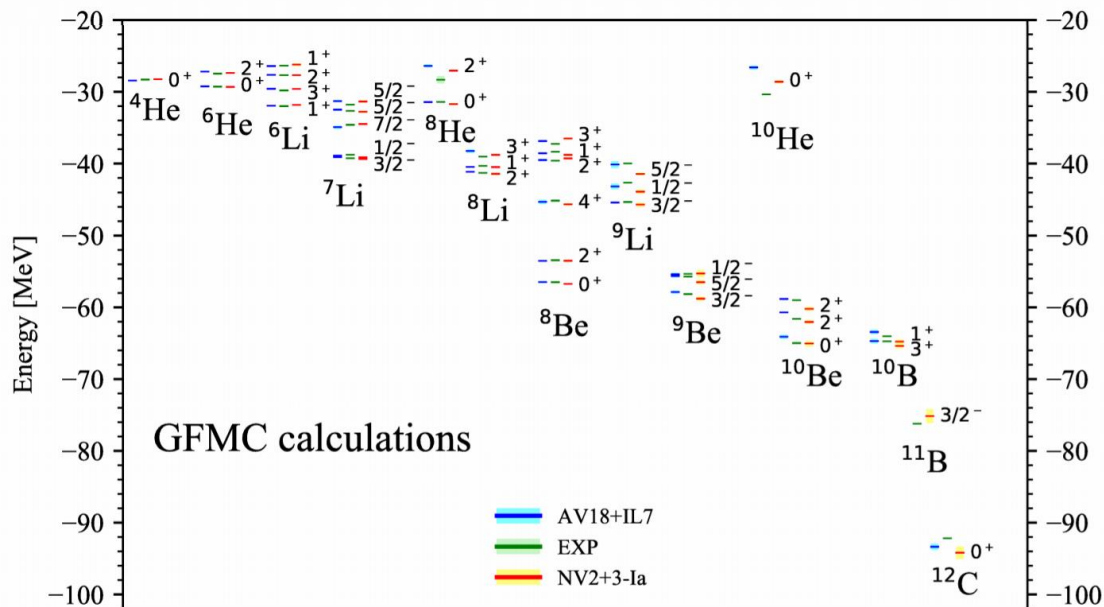
The Norfolk (NV2+3) interaction

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

Semi-phenomenological model based on χ EFT 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)



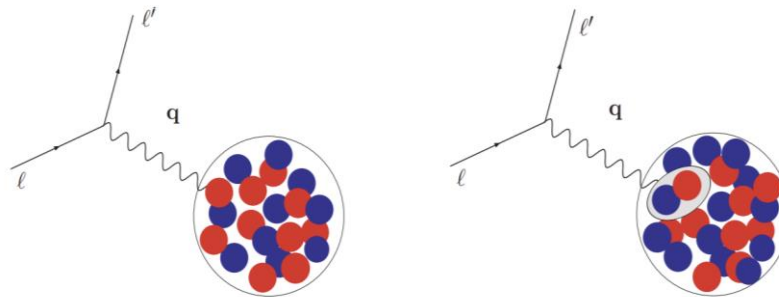
Electroweak charge and currents

Need nuclear electroweak charge and current operators as well

Schematically:

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

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), ...



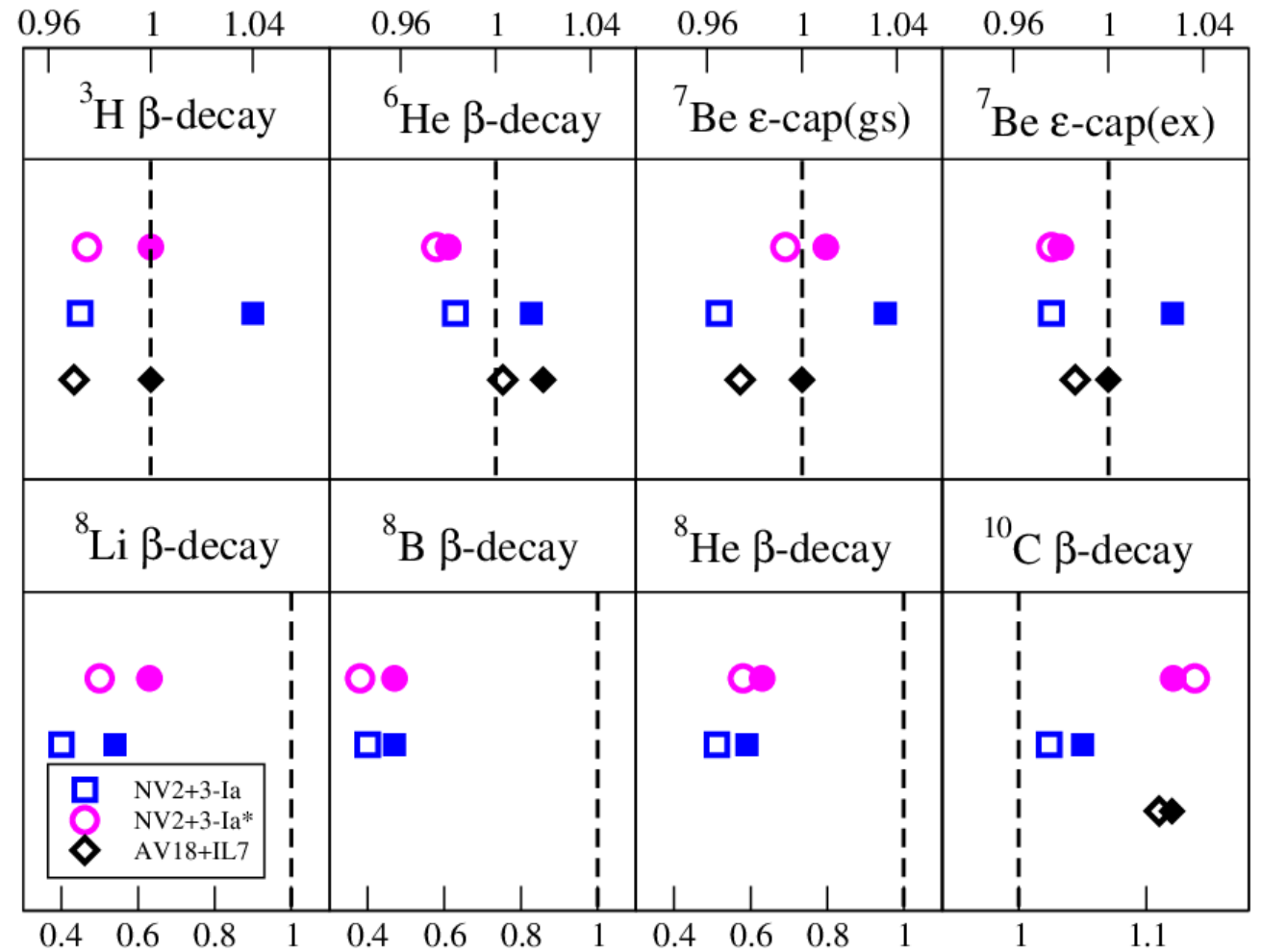
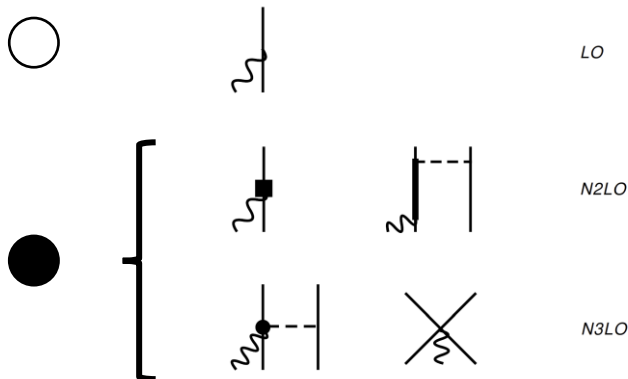
Model Validation

Beta-decay: Gamow-Teller matrix elements

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

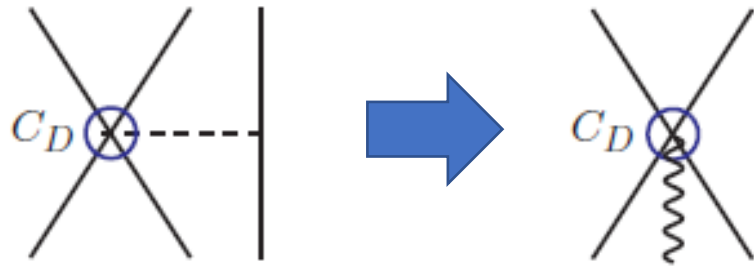
Correlations provide bulk of quenching

Two-body almost always enhances





Three-body LECs and N3LO-CT



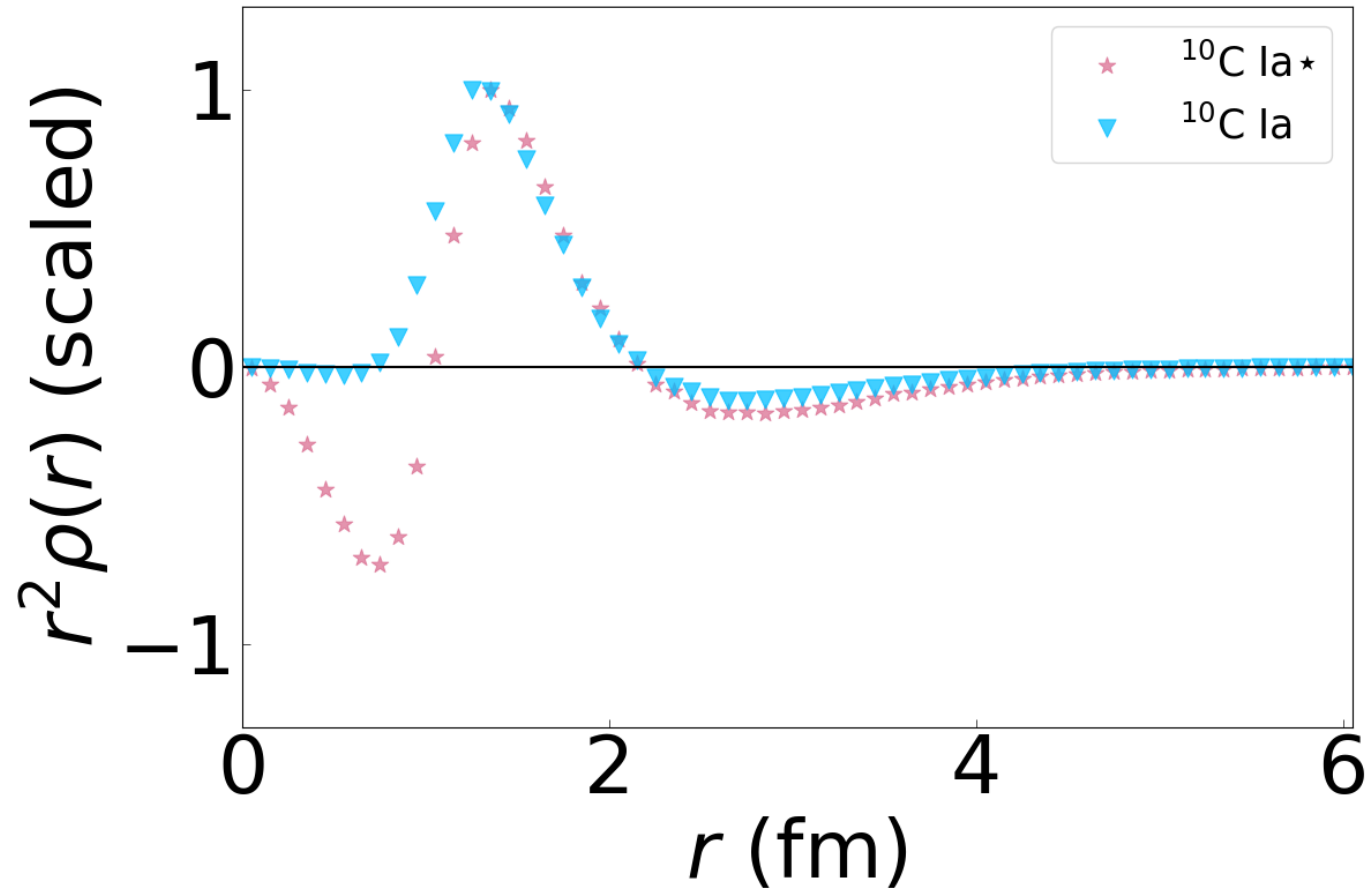
$$\mathbf{j}_{5,a}^{\text{N3LO}}(\mathbf{q}; \text{CT}) = z_0 \mathcal{O}_{ij}(\mathbf{q})$$

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

The NV2+3-1a model fits c_D using *strong interaction data only*

The NV2+3-1a* model fits c_D with *strong and weak interaction data*

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

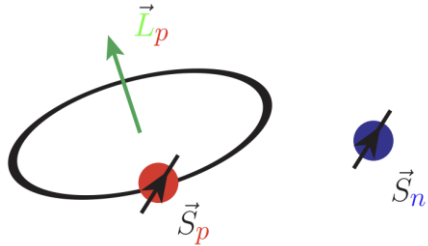
$$M_{GT}^{2b} = \int dr_{ij} 4\pi r_{ij}^2 \rho_{GT}^{2b}(r_{ij})$$



Magnetic structure: two-body currents

One-body picture:

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



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

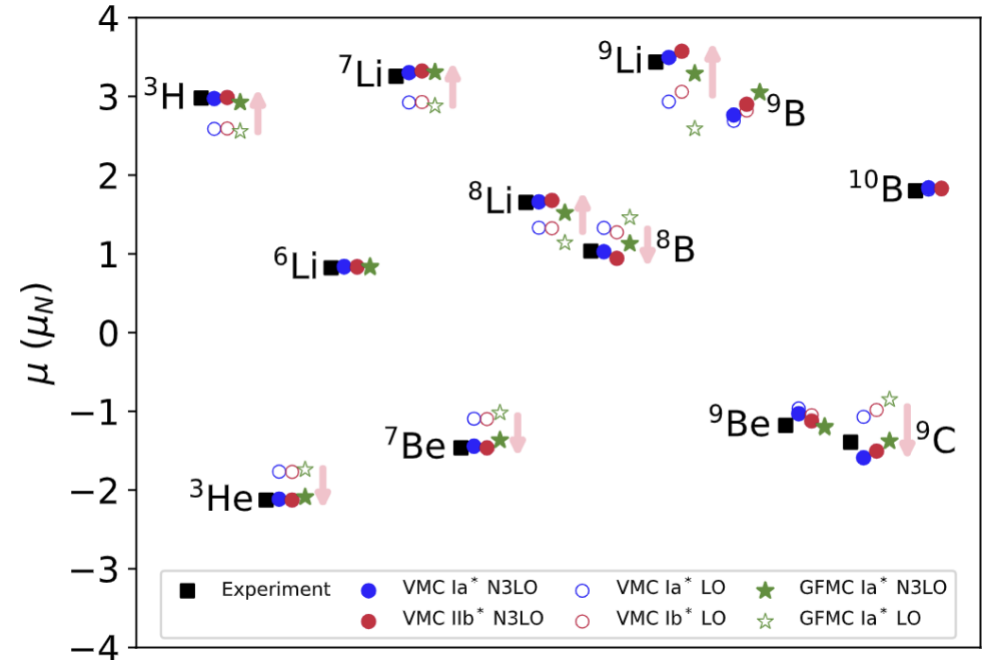
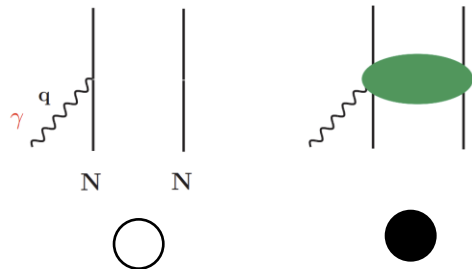


Figure courtesy of G. Chambers-Wall



Magnetic structure: two-body currents

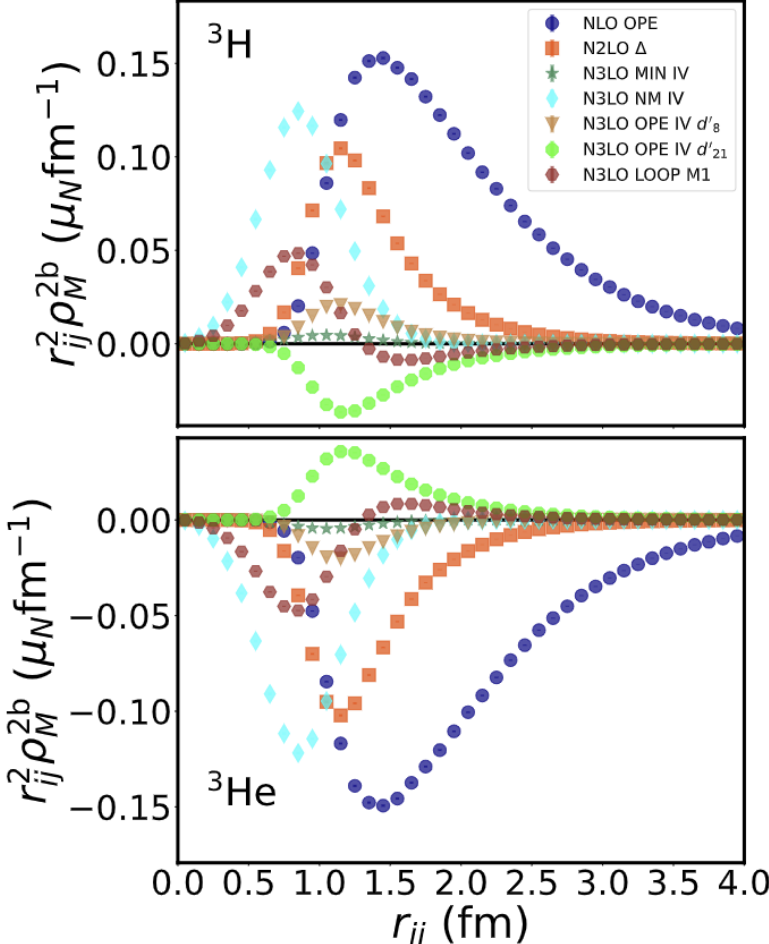
NV2+3-IIb*

Non-minimal (NM) contact term should naively be suppressed by Q^3

It is in fact order $\sim Q^{1.5}$, resulting in larger-than-expected N3LO contribution

Summed contributions agree with data, but power counting is not converging order-by-order

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



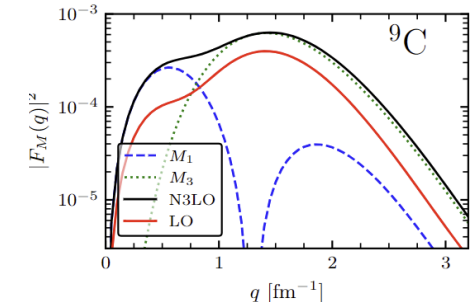
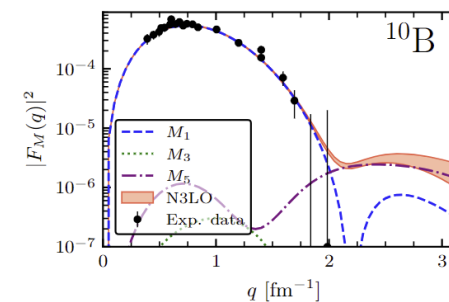
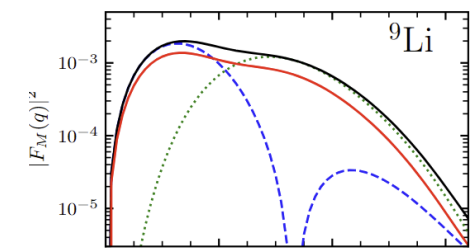
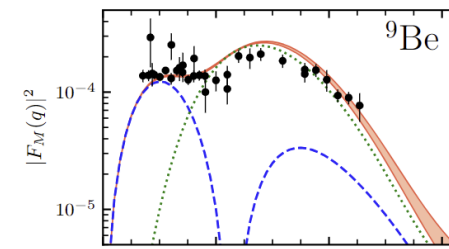
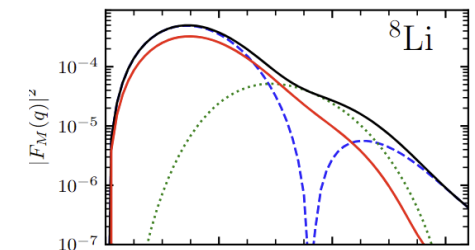
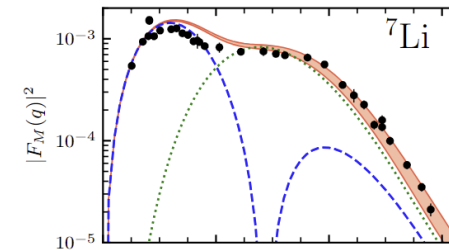
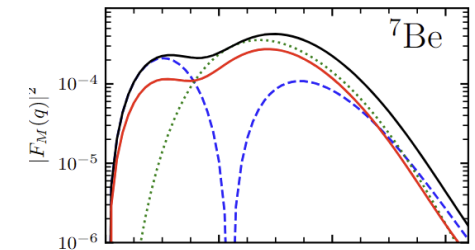
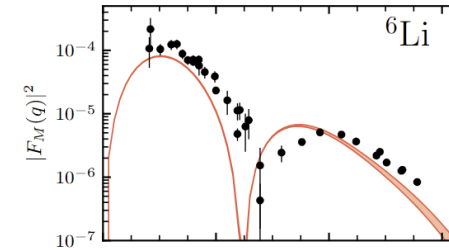


Magnetic structure: form factors

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

In some cases, good quantitative agreement at large momentum transfer

Two-body effects $\sim 20\%$ to 50% at large momentum transfer in various radioisotopes





Prediction: ${}^6\text{He}$ β -decay spectrum



${}^6\text{He}$ beta decay spectrum: Overview

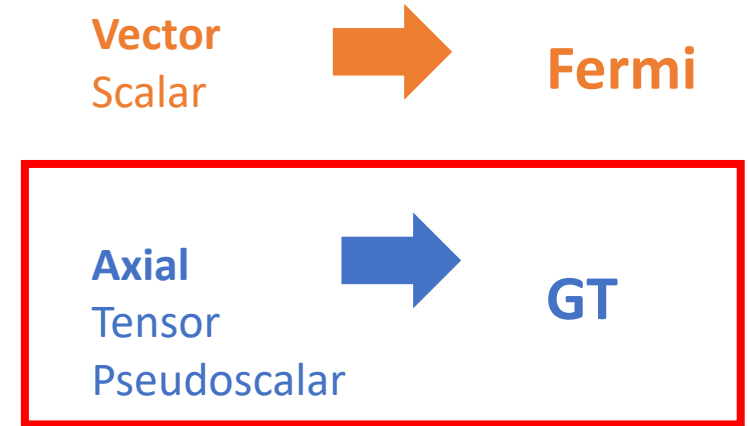
Differential rate: $d\Gamma_\beta = |M_\beta(q)|^2 \times (\text{kinematic factors})$

In the $q \rightarrow 0$ limit:

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

SM ($q \rightarrow 0$):

$$b = 0$$





${}^6\text{He}$ beta decay spectrum: Overview

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

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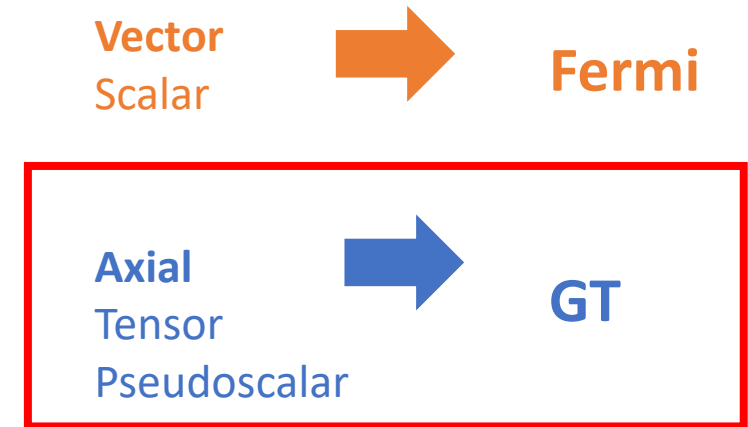
$$\frac{d\Gamma_\beta}{dE_e} = \frac{d\Gamma_0}{dE_e} \left[1 + b \frac{m_e}{E_e} \right]$$

SM ($q \rightarrow 0$):

$$b = 0$$

SM (with recoil):

$$b = 0 + \Delta b$$



${}^6\text{He}$ beta decay spectrum: SM results

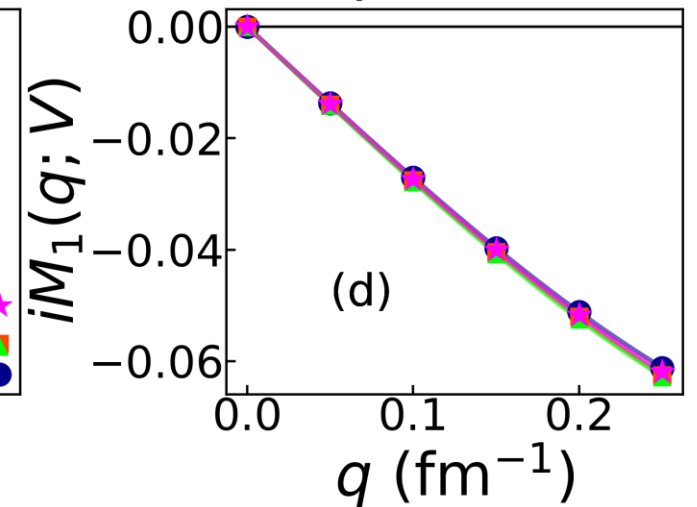
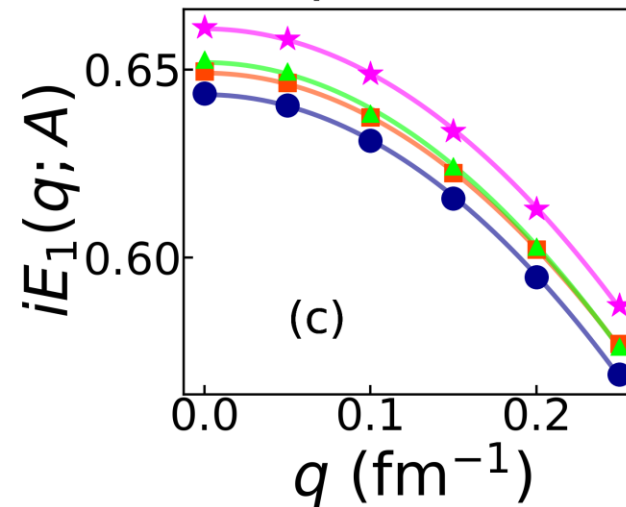
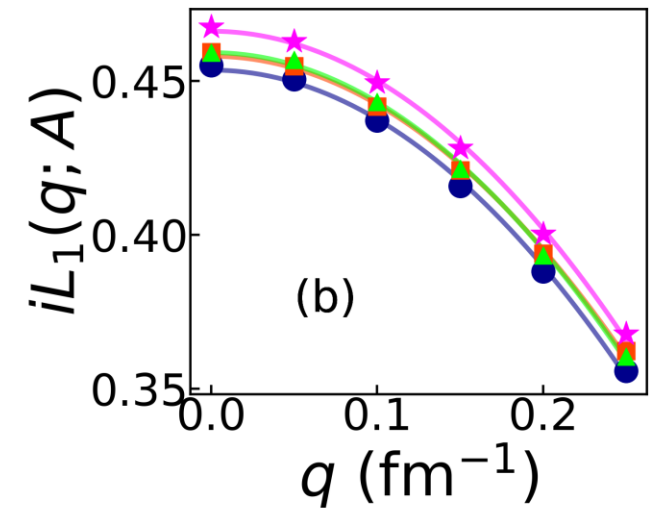
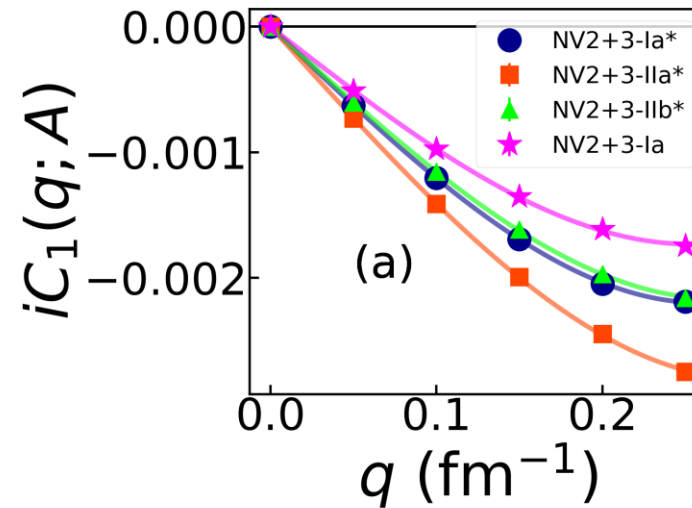
Fully retain two-body physics by leveraging low- q behavior

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

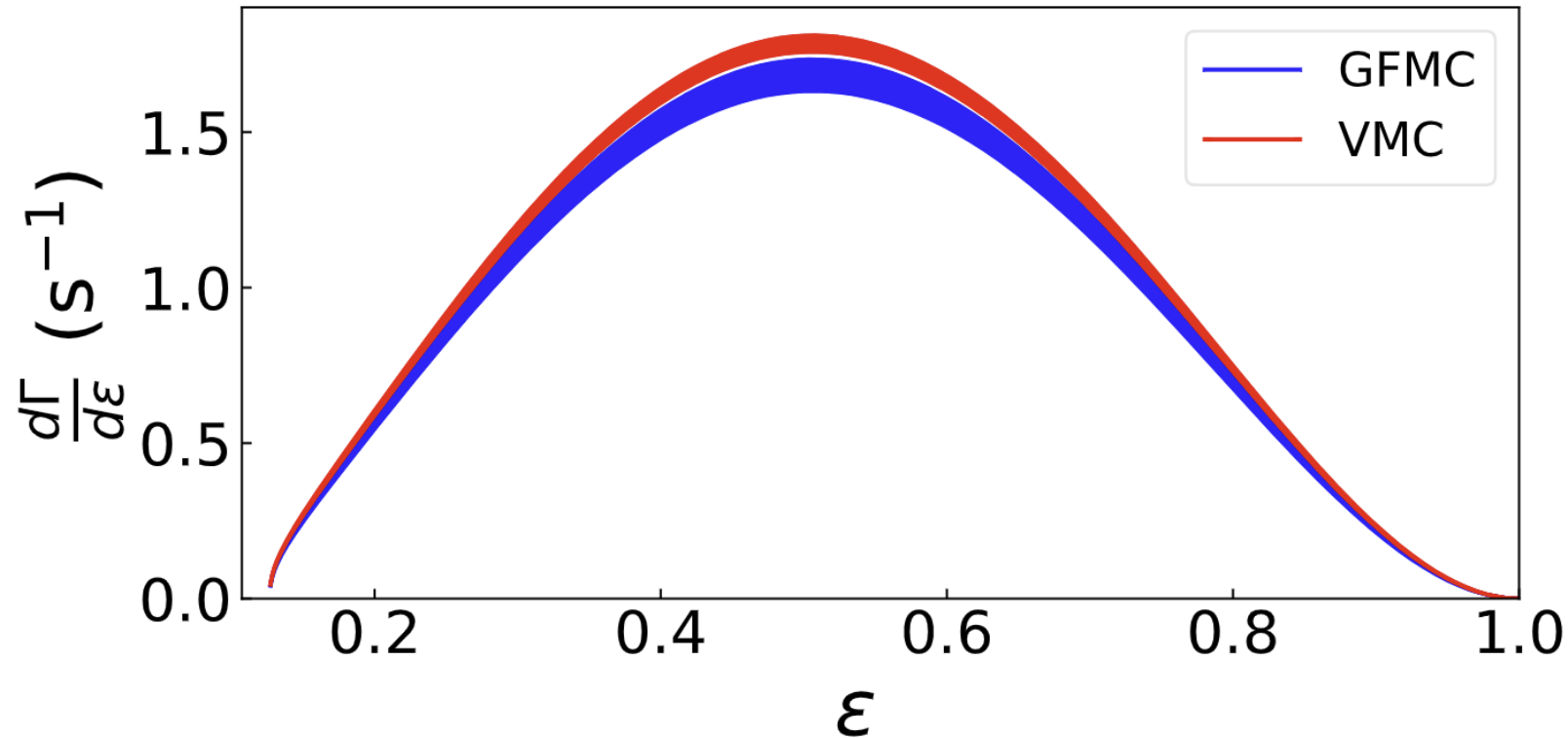
$$L_1(q; A) = \frac{i}{\sqrt{4\pi}} \langle {}^6\text{Li}, 10 | \hat{\mathbf{z}} \cdot \mathbf{j}_+^\dagger(q\hat{\mathbf{z}}; A) | {}^6\text{He}, 00 \rangle$$

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

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



${}^6\text{He}$ beta decay spectrum: SM results



$$\tau_{\text{VMC}} = 762 \pm 11 \text{ ms}$$

$$\tau_{\text{GFMC}} = 808 \pm 24 \text{ ms}$$

$$\tau_{\text{Expt.}} = 807.25 \pm 0.16 \pm 0.11 \text{ ms}$$

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

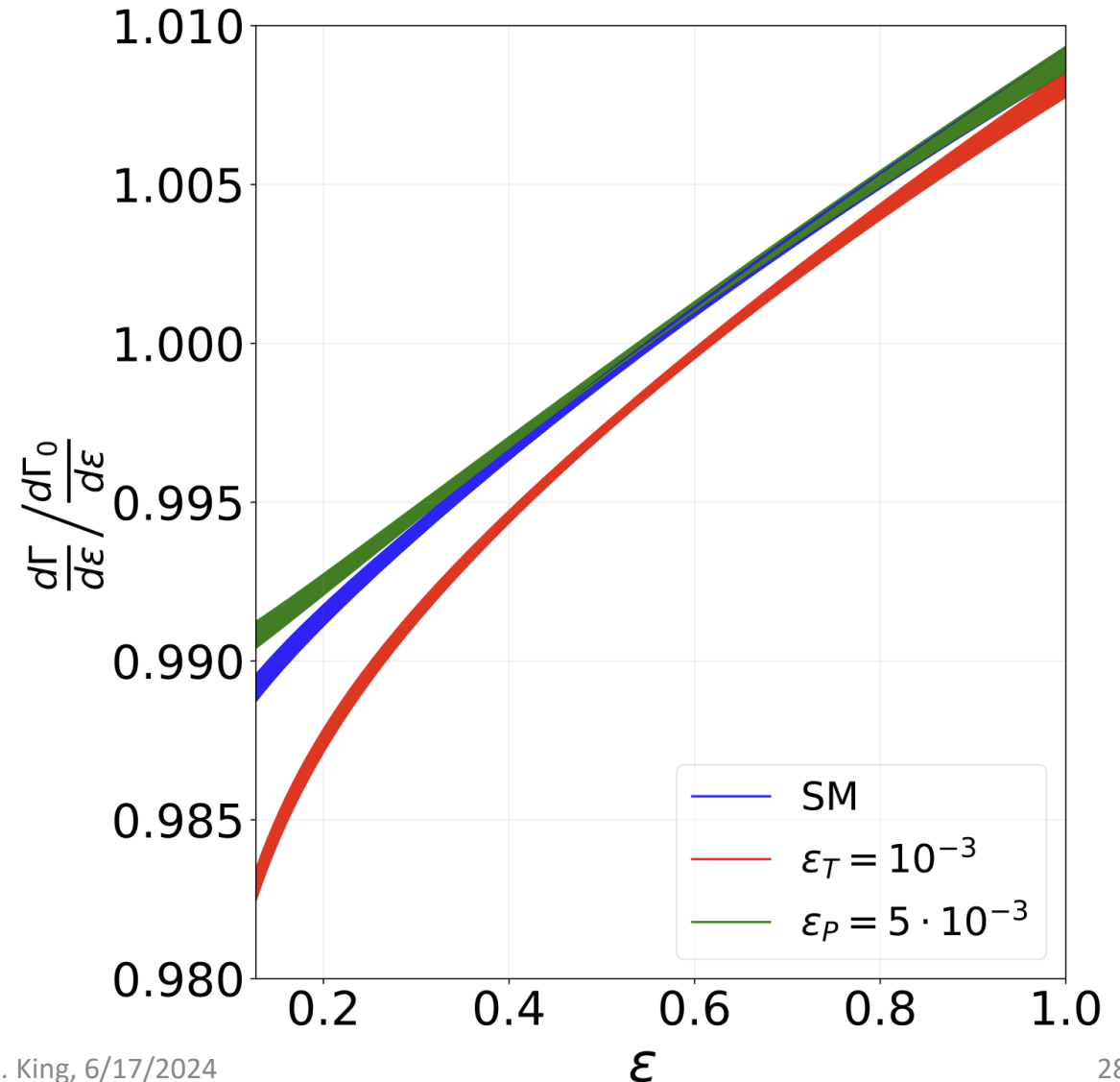
$$\varepsilon = \frac{E_e}{W_0}$$

${}^6\text{He}$ beta decay spectrum: BSM connections

Include new physics with strengths ϵ_i allowed from current analyses

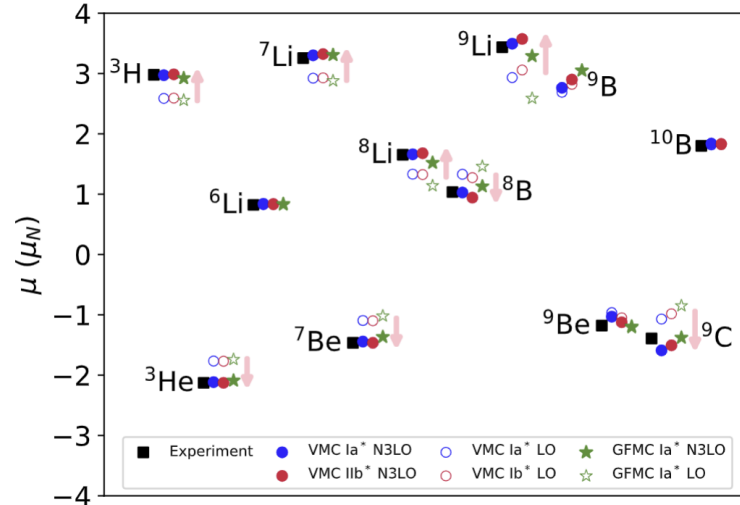
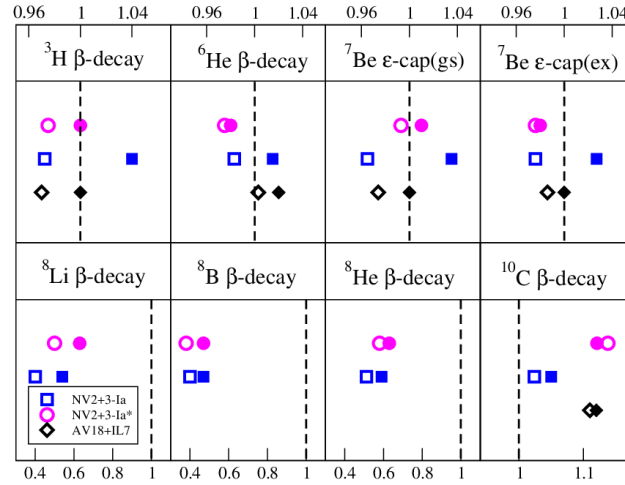
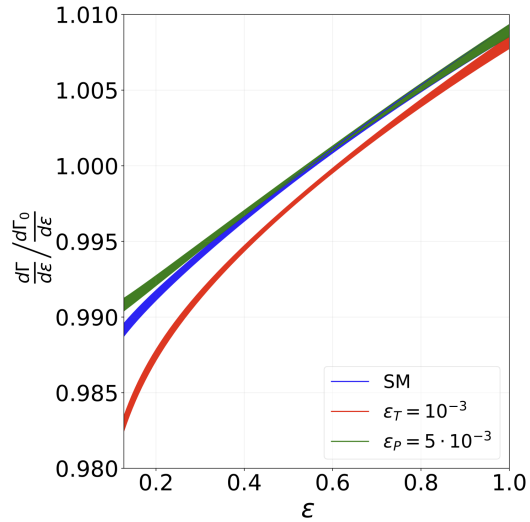
With permille precision, it will be possible to further constrain new physics

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





Conclusions



Many-body plus χ EFT is a powerful tool 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

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



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JLab+ODU: Gnech, Schiavilla

LANL: Carlson, Gandolfi, Mereghetti

LPC Caen: Hayen

ORNL: Baroni

UW: Cirigliano

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STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

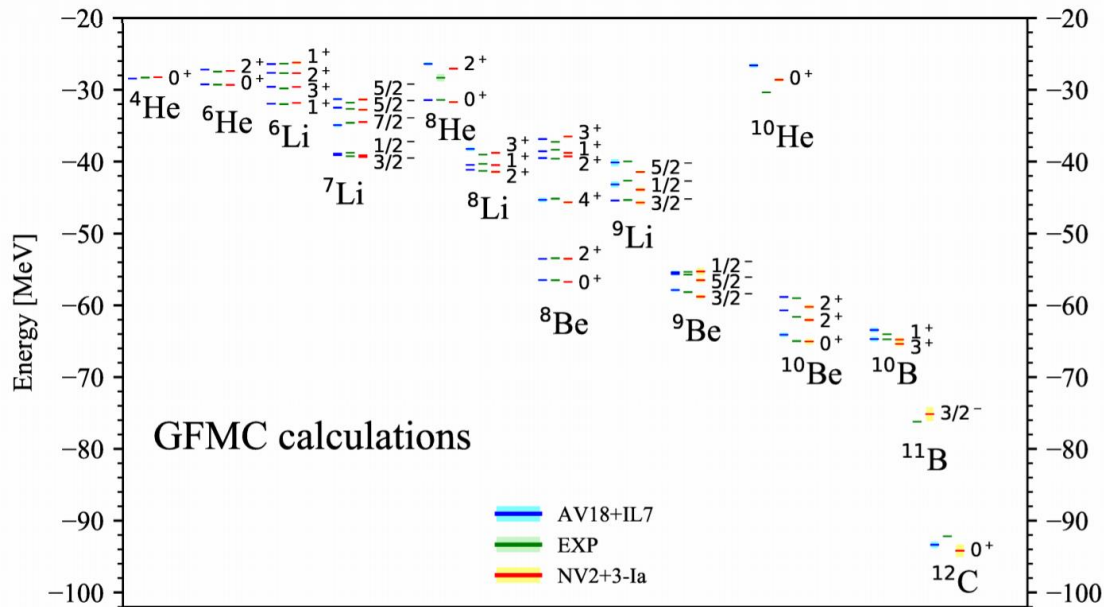


Additional Slides



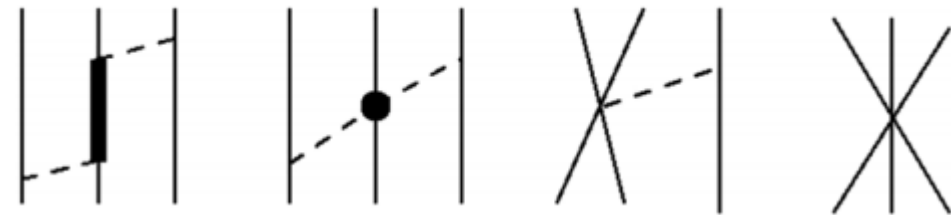
The Norfolk (NV2+3) Interaction

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



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



Piarulli et al. PRL 120, 052503 (2018)



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

Optimize when you minimize:

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



Green's Function Monte Carlo (GFMC)

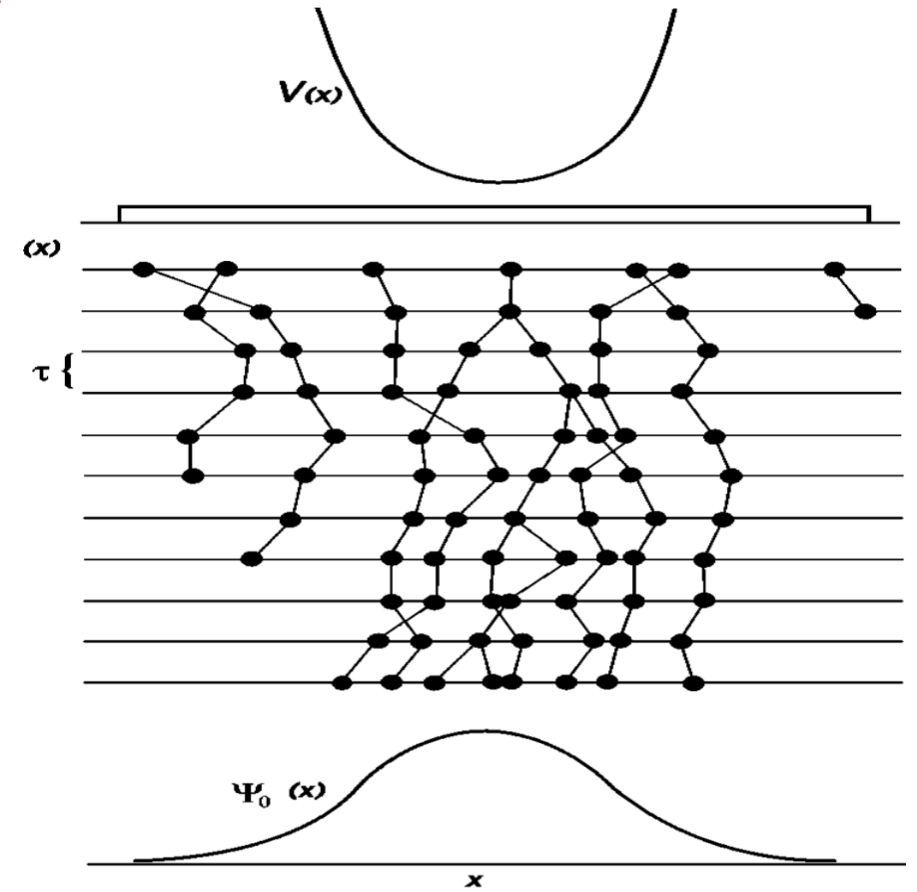
Can expand in exact states H : $|\Psi_V\rangle = c_0\psi_0 + \sum_{i=1}^n c_n|\psi_n\rangle$

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**

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



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



Mixed estimate

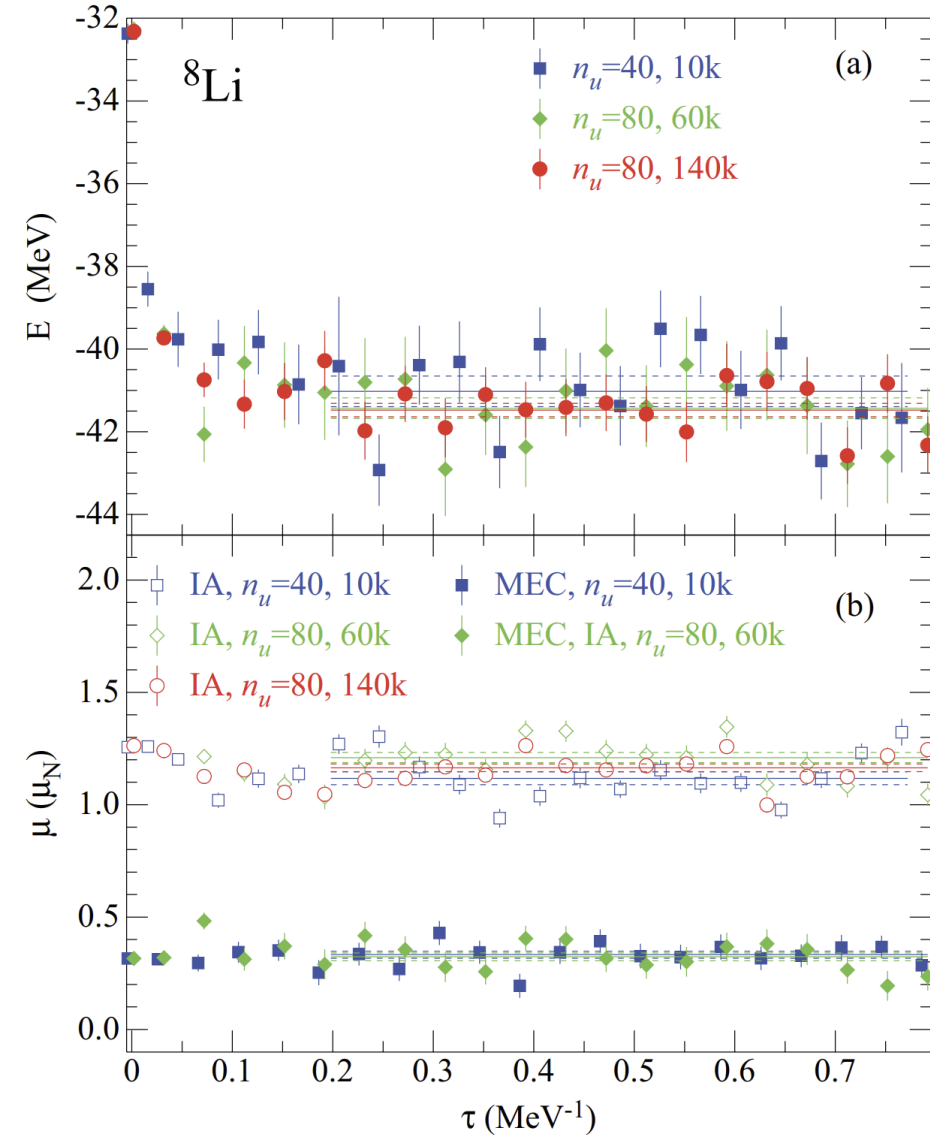
Assume small correction to VMC:

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

To first order in the correction:

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

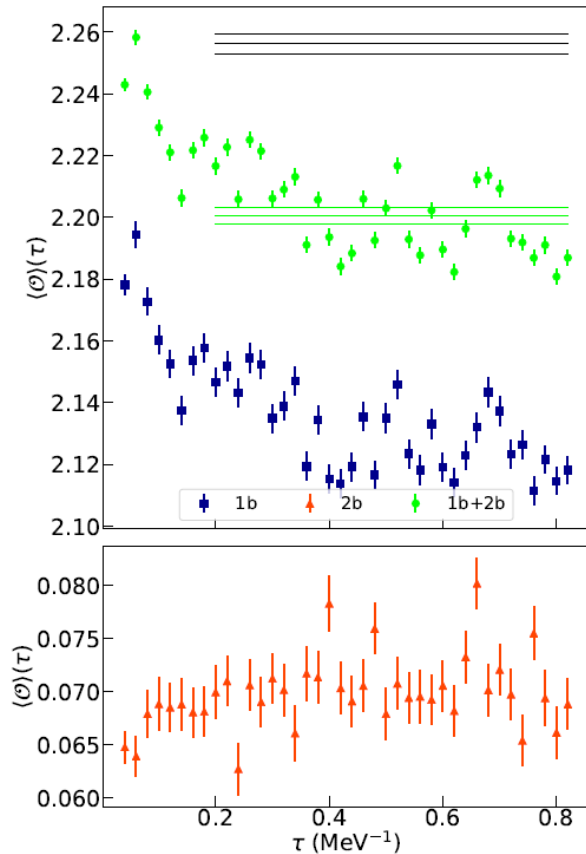
Pastore et al. PRC 87, 035503





Off-diagonal mixed estimate

${}^6\text{He} \rightarrow {}^6\text{Li}$ GT RME extrapolation



Mixed estimate for off-diagonal transitions:

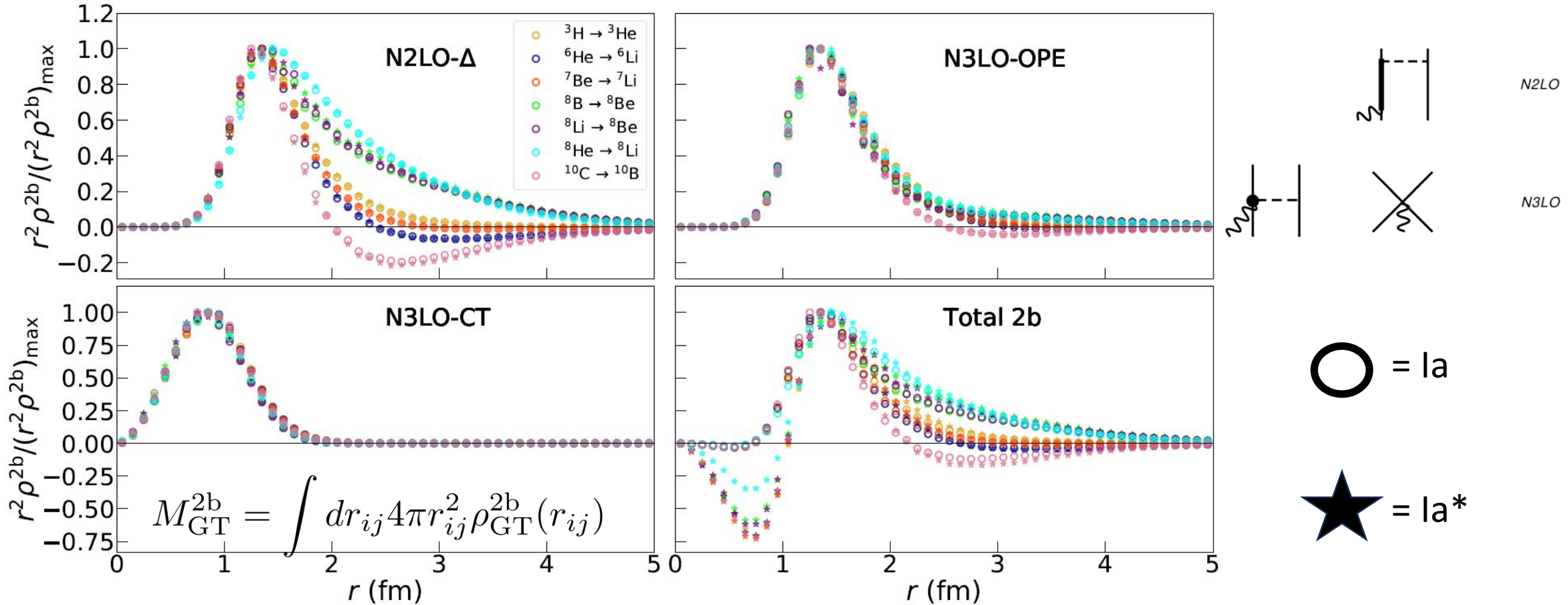
$$\langle \mathcal{O}(\tau) \rangle = \frac{\langle \Psi^f(\tau) | \mathcal{O} | \Psi^i(\tau) \rangle}{\sqrt{\langle \Psi^f(\tau) | \Psi^f(\tau) \rangle} \sqrt{\langle \Psi^i(\tau) | \Psi^i(\tau) \rangle}}$$

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

where

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

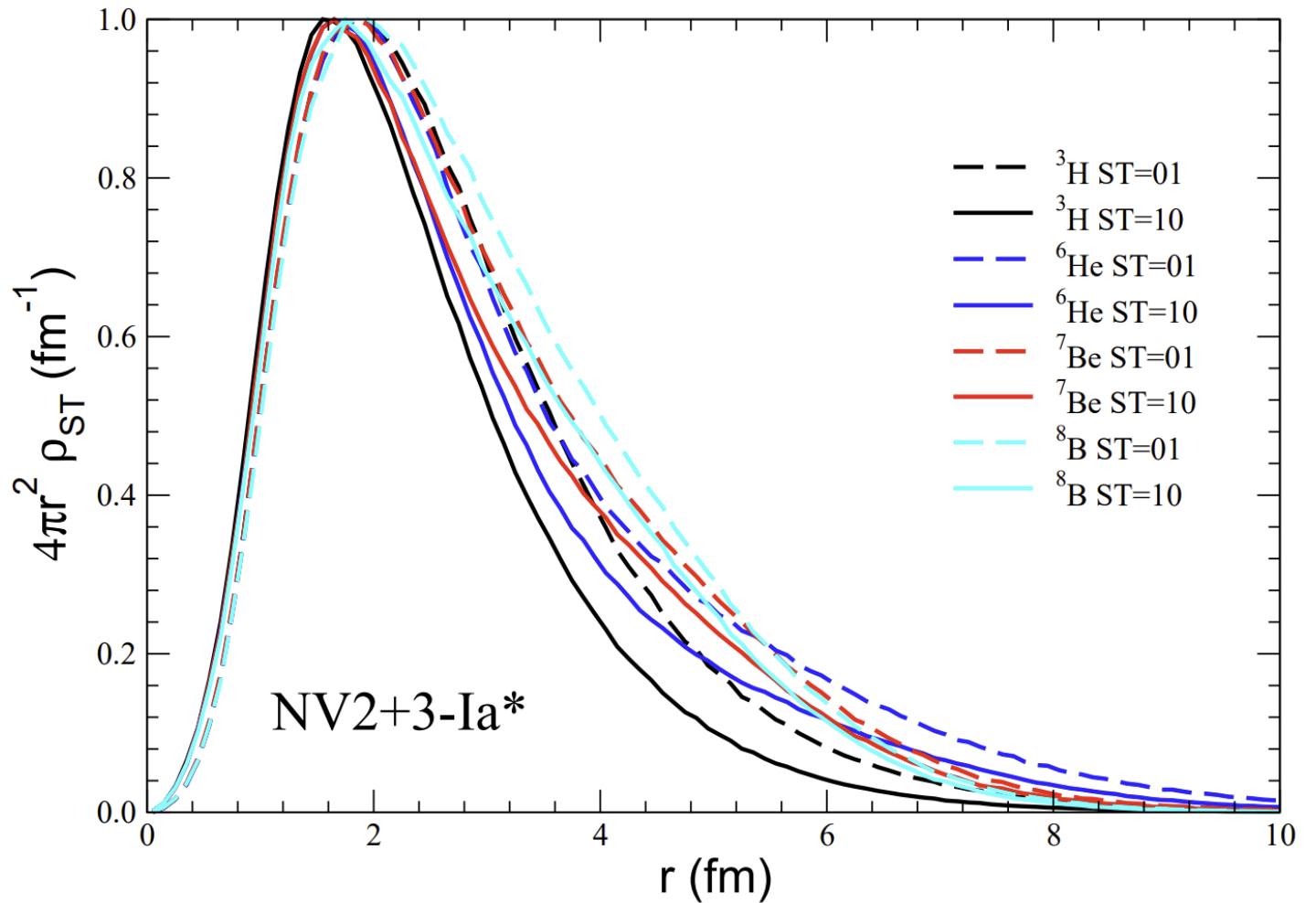
Scaled two-body transition densities



Explanation of universal scaling behaviors

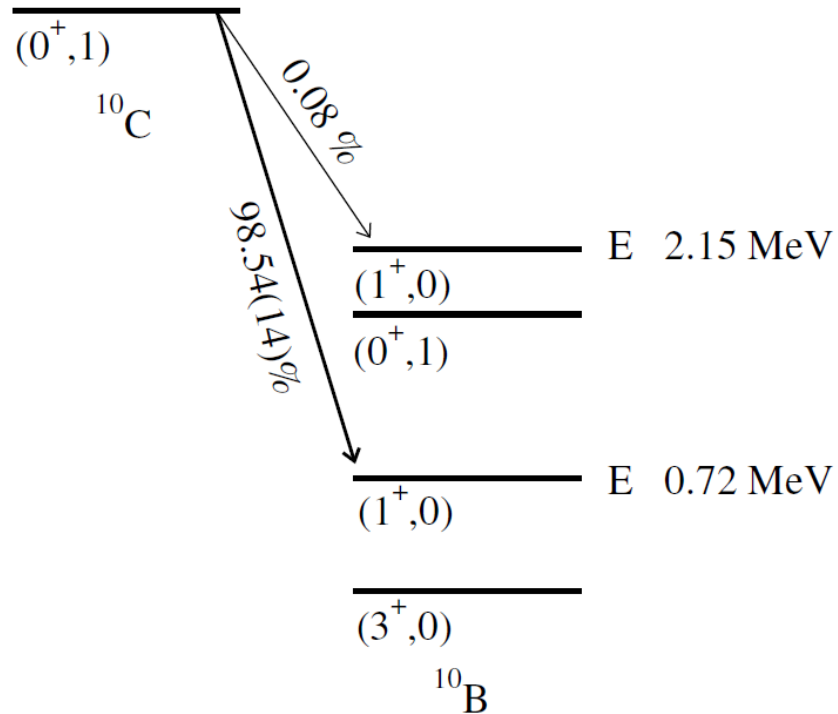
ST=01 and 10 pairs dominate short distances due to suppression of P-waves

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





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



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

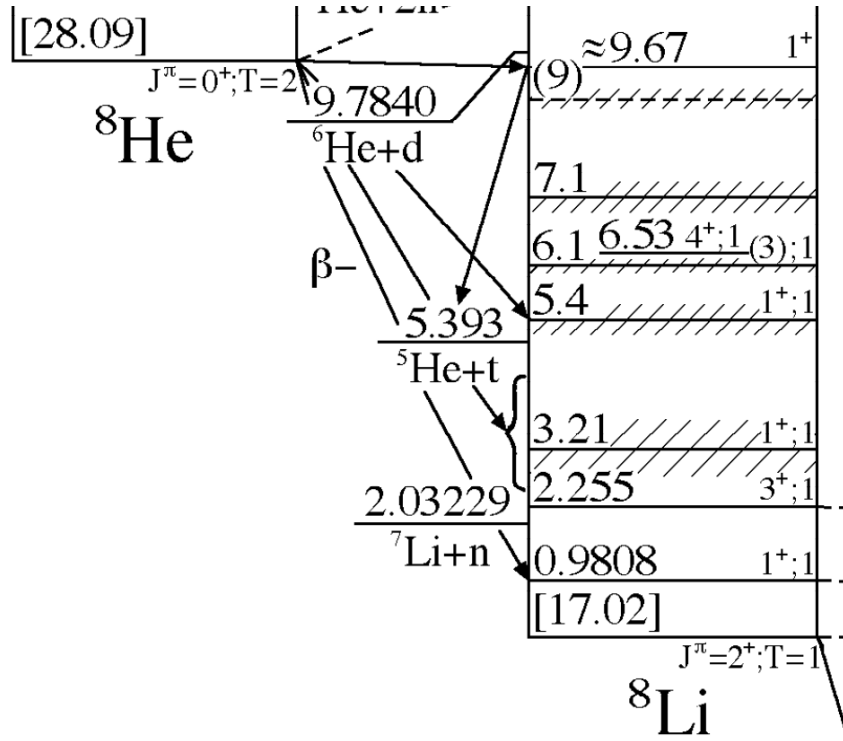
Two states of the same quantum numbers nearby

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



^8He to ^8Li GT beta decay



Three (1⁺;1) states within a few MeV

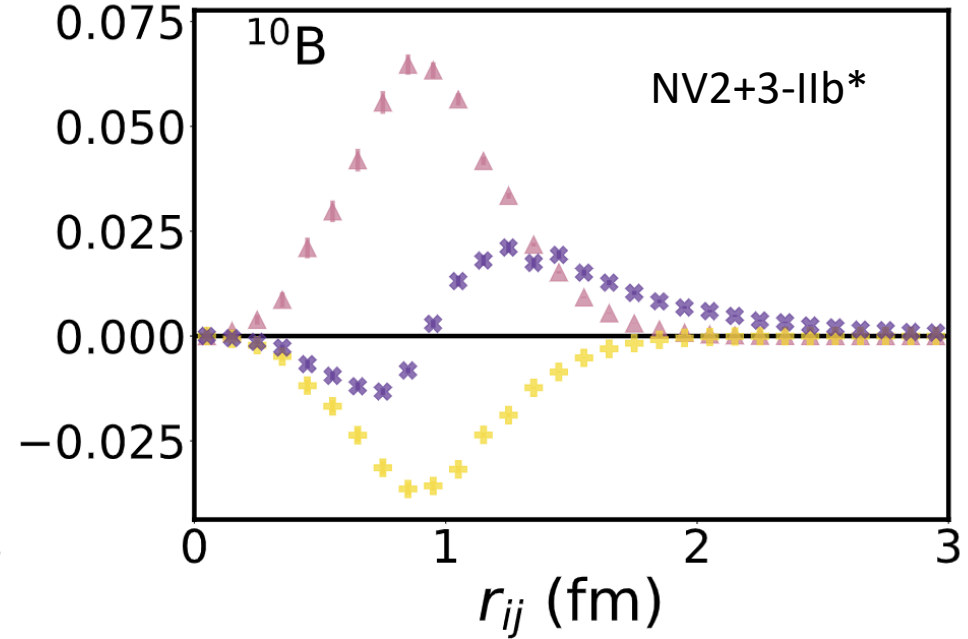
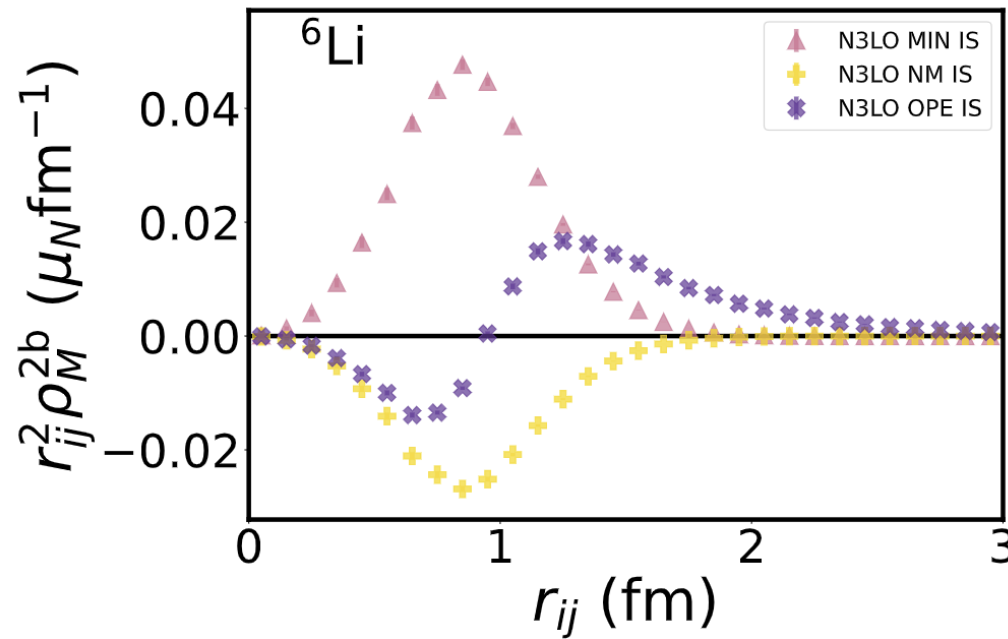
Different dominant spatial symmetries → sensitivity to the precise mixing of small components in the wave function

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

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



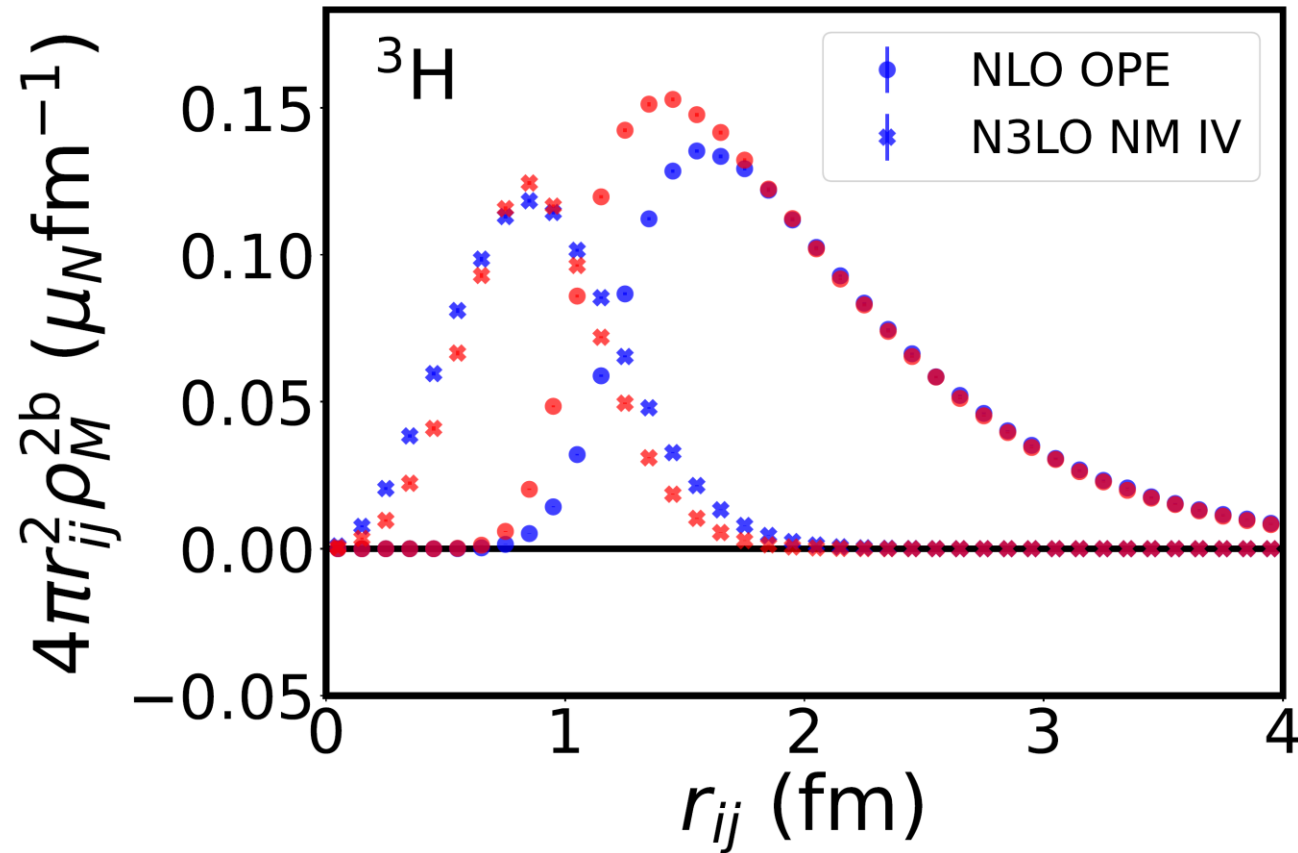
Isoscalar (IS) two-body magnetic densities



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



Cutoff dependence: magnetic currents



Regulator choice between model **la*** and **llb*** strongly influences the short-range dynamics



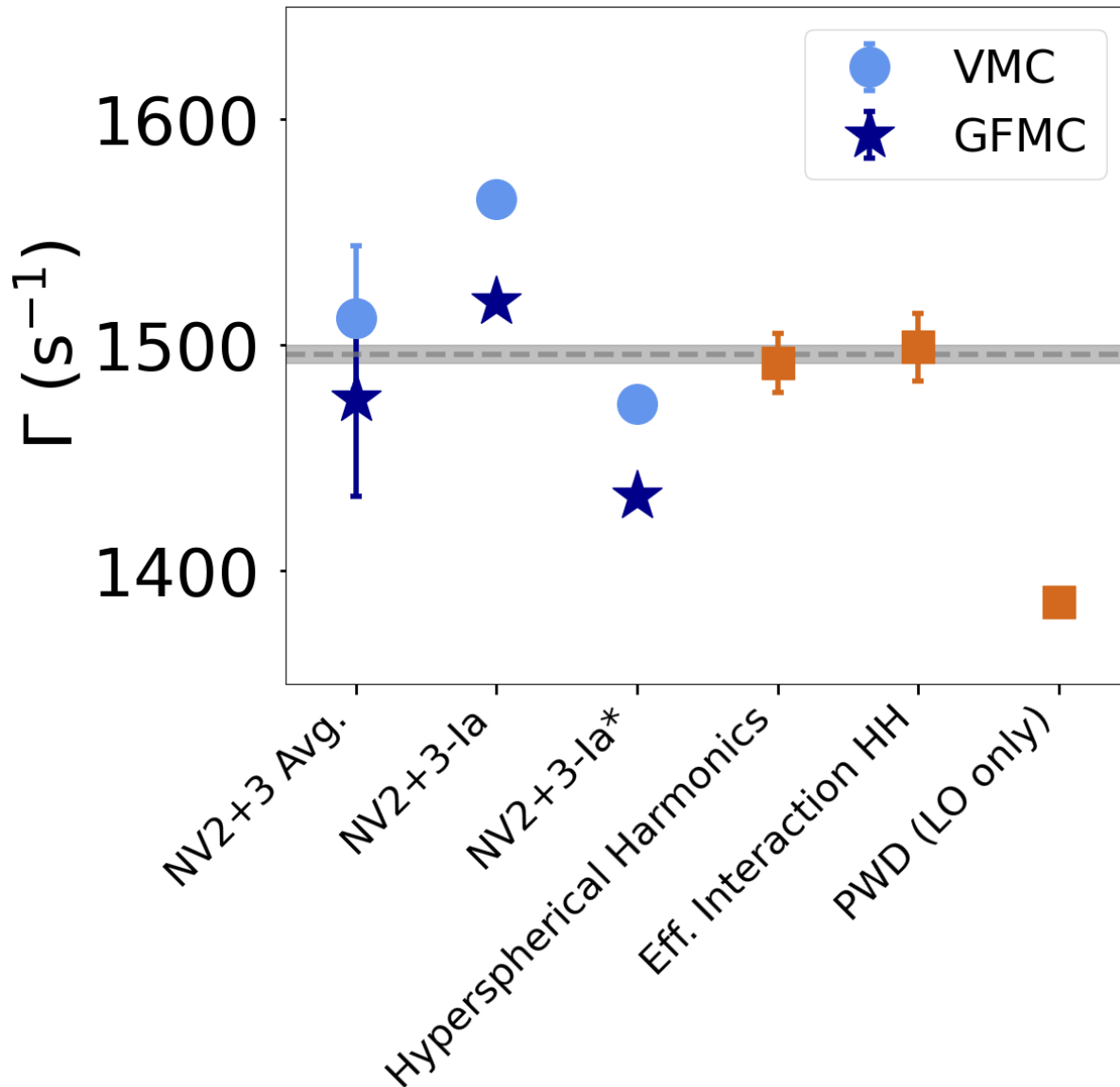
Partial Muon Capture Rates with QMC

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

$$\begin{aligned} \Gamma = & \frac{G_V^2}{2\pi} \frac{|\psi_{1s}^{\text{av}}|^2}{(2J_i + 1)} \frac{E_\nu^{*2}}{\text{recoil}} \sum_{M_f, M_i} \left[|\langle J_f, M_f | \rho(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2 + |\langle J_f, M_f | \mathbf{j}_z(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2 \right. \\ & + 2 \text{Re} \left[\langle J_f, M_f | \rho(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle \langle J_f, M_f | \mathbf{j}_z(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle^* \right] + |\langle J_f, M_f | \mathbf{j}_x(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2 \\ & \left. + |\langle J_f, M_f | \mathbf{j}_y(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2 - 2 \text{Im} \left[\langle J_f, M_f | \mathbf{j}_x(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle \langle J_f, M_f | \mathbf{j}_y(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle^* \right] \right] \end{aligned}$$



Partial muon capture rates with QMC



${}^3\text{He}(1/2^+;1/2) \rightarrow {}^3\text{H}(1/2^+;1/2)$ 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

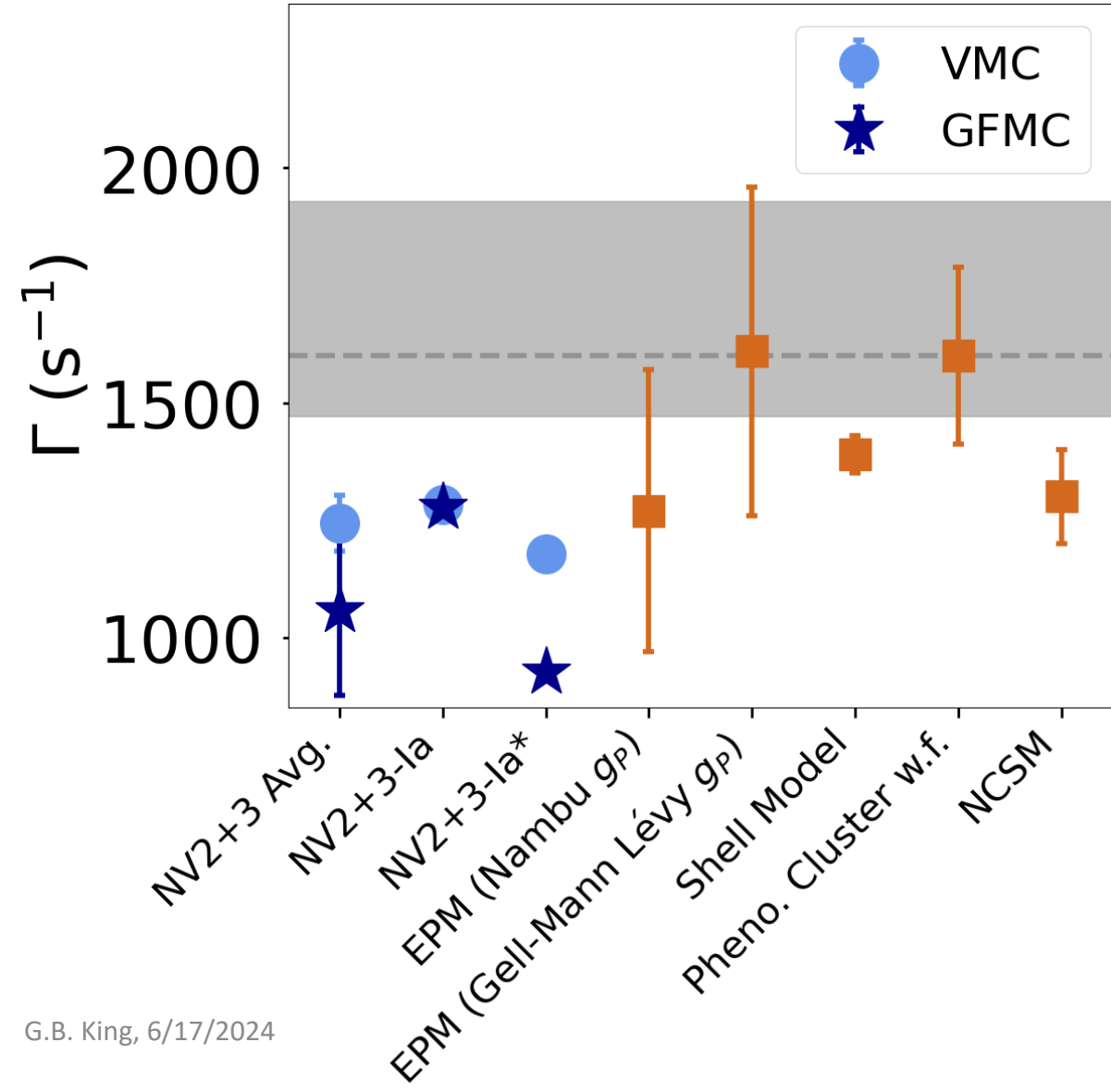


Partial muon capture rates with QMC

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

Subsequent NCSM evaluation agrees with QMC results

Could merit further attention





${}^6\text{He}$ Beta Decay Spectrum: Multipoles

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

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

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

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

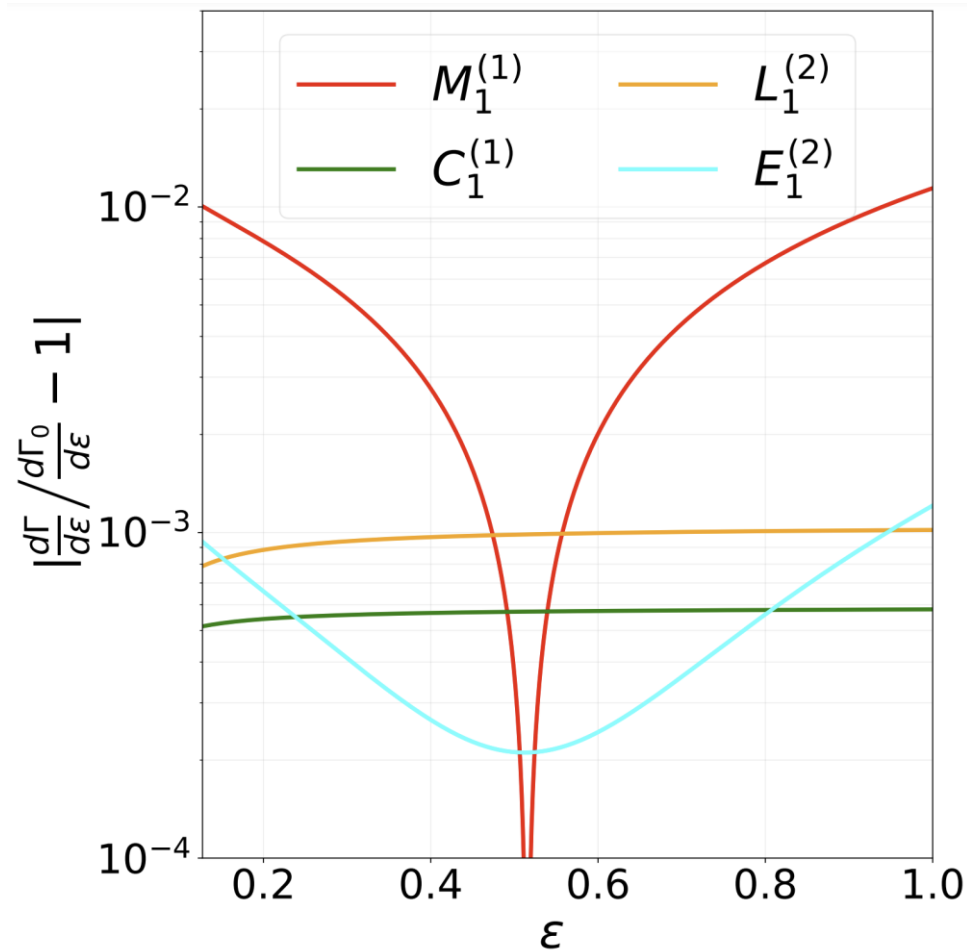
$$L_{JM}(q) = \frac{i}{q} \int d^3x \{ \nabla [j_J(qx) Y_{JM}(\Omega_x)] \} \cdot (\mathbf{j}(\mathbf{x}; V) + \mathbf{j}(\mathbf{x}; A))$$

$$E_{JM}(q) = \frac{1}{q} \int d^3x [\nabla \times j_J(qx) \mathcal{Y}_{JJ_1}^M(\Omega_x)] \cdot (\mathbf{j}(\mathbf{x}; V) + \mathbf{j}(\mathbf{x}; A))$$

$$M_{JM}(q) = \int d^3x [j_j(qx) \mathcal{Y}_{JJ_1}^M(\Omega_x)] \cdot (\mathbf{j}(\mathbf{x}; V) + \mathbf{j}(\mathbf{x}; A))$$

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

${}^6\text{He}$ beta decay spectrum: SM results



$$\tau_{\text{VMC}} = 762 \pm 11 \text{ ms}$$

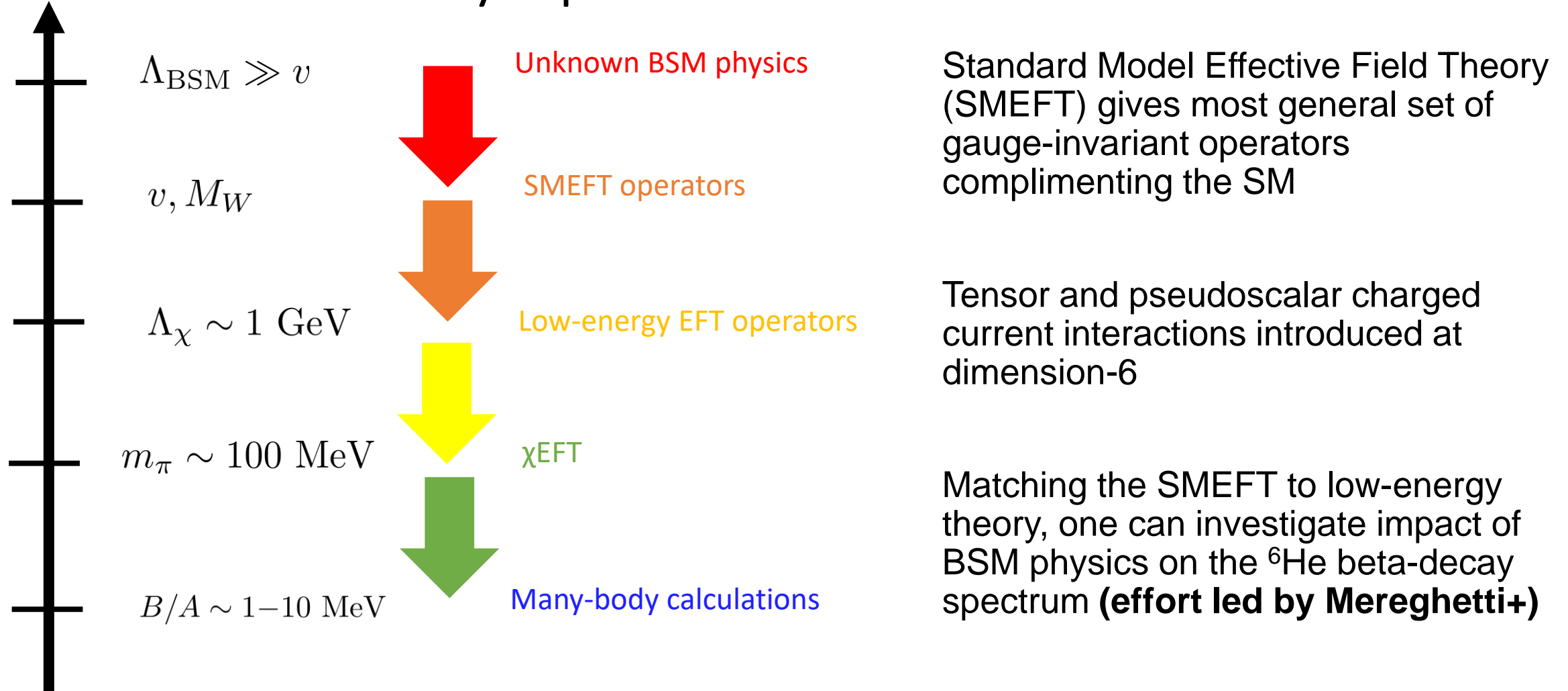
$$\tau_{\text{GFMC}} = 808 \pm 24 \text{ ms}$$

$$\tau_{\text{Expt.}} = 807.25 \pm 0.16 \pm 0.11 \text{ ms}$$

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

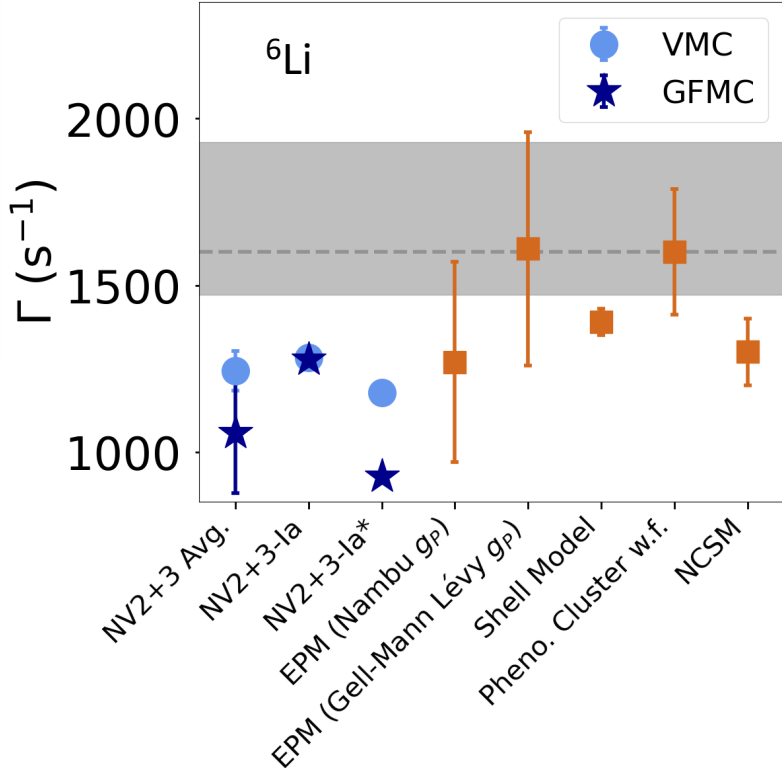
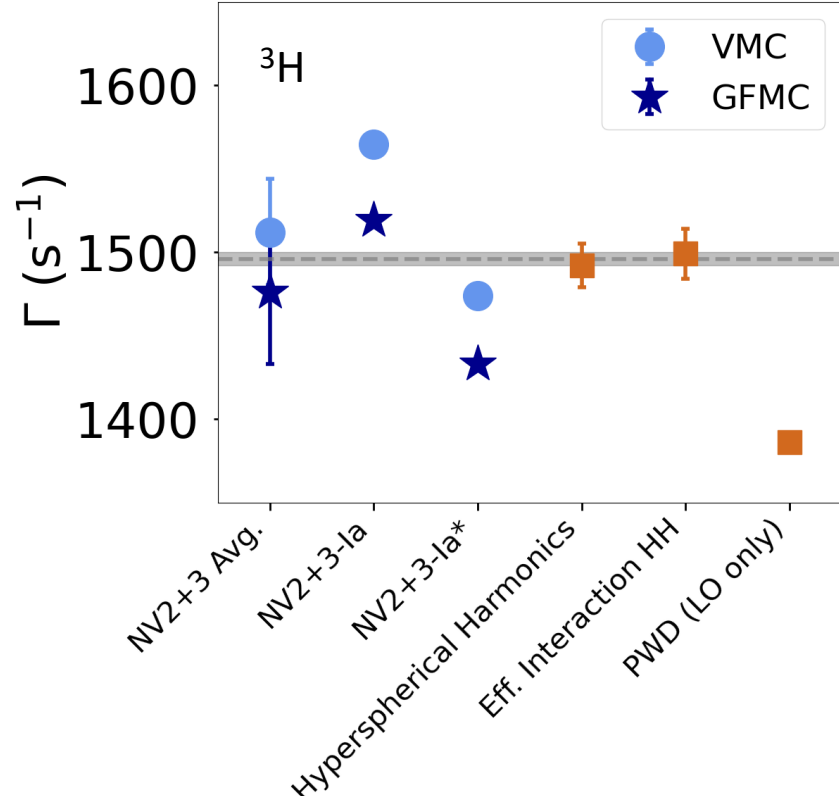
$$\varepsilon = \frac{E_e}{\omega}$$

${}^6\text{He}$ Beta Decay Spectrum: BSM Connections





Muon capture: non-zero momentum transfer



Momentum transfer ~ 100 MeV/c

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

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

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