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Electroweak processes with quantum Monte Carlo methods

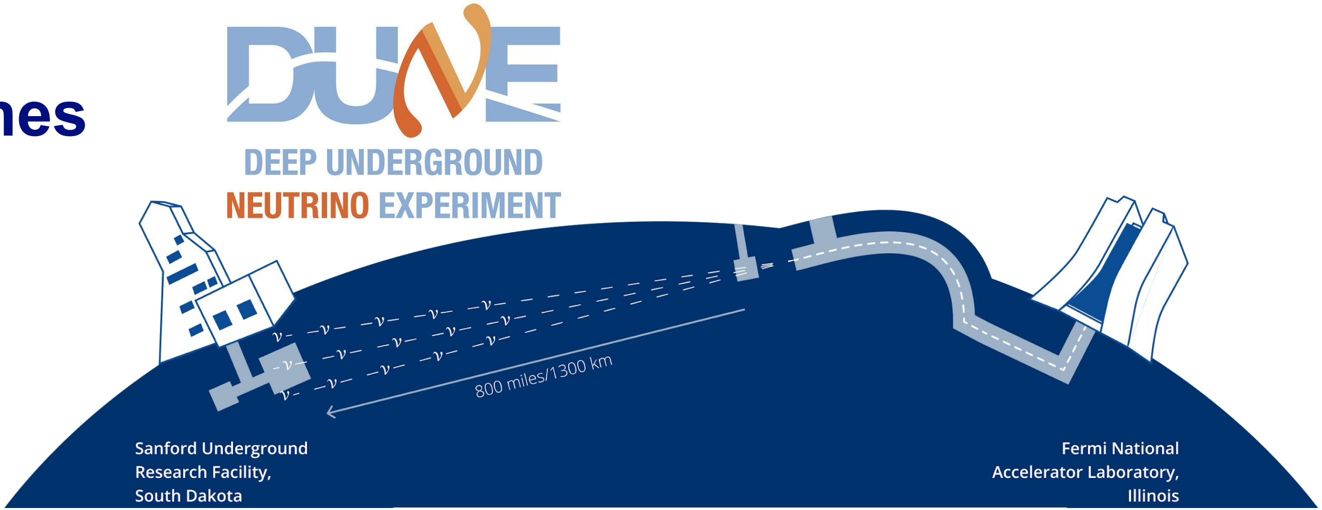
Garrett King

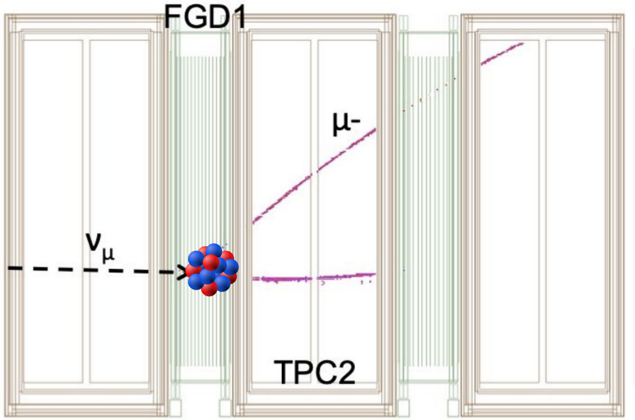
NISMB 2025
Mainz, Germany
5/13/2025

LA-UR-25-24452

Neutrino searches

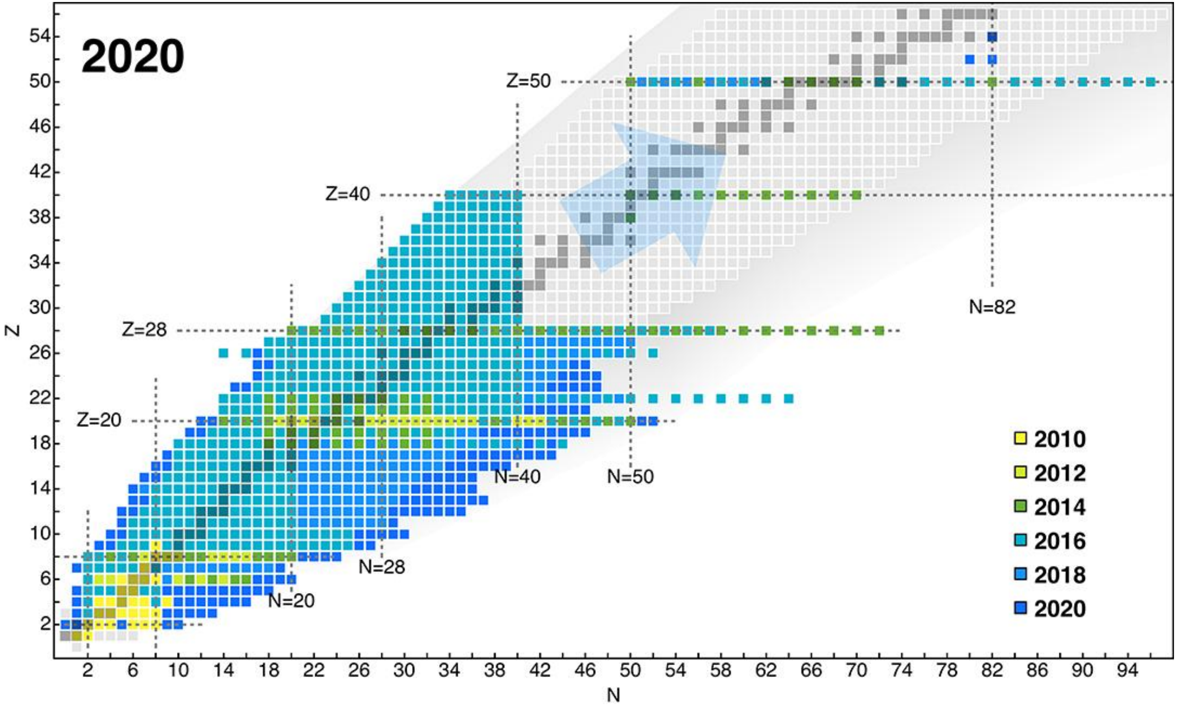
Fermilab / Sandbox Studio, Chicago





Adapted from K. Mahn,
"The Theoretical Cross Section Needs of Future Long Baseline Experiments"
at INT WORKSHOP INT-23-86W

Growing reach of many-body methods

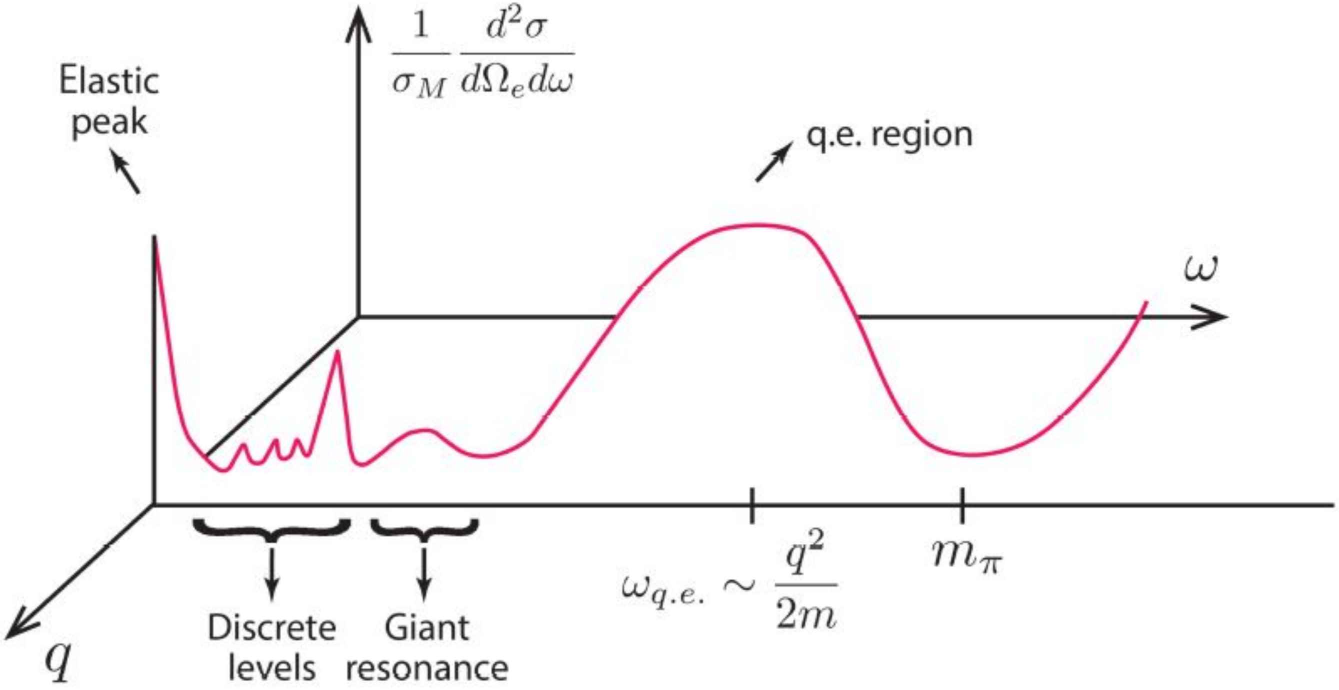


H. Hergert, J. Front. Phys. 8 (2020)

The reach of many-body approaches has also expanded greatly in the last decade

We can now study nuclei that intersect with the frontiers probed by experiment

The theoretical picture



Microscopic description of nuclei

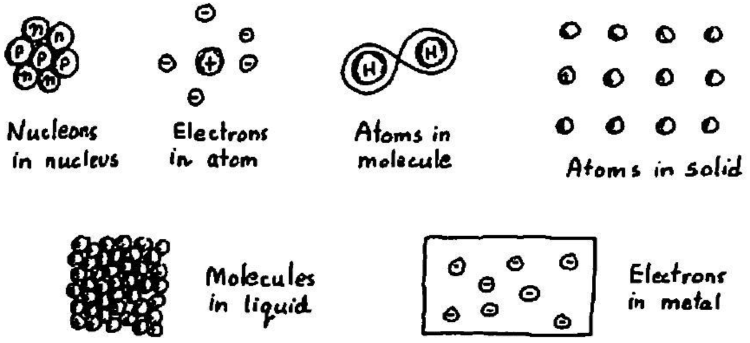
The quantum many-body problem

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

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The quantum many-body problem

Wave function of ***A* nucleons** containing information about ***coordinates*, *spins*, *and isospins***

$$\Psi(r_1, r_2, \ldots, r_A; s_1, s_2, \ldots, s_A; t_1, t_2, \ldots, t_A)$$

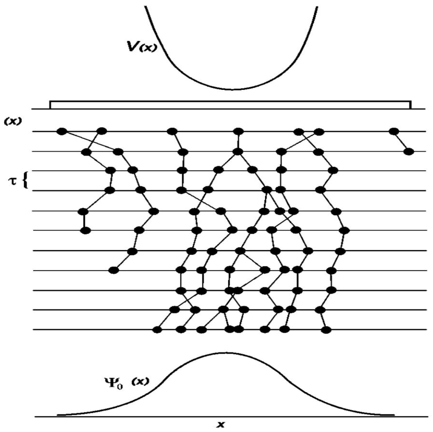
$$\dim(\Psi) = 3A \times 2^A \times \frac{A!}{N!Z!}$$

Turn to numerical approaches; In this talk, **Quantum Monte Carlo**

Quantum Monte Carlo

Solving the many-body problem using random sampling to compute integrals

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***

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

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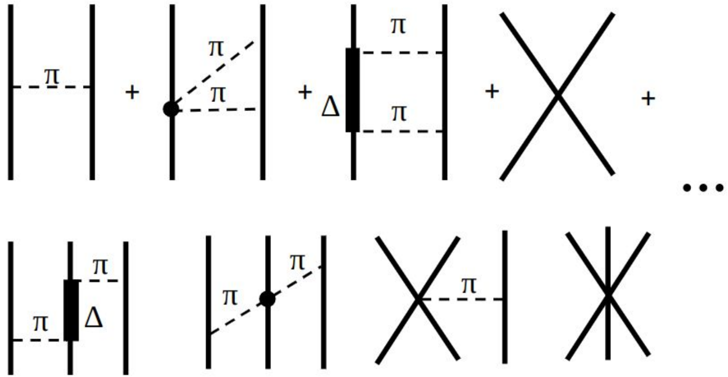
Foulkes et al. Rev. Mod. Phys. 73, 33 (2001)

Nuclear interactions

$$H = \sum_i T_i + \sum_{ij} v_{ij} + \sum_{ijk} V_{ijk} + \ldots$$



Contains kinetic energies, plus two-body and three-body interactions

Long-range attraction mediated by the lightest meson, the pion (π)

Intermediate range attraction involving two pions, and sometimes excitation of nucleons (ex: the Δ)

Short-range repulsion from heavier intermediaries represented by “contact” terms

Need for three-body forces to bind light systems

Electroweak charge and current operators

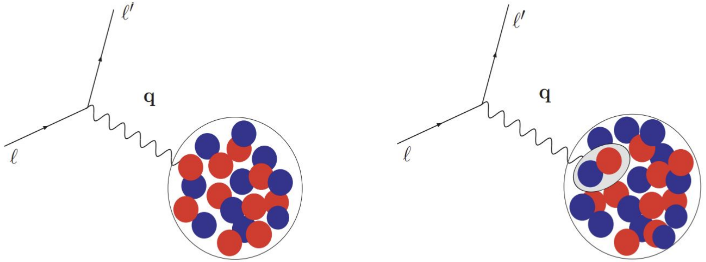
Need electromagnetic and weak current operators to study decays

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)

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Electron scattering

Cross section

$$\frac{d\sigma}{d\Omega} = 4\pi\sigma_M f_{\rm rec}^{-1} \left[\frac{Q^4}{q^4} F_L^2(q) + \left(\frac{Q^2}{2q^2} + \tan^2\theta_e/2 \right) F_T^2(q) \right]$$

In elastic scattering:

$$F_T^2(q) = F_M^2(q) = \frac{1}{2J_i+1} \sum_{L=1}^{\infty} |\langle J_f || M_L(q) || J_i \rangle|^2 \qquad F_L^2(q) = \frac{1}{2J_i+1} \sum_{L=0}^{\infty} |\langle J_f || C_L(q) || J_i \rangle|^2$$

Cross section

$$\frac{d\sigma}{d\Omega} = 4\pi\sigma_M f_{\rm rec}^{-1} \left[\frac{Q^4}{q^4} F_L^2(q) + \left(\frac{Q^2}{2q^2} + \tan^2\theta_e/2\right) F_T^2(q)\right]$$

In elastic scattering:

$$\boxed{F_T^2(q) = F_M^2(q)} = \frac{1}{2J_i+1}\sum_{L=1}^{\infty} |\langle J_f||M_L(q)||J_i\rangle|^2$$

Sensitive to single particle structure

$$\boxed{F_L^2(q)} = \frac{1}{2J_i+1}\sum_{L=0}^{\infty} |\langle J_f||C_L(q)||J_i\rangle|^2$$

Sensitive to global properties

Cross section

$$\frac{d\sigma}{d\Omega} = 4\pi\sigma_M f_{\text{rec}}^{-1} \left[\frac{Q^4}{q^4} F_L^2(q) + \left(\frac{Q^2}{2q^2} + \tan^2\theta_e/2 \right) F_T^2(q) \right]$$

In elastic scattering:

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QMC is used to compute reduced multipoles

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Cross section

$$\frac{d\sigma}{d\Omega d\omega} = 4\pi\sigma_M f_{\mathrm{rec}}^{-1}\left[\frac{Q^4}{q^4}R_L(q,\omega) + \left(\frac{Q^2}{2q^2} + \tan^2\theta_e/2\right)R_T(q,\omega)\right]$$

In quasi-elastic scattering:

$$R_L(q,\omega) = \sum_f |\langle\Psi_f|\rho(q,\omega)|\Psi_0\rangle|^2$$

$$R_T(q,\omega) = \sum_{\alpha,f} |\langle\Psi_f|j_\alpha(q,\omega)|\Psi_0\rangle|^2$$

Elastic scattering

Computation of reduced multipoles

Reduced multipoles are defined by **[Carlson and Schiavilla RMP 70 (1998)]**:

$$\begin{aligned}
\langle J_f M|\rho^\dagger(q)|J_i M\rangle &= (-1)^{J_i-M}\sum_L \sqrt{4\pi}(-i)^L P_L(\cos\theta) c^M_{J_f J_i L} C_L(q)\,, \\
\langle J_f M|\hat{\mathbf{e}}^*_\lambda \cdot \mathbf{j}^\dagger(q)|J_i M\rangle &= (-1)^{J_i-M+1}\sum_{L\geq 1} \sqrt{8\pi^2}\frac{(-i)^L}{\sqrt{2L+1}} Y^*_{LM}(\theta,\phi) c^M_{J_f J_i L} M_L(q)
\end{aligned}$$

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Computation of reduced multipoles

Reduced multipoles are defined by **[Carlson and Schiavilla RMP 70 (1998)]**:

$$\boxed{\langle J_f M|\rho^\dagger(q)|J_i M\rangle} = \boxed{(-1)^{J_i-M}\sum_L \sqrt{4\pi}(-i)^L P_L(\cos\theta)c^M_{J_f J_i L}}\boxed{C_L(q)}\,,$$

$$\langle J_f M|\hat{\mathbf{e}}^*_\lambda\cdot\mathbf{j}^\dagger(q)|J_i M\rangle = \boxed{(-1)^{J_i-M+1}\sum_{L\geq 1}\sqrt{8\pi^2}\frac{(-i)^L}{\sqrt{2L+1}}Y^*_{LM}(\theta,\phi)c^M_{J_f J_i L}}\boxed{M_L(q)}$$

Complex value calculable with QMC techniques

A complex coefficient

Obtained by inverting system of equations generated by independent choices of q

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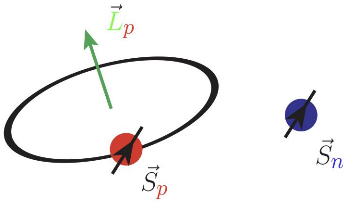
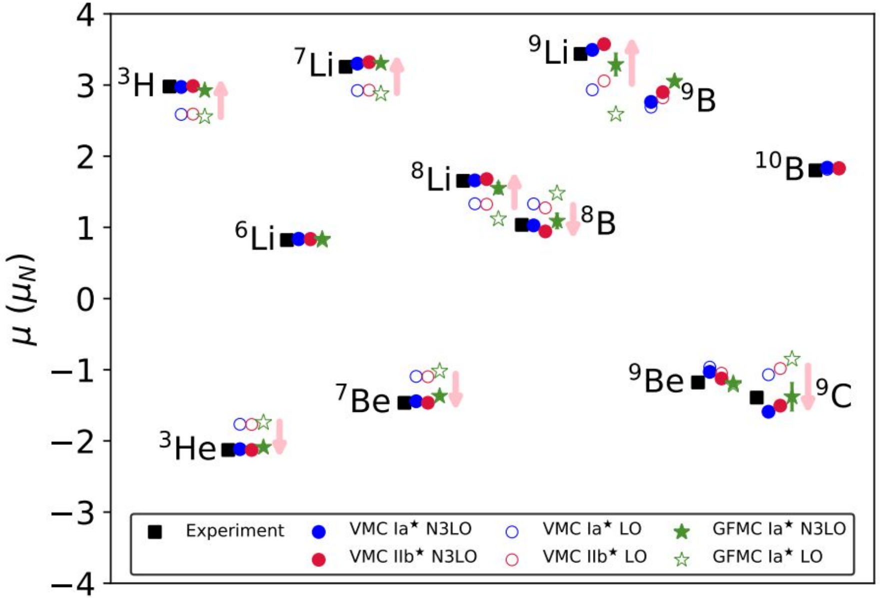
Magnetic moments

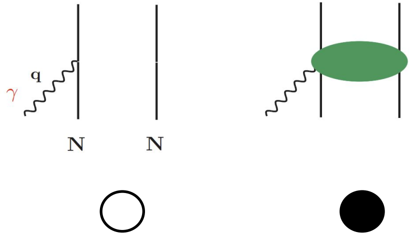
One-body picture:

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



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





Chambers-Wall et al. PRL 133, 212501 (2024)
Chambers-Wall et al. PRC 110, 054316 (2024)

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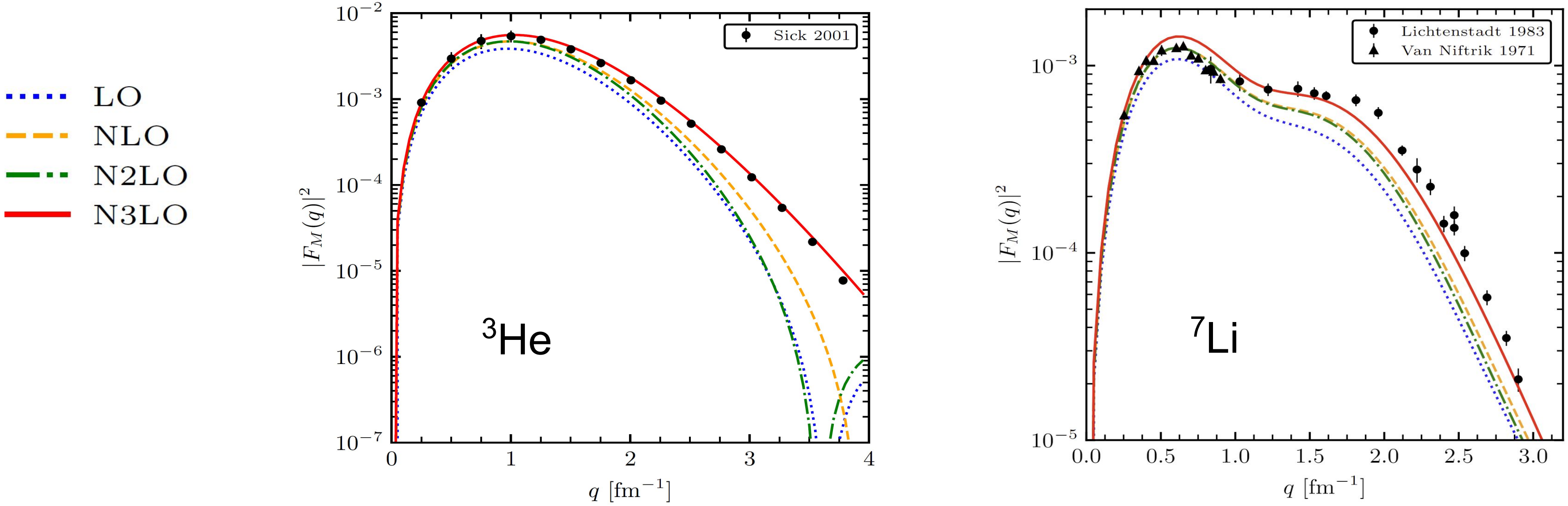
VMC magnetic form factors

NV2+3-IIb*

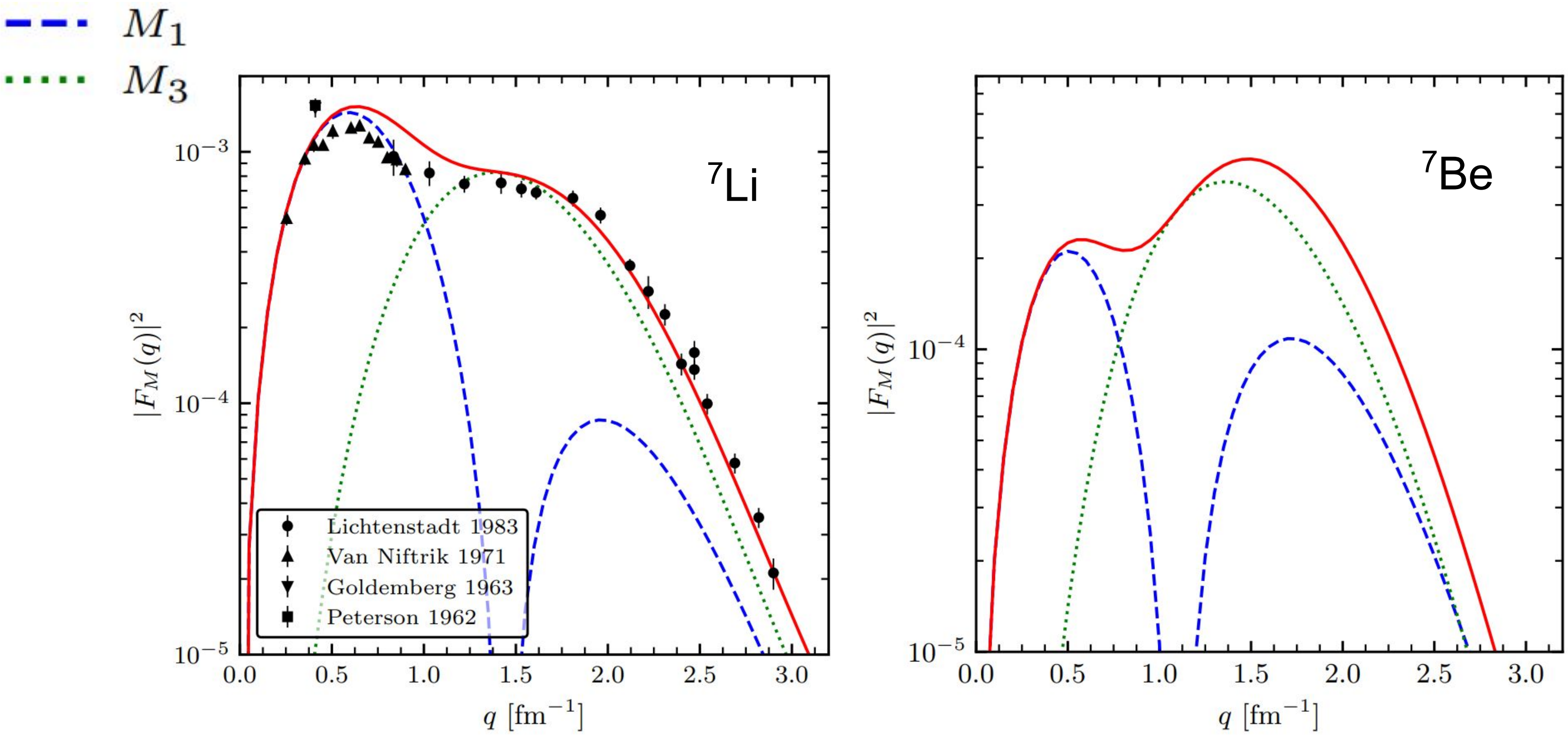


Two-body effects needed to describe data up to q ~ 600 MeV

Minimal model dependence in total form factor for A = 3 – 10

Chambers-Wall et al. PRL 133, 212501 (2024)
Chambers-Wall et al. PRC 110, 054316 (2024)

Magnetic form factors for mirror nuclei



Chambers-Wall et al. PRL 133, 212501 (2024)
Chambers-Wall et al. PRC 110, 054316 (2024)

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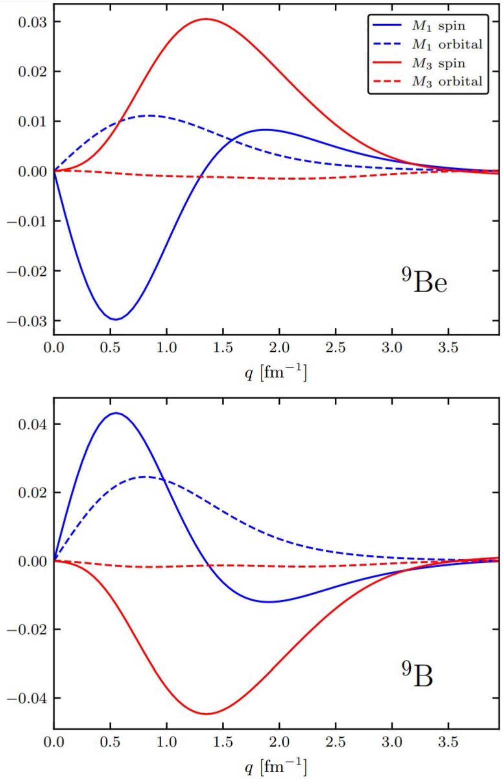
Spin-orbit interference in M1



Orbital contribution generates positive contribution to M1

Spin can be positive or negative, depending on single particle structure

Minimal contribution orbital contribution to M3

Destructive interference between spin and orbit present in nuclei with smaller M1 peak than M3

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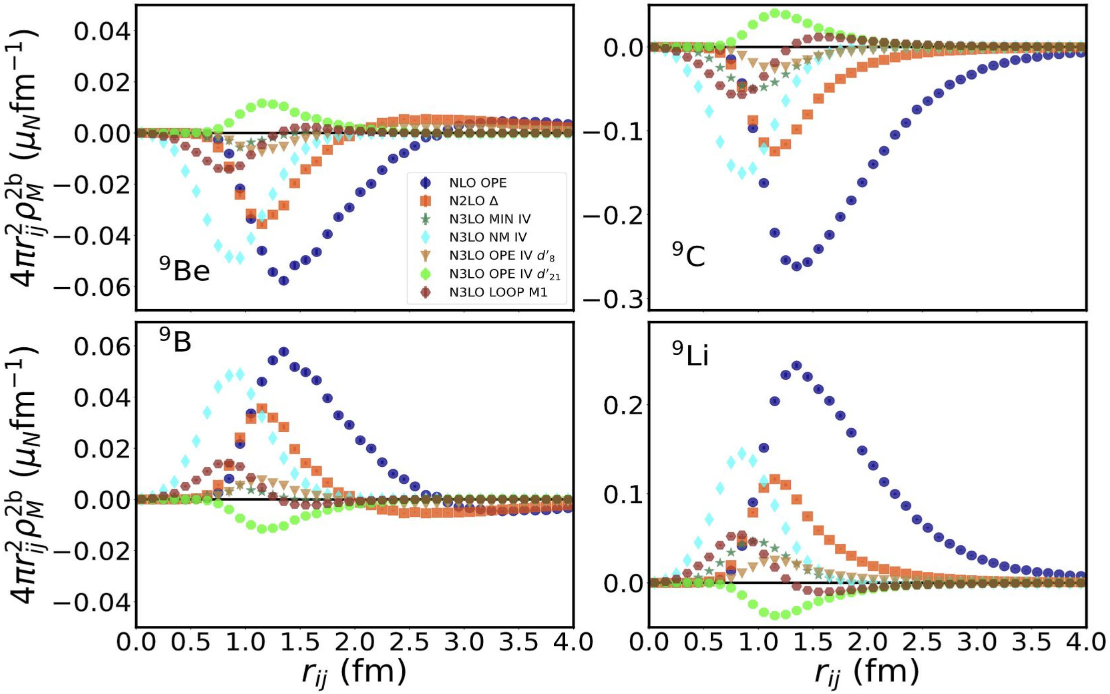
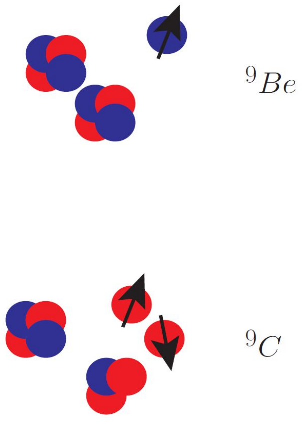
Chambers-Wall et al. PRL 133, 212501 (2024)
Chambers-Wall et al. PRC 110, 054316 (2024)

Structural effects in two-body currents

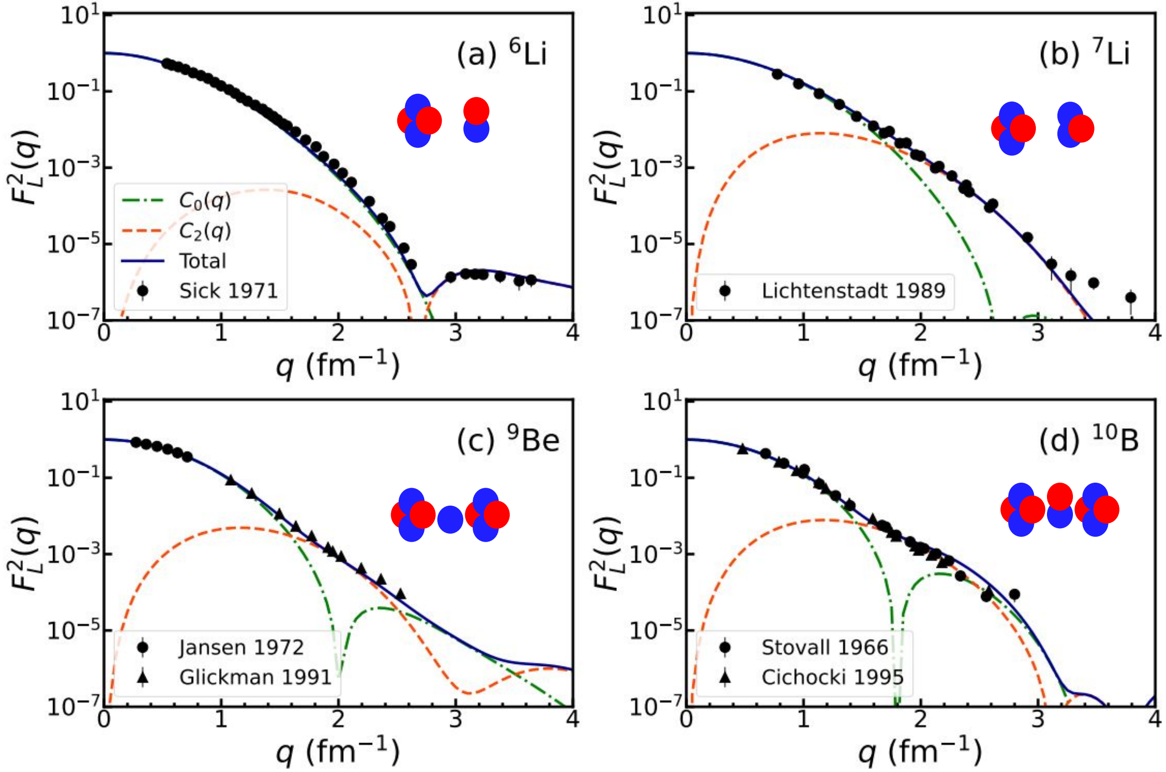




$$\mu^{2b} = \int dr_{ij} 4\pi r_{ij}^2 \rho_M^{2b}(r_{ij})$$

Chambers-Wall et al. PRL 133, 212501 (2024)
Chambers-Wall et al. PRC 110, 054316 (2024)

Charge form factors



Charge form factor depends on sum of excited "multipolarities"

The l=0 term is related to spherically averaged charge density

l=2 is sensitive to quadrupole deformation of the nucleus

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King et al. PRC 110, 054325 (2024)

Heavier systems: Auxiliary Field Diffusion Monte Carlo

Use the single particle basis: $\langle S|\Psi\rangle \propto \xi_{\alpha_1}(s_1)\,\xi_{\alpha_2}(s_2)\ldots\,\xi_{\alpha_A}(s_A)$

Advantage of a polynomial scaling with A

Technically more complicated to operate on wave function

Cost is a simpler correlation structure in the wave function

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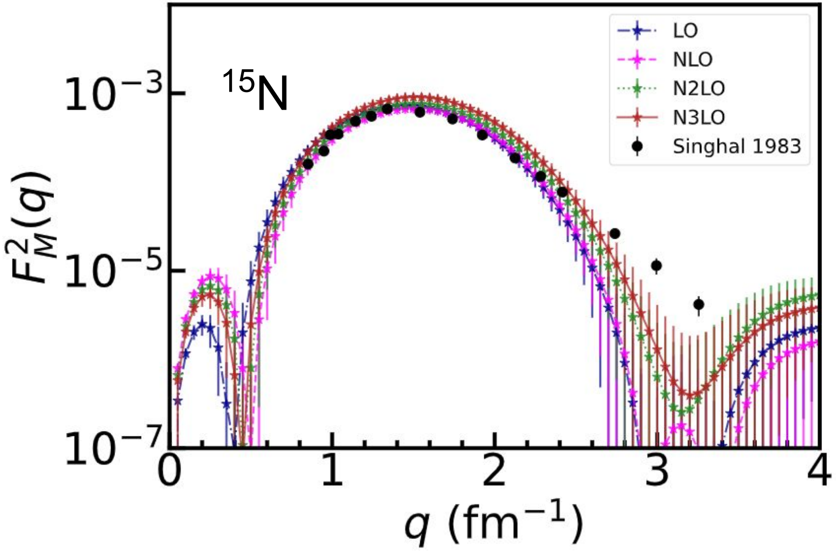
Lonardoni *et al.*, PRC 97, 044318 (2018)

Outlook: A ≥ 15 nuclei with AFDMC

Preliminary



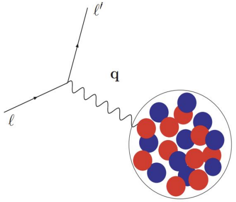
In collaboration with: Carlson (LANL), Gandolfi (LANL), Martin (LANL), Novario (WUSTL), Tews (LANL), ***in preparation***

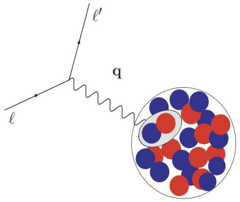
Quasi-elastic scattering

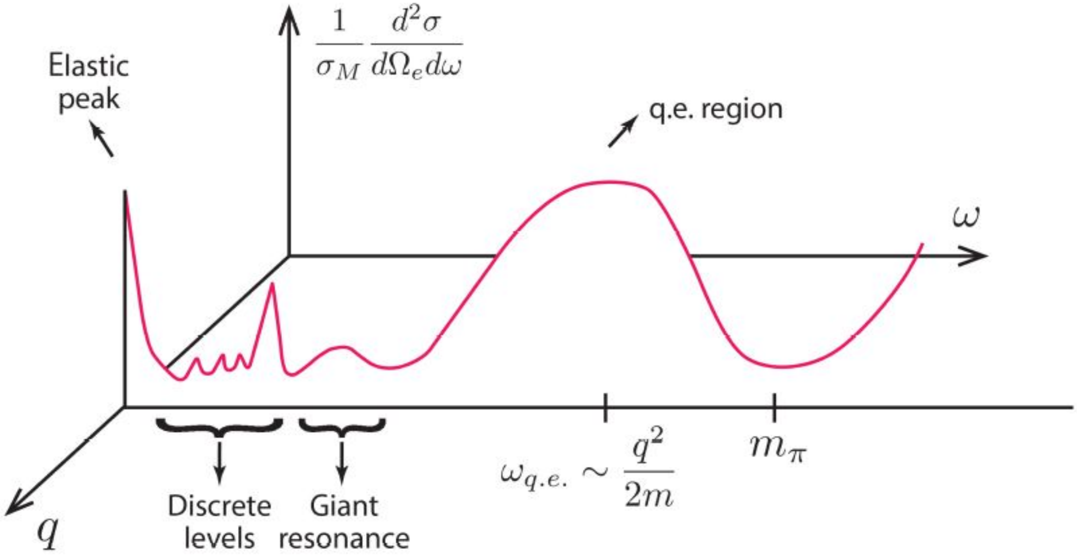
Quasi-elastic electron scattering

Electron strikes "quasi-free nucleon"

Two-body currents can enhance the response to external probe







Short-time approximation in electron scattering

Response function: $$R(\mathbf{q},\omega) = \frac{1}{2\pi}\int dt e^{i(\omega+E_0)t}\,\langle 0|\mathcal{O}^\dagger(\mathbf{q},\omega)e^{-iHt}\mathcal{O}(\mathbf{q},\omega)|0\rangle$$

To first order in time: $$e^{-iHt} \approx 1 - it\left(\sum_i T_i + \sum_{ij} v_{ij} + \dots\right) + \mathcal{O}(t^2)$$

When times satisfies $t \ll \omega^{-1}$:

$$\langle \mathcal{O}^\dagger \mathcal{O}\rangle \approx \sum_i \mathcal{O}_i^\dagger \mathcal{O}_i + \sum_{i\neq j} \mathcal{O}_i^\dagger \mathcal{O}_j + \sum_{i\neq j} \mathcal{O}_{ij}^\dagger \mathcal{O}_{ij} + \sum_{i\neq j}\left(\mathcal{O}_i^\dagger \mathcal{O}_{ij} + i \rightleftharpoons j\right)$$

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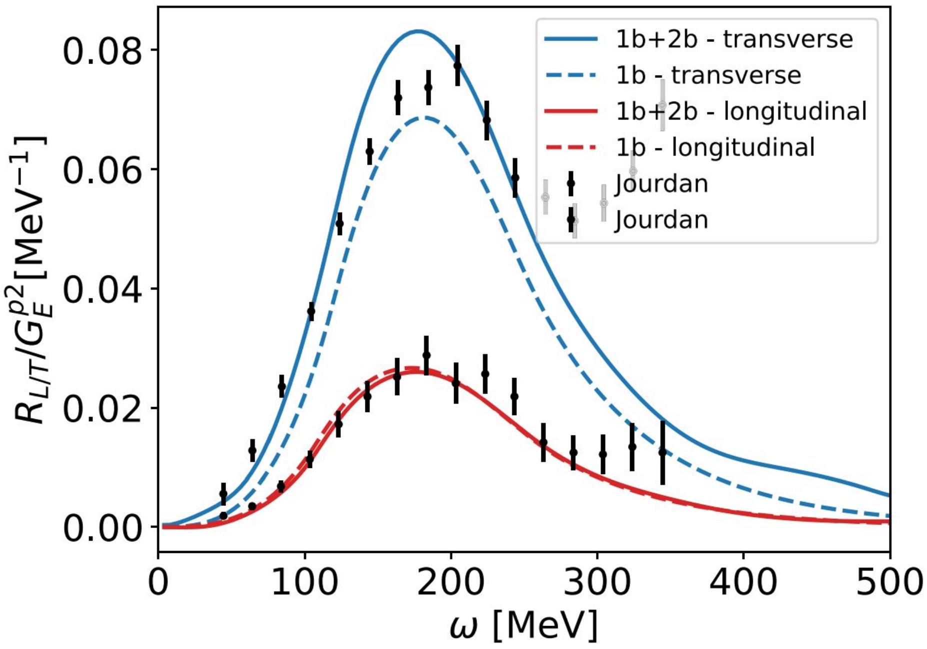
Quasi-elastic response functions

AV18+IL7



Can break down responses in terms of the one- and two-body contributions

Ex: ^{12}C at q=570 MeV/c

Longitudinal response receives 5% contribution, while transverse response gets ~30% enhancement

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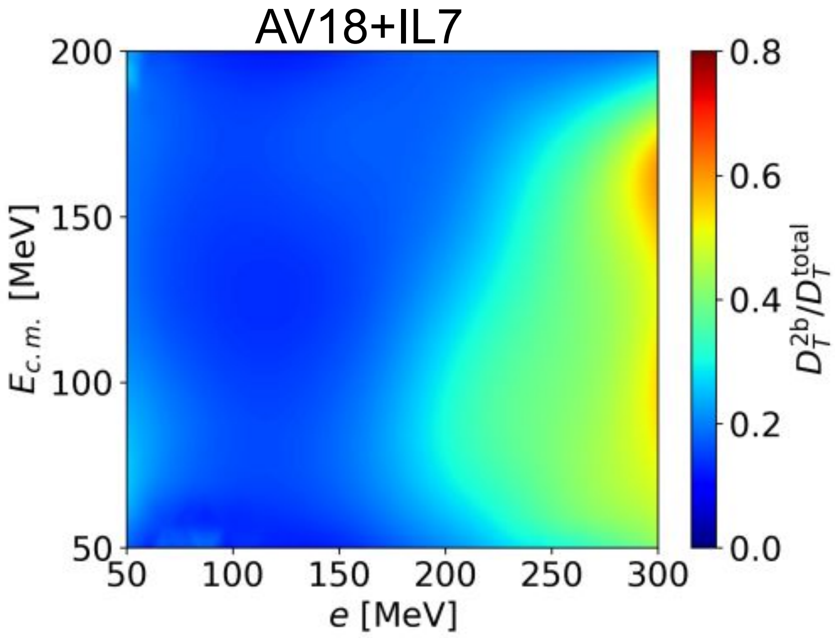
Andreoli et al. PRC 110, 064004 (2024)

Two-body response densities



Can break down the kinematics of important two body contributions by studying response densities

$$R(\mathbf{q},\omega) = \int de dE D(e,E)\delta(\omega - (e + E - E_0)$$

Ex: Two-body contribution to the ^{12}C transverse response made up by large relative energy pairs

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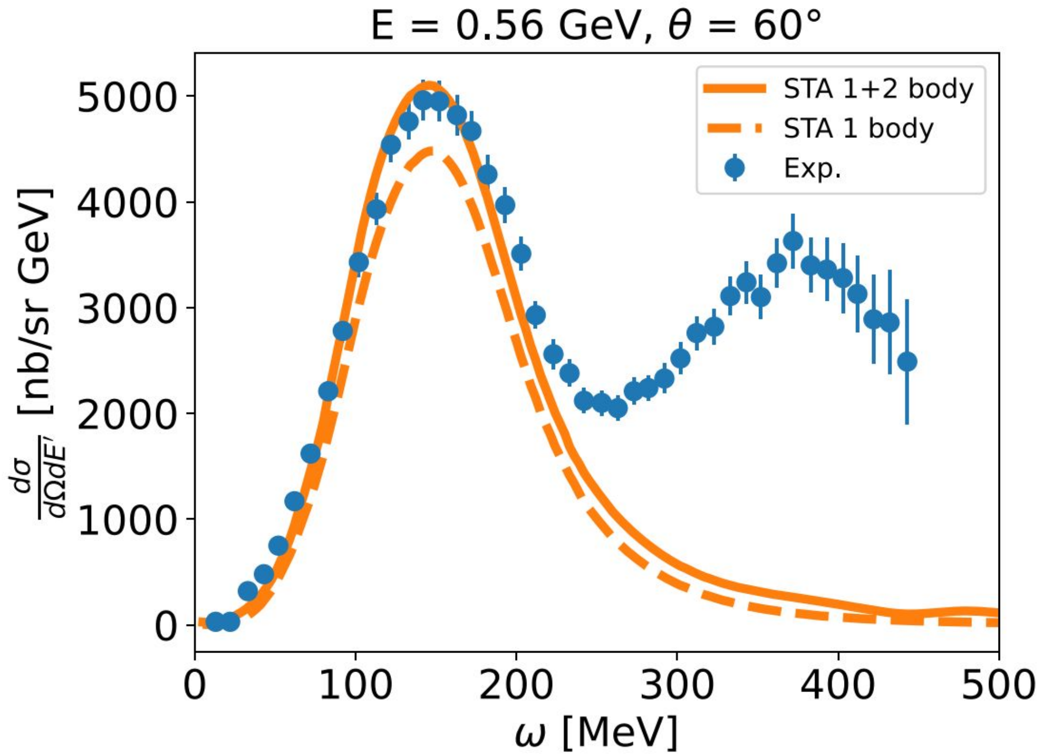
Andreoli et al. PRC 110, 064004 (2024)

Quasi-elastic electron scattering on ^{12}C

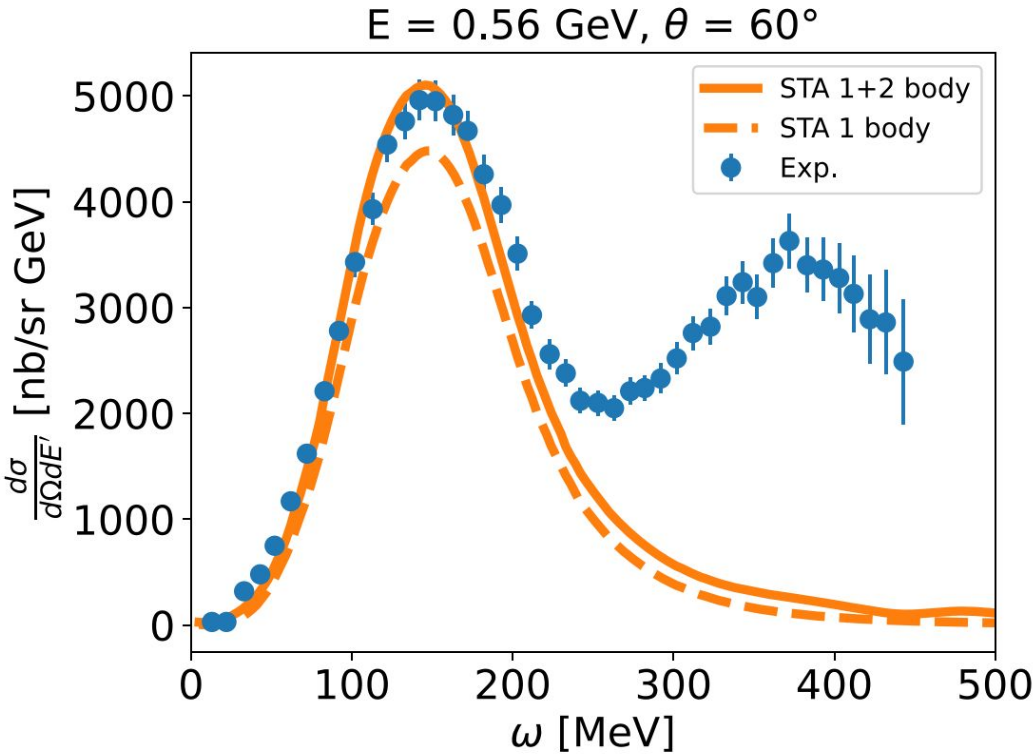


Two-body physics plays an important role in describing quasi-elastic cross sections

Roughly 5% to 15% enhancement for E = [0.3,2.5] GeV and scattering angles up to 60 degrees

Andreoli et al. PRC 110, 064004 (2024)

Quasi-elastic electron scattering on ^{12}C



Two-body physics plays an important role in describing quasi-elastic cross sections

Outlook:
Study of quasi-elastic neutrino scattering and inclusion of pion production

Andreoli et al. PRC 110, 064004 (2024)

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β-decay searches for beyond the Standard Model physics

34

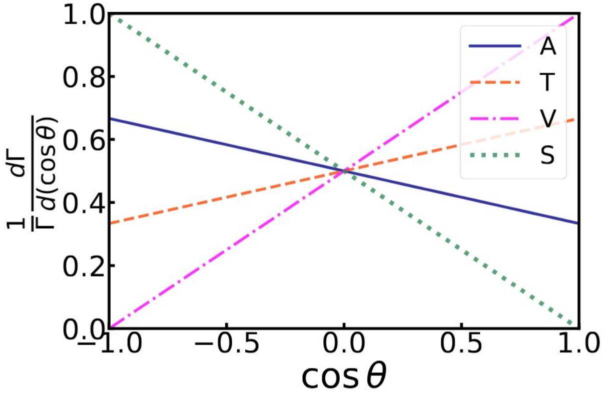
β-decays as a bridge to new physics

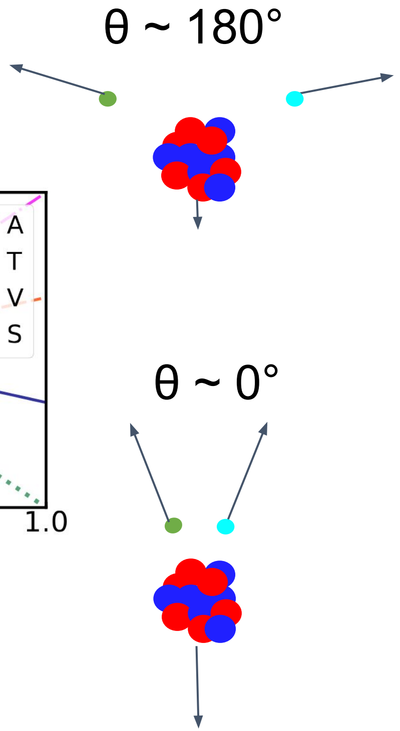
Weak currents with different transformation properties prefer different lepton angles

Standard Model is a vector minus axial theory

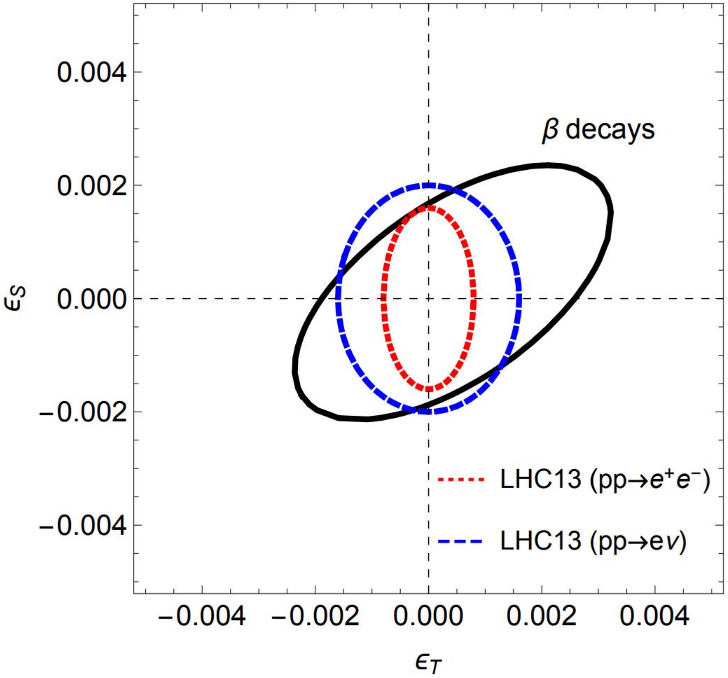
BSM tensor and scalar currents could interfere with standard current, changing kinematics

Neutrino mass would remove some phase space for the outgoing electron





New physics impact of nuclear β-decays



Falkowski et al, JHEP04 (2021) 126

Competitive bounds on BSM currents that complement high-energy searches

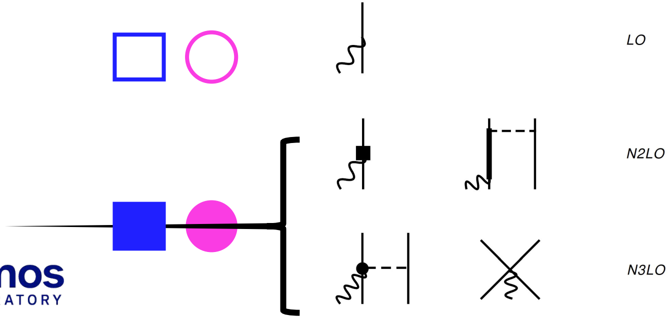
β-decay rates

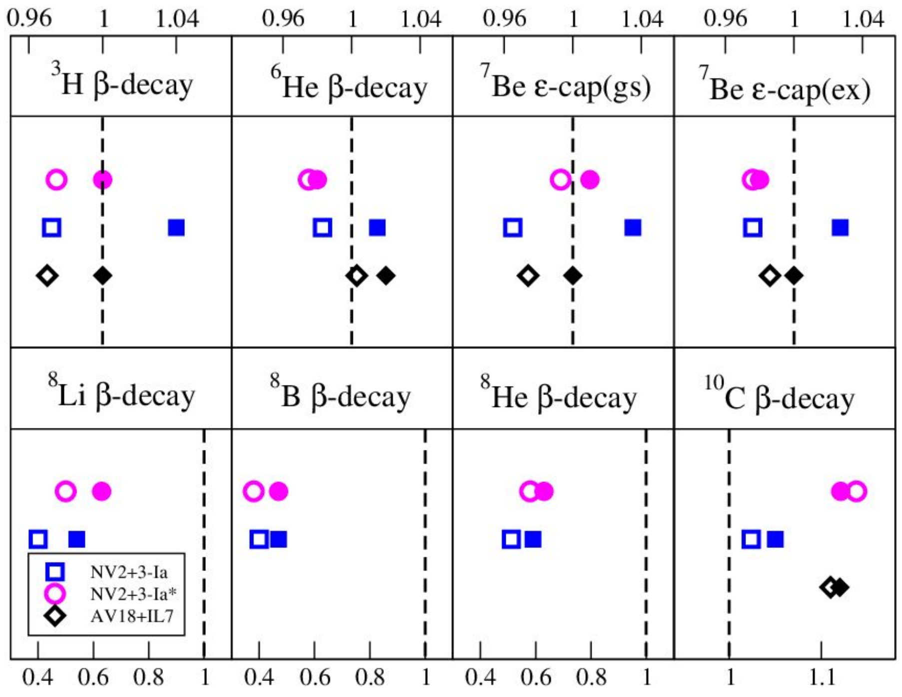
Computed with two models:

Fit to 3H beta decay or purely strong data

Many-body correlations important

Two-body can be ~few % to several %





King et al. PRC 121, 025501 (2020)

^{6}He β-decay spectrum: Overview

Differential rate:

$$\frac{d\Gamma_0}{dE_e} = |M|^2 G_\beta(E)$$

New physics can distort this:

$$\frac{d\Gamma}{dE_e} = \frac{d\Gamma_0}{dE_e}[1 + \Delta(E)]$$

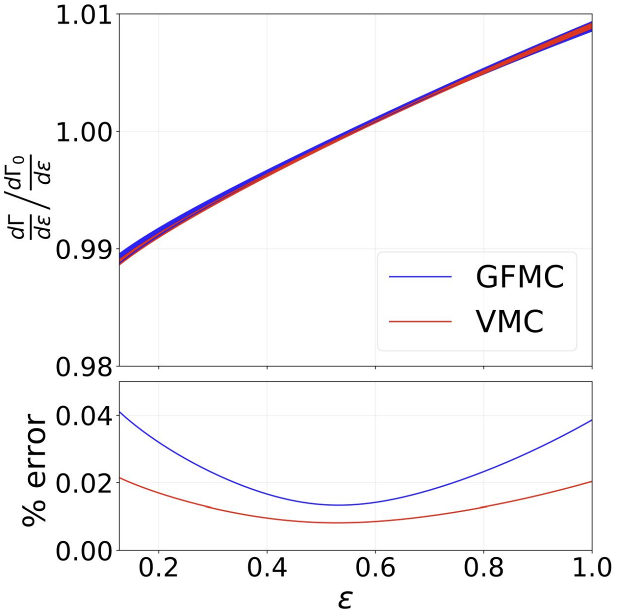
Similar distortions can be generated when accounting for nuclear recoil

Performed calculation with recoil corrections and two-body physics effects

Vector
Scalar $\rightarrow$ **Fermi**

Axial
Tensor
Pseudoscalar $\rightarrow$ **GT**

^{6}He β-decay spectrum: Standard Model results



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

Model uncertainty plus two-body contribution brings theory precision within needs of experiment

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)]

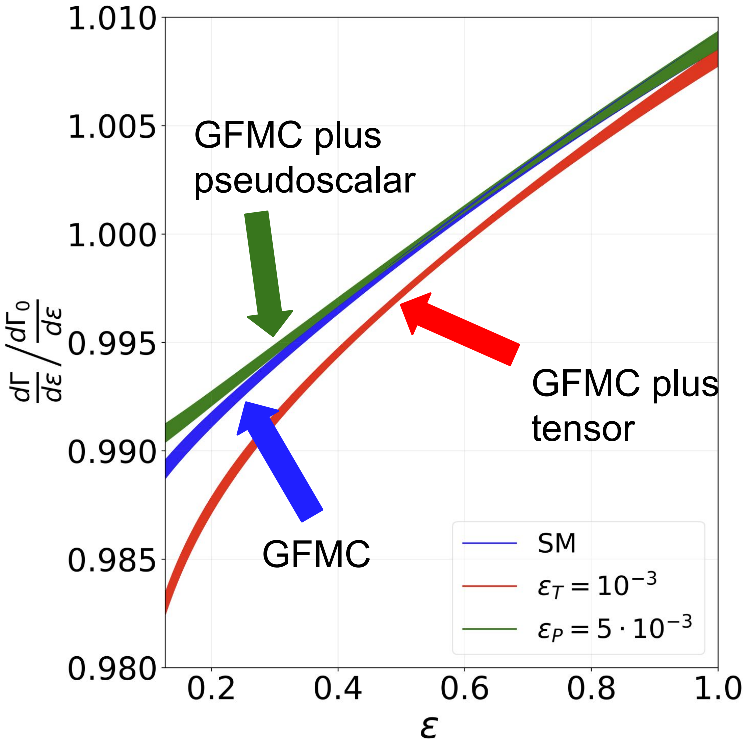
King et al. PRC 107, 015503 (2023)

^{6}He β-decay spectrum: Probing new forces

Included transition operators associated with new physics

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

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



FRIB

lpc caen

^{6}He-CRES

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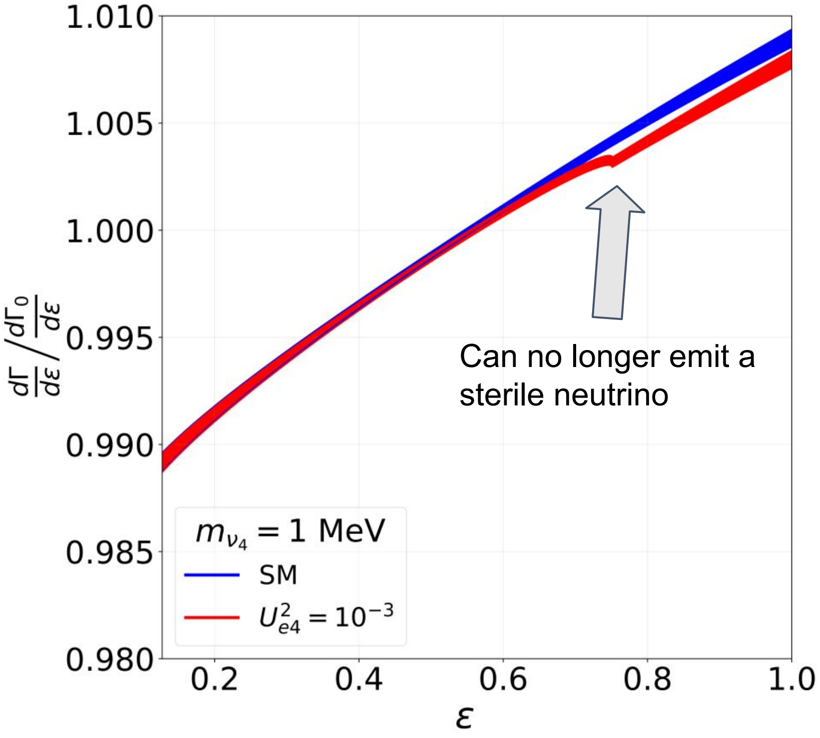
King et al. PRC 107, 015503 (2023)

^{6}He β-decay spectrum: Probing neutrino physics

Can also investigate impacts from production of ~1 MeV sterile neutrinos

The shape of the decay endpoint can exclude some parameter space and probe BSM scenarios



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^{6}He-CRES

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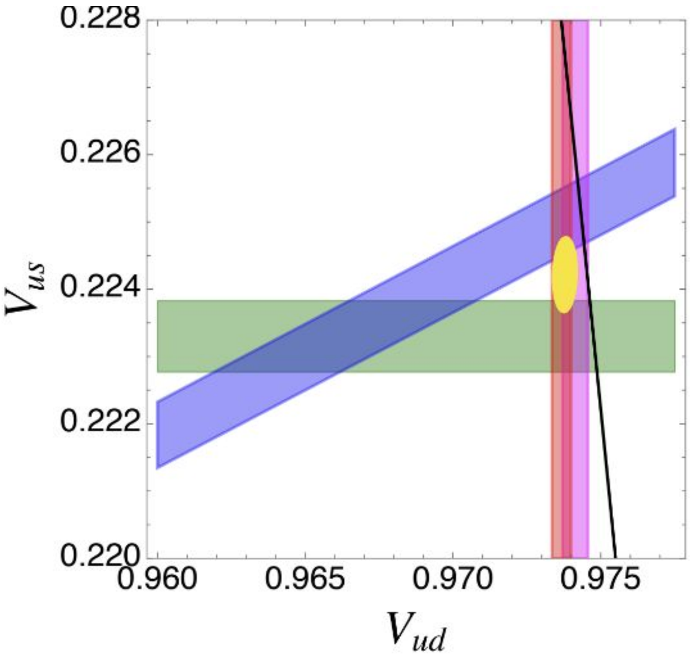
King et al. PRC 107, 015503 (2023)

Superallowed 0+ to 0+ β-decays



Cirigliano et al., PLB 838 (2023) 137748

Competitive bounds on BSM currents that complement high-energy searches

Tests of CKM unitarity

$$V_{\mathrm{CKM}} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$$

$$|V_{ud}|^2 + |V_{us}|^2 + \cancel{|V_{ub}|^2} = 1$$

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Role of nuclear structure

For a 0+ to 0+ transition: $\langle TT_z \pm 1 | T_\pm | TT_z \rangle = 2 = \text{const}$

If there were perfect symmetry between proton and neutron without radiative corrections:

$$ft = \frac{K}{2G_F^2 V_{ud}^2}$$

In reality:

$$\mathcal{F}t = \frac{K}{2G_F^2 V_{ud}^2 (1 + \Delta_R^V)} = ft(1 + \delta_R')(1 + \delta_{\mathrm{NS}} - \delta_{\mathrm{C}})$$

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$^{10}C(0+) \to {}^{10}B(0+)$ β-decay

In an effective field theory approach:

$$\delta_{\rm NS} = \sum_{m,n,i} \alpha^m E_0^n c_{m,n} M^i_{m,n}$$

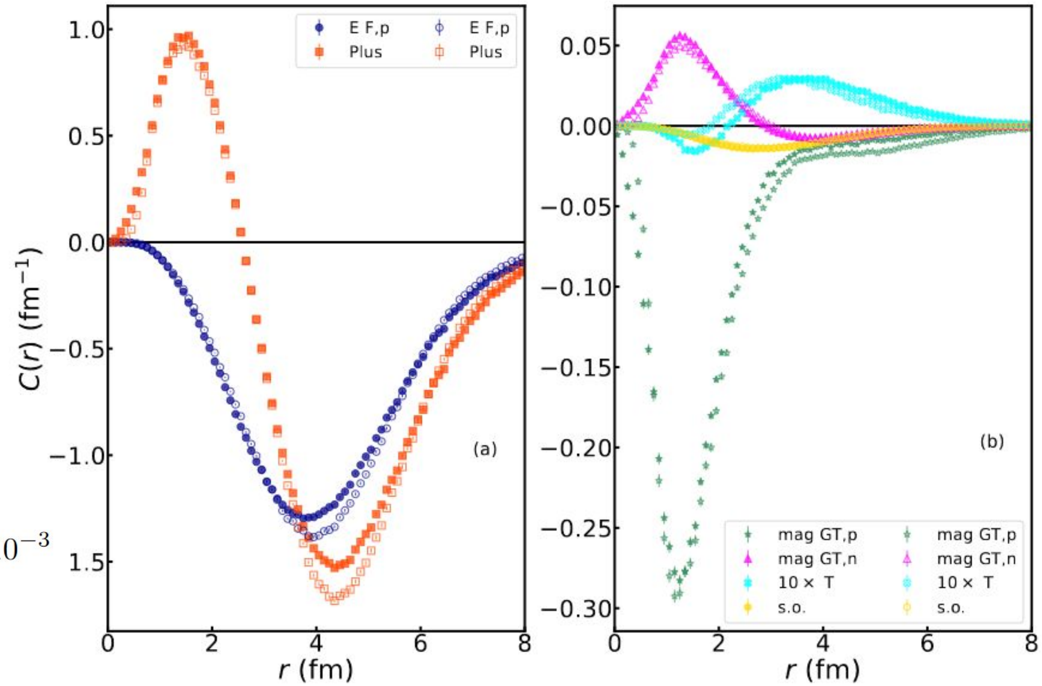
Can also evaluate:

$$M = \int dr C(r)$$

At *VMC* level: $\delta_{\rm NS} = -5.2(6) \times 10^{-3}$ to $-4.7(7) \times 10^{-3}$

Standard value: $\delta_{\rm NS} = -4.0(5) \times 10^{-3}$

VMC with chiral (filled) and AV18+UX (open)



In collaboration with: **Mereghetti (LANL)**, Carlson (LANL), Flores (WUSTL), Gandolfi (LANL), Pastore (WUSTL), Piarulli (WUSTL)

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Outlook: Joint analysis with QMC + Coupled-cluster

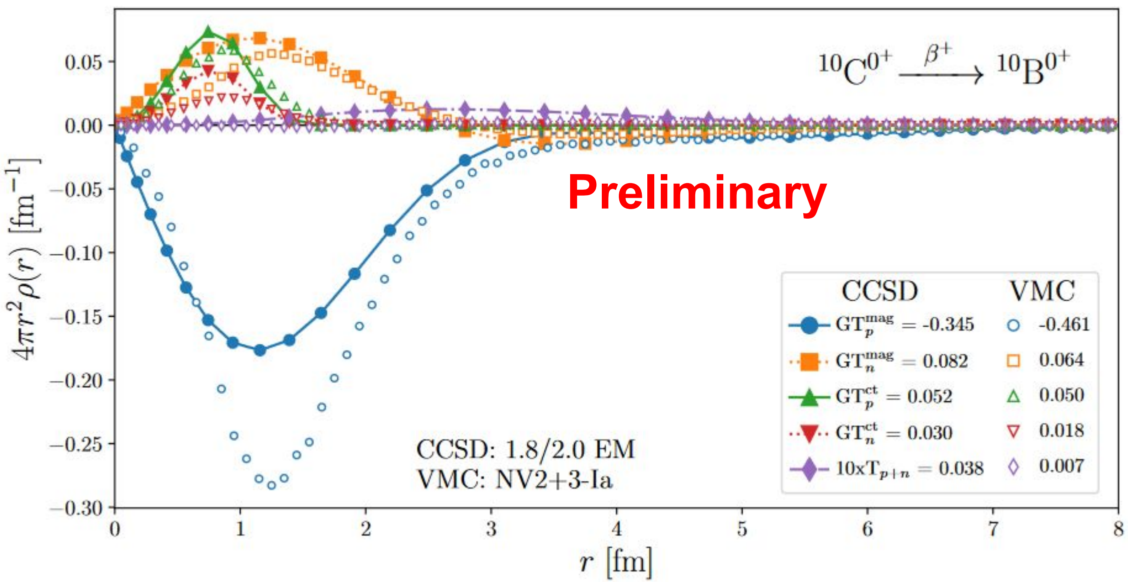

Figure courtesy of Sam Novario

Benchmarking different models, methods in first step toward global analysis

Calculations performed with different nuclear interactions, methods

Qualitative agreement, but further analysis necessary

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Conclusions

Accurate many-body calculations help to understand the impact of the nuclear dynamics on electromagnetic structure

Framework developed for QMC calculations of form factors, cross sections

Collaboration with other many-body practitioners can inform new physics searches

Outlook: heavier systems with AFDMC, relativistic corrections to quasi-elastic scattering **(cf. talk by Graham next week)**, neutrino response with STA

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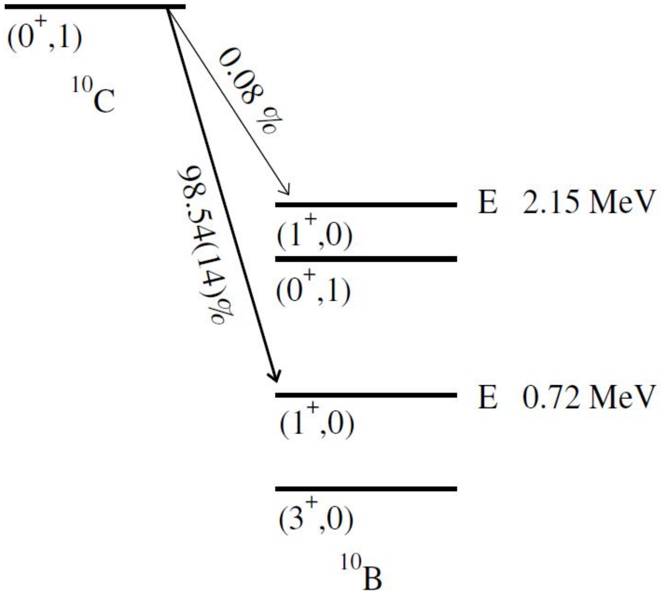
Additional slides

^{10}B β-decay



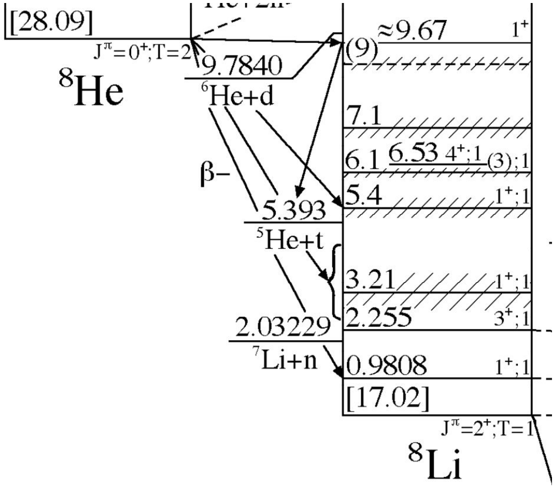
https://nucldata.tunl.duke.edu/

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 β-decay



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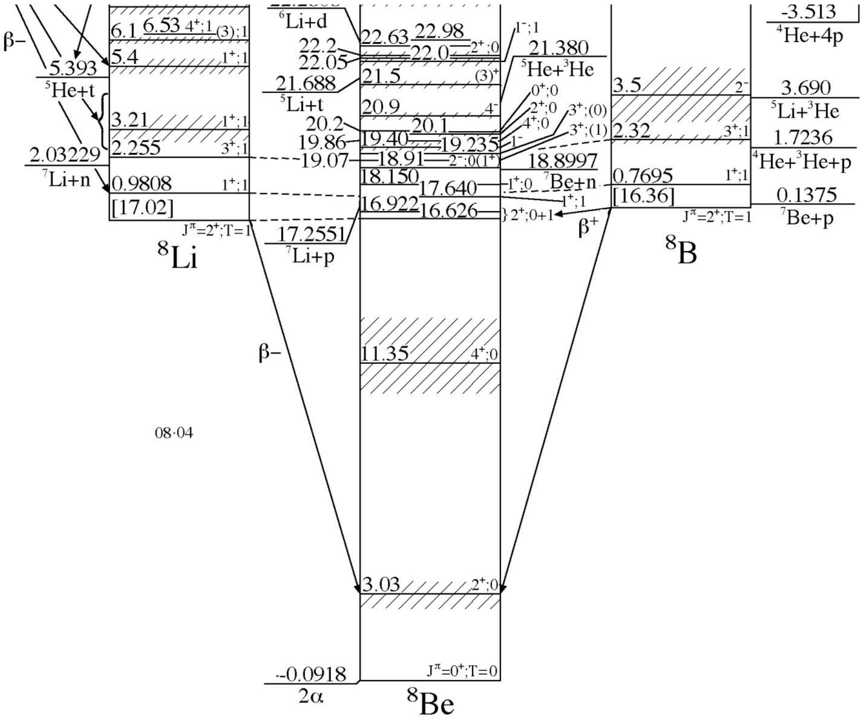
Three (1$^+$;1) states within a few MeV

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.

A=8 level scheme



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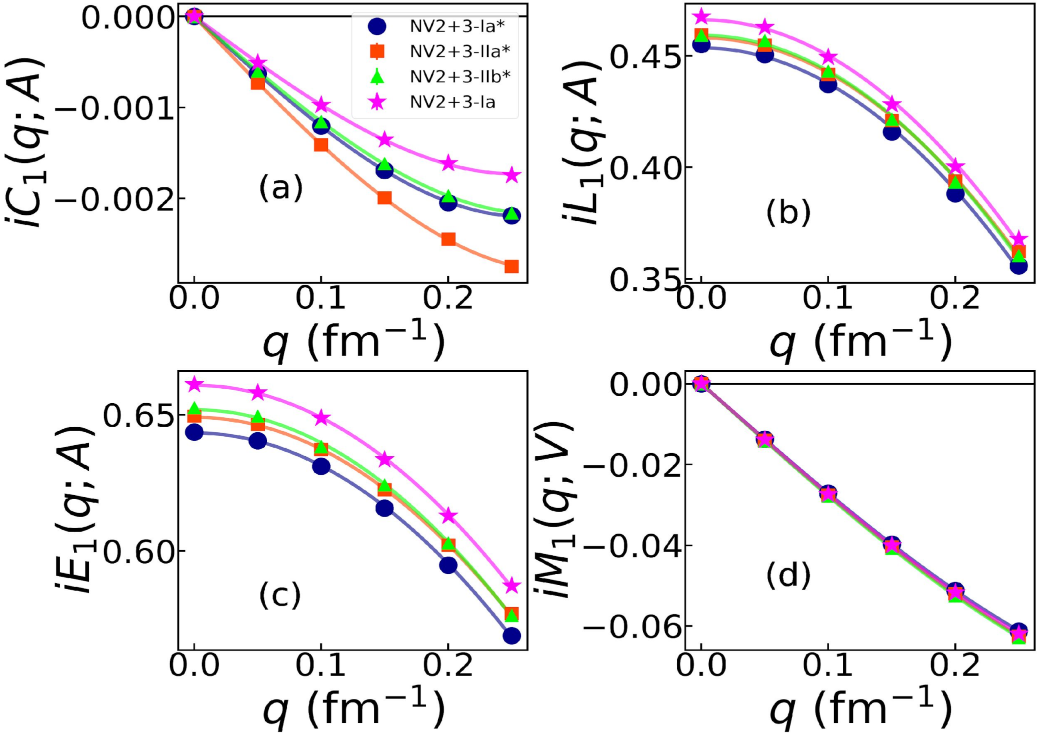
^{6}He β-decay spectrum: Multipoles

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

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

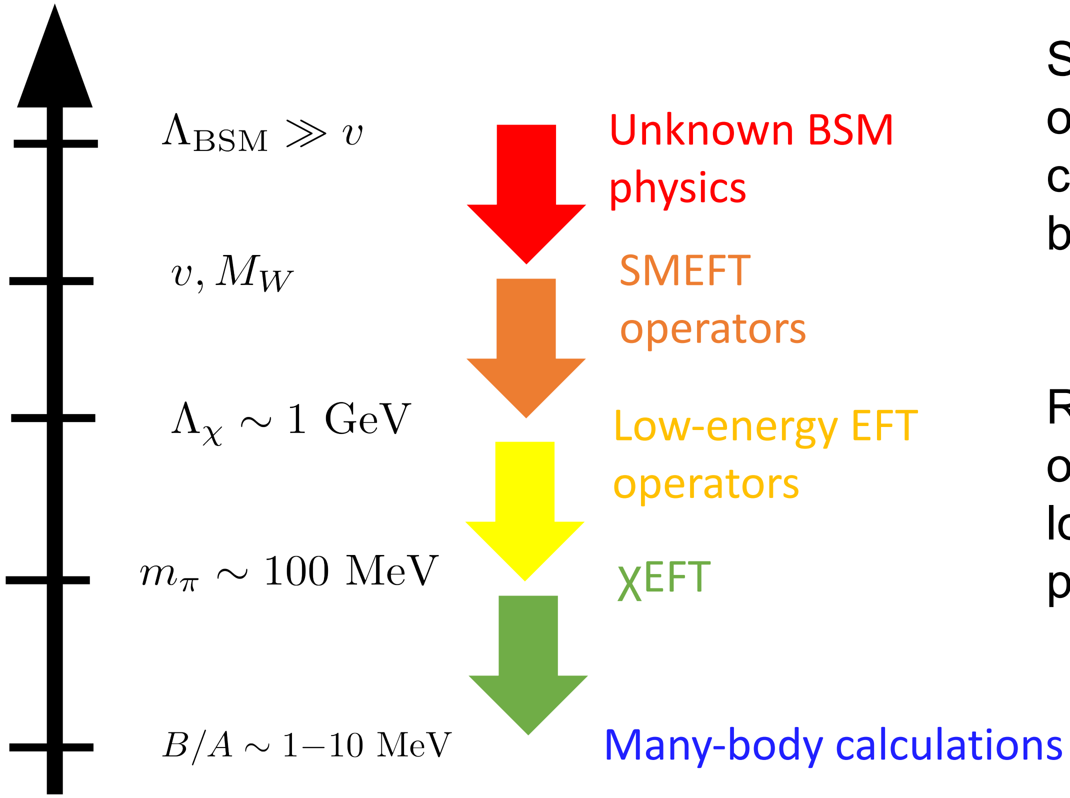
$$E_1(q;A) = -\frac{i}{\sqrt{2\pi}}\langle {}^6\mathrm{Li}, 10|\hat{\mathbf{z}}\cdot\mathbf{j}_+^\dagger(q\hat{\mathbf{x}};A)|{}^6\mathrm{He}, 00\rangle$$

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



King et al. PRC 107, 015503 (2023)

^{6}He β-decay spectrum: SMEFT



Start with most general operators in SMEFT that can contribute to GT beta decay

Run the coupling and obtain operators at the low-energy nuclear physics scale

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