

Fundamental Physics with Nuclei

EMMI Workshop and International Workshop XLIX on Gross Properties of Nuclei and Nuclear Excitations

16 January 2023 Saori Pastore

https://physics.wustl.edu/quantum-monte-carlo-group

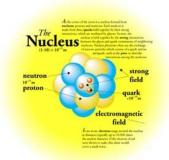
Quantum Monte Carlo Group @ WashU Lorenzo Andreoli (PD) Jason Bub (GS) Garrett King (GS) Maria Piarulli and Saori Pastore

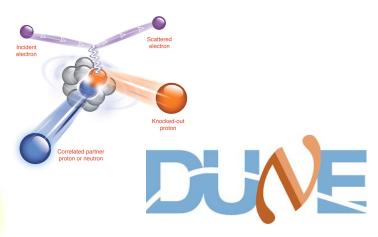
Computational Resources awarded by the DOE ALCC and INCITE programs

Understand Nuclei to Understand the Cosmos



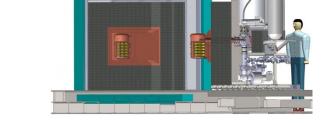








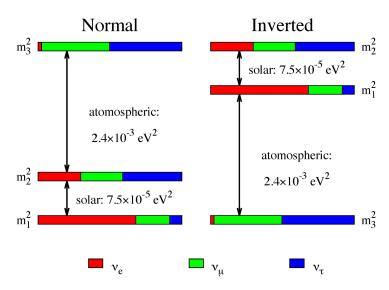




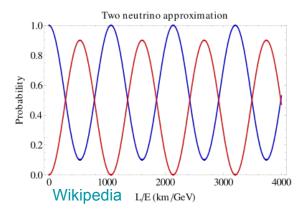
ESA, XMM-Newton, Gastaldello, CFHTL

Neutrino Oscillations

Neutrinos oscillate → they have a tiny mass **Beyond the Standard Model** physics



J.Phys.G43(2016)030401



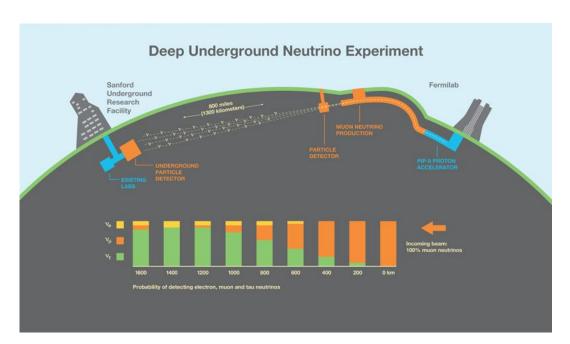
Simplified two-flavour picture

$$\begin{pmatrix} |\mathbf{v}_e\rangle \\ |\mathbf{v}_{\mu}\rangle \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} |\mathbf{v}_1\rangle \\ |\mathbf{v}_2\rangle \end{pmatrix}$$

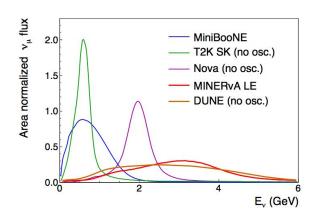
Probability of conversion

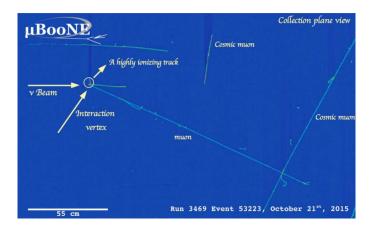
$$P(\mathbf{v_{\mu}} \rightarrow \mathbf{v_{e}}) = \sin^2 2\theta \sin^2 \left(\frac{\left(m_2^2 - m_1^2\right)L}{2E_{\mathbf{v}}}\right)$$

Accelerator Neutrinos' Experiments

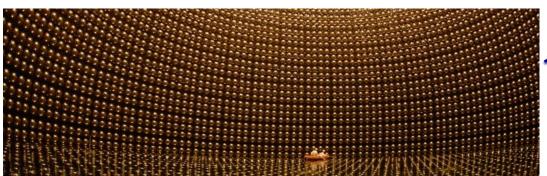


DUNE - Fermilab

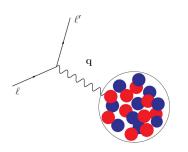




Nuclei for Neutrino Oscillations' Experiments



$$P(\nu_{\mu} \to \nu_{e}) = \sin^{2}2\theta \sin^{2}\left(\frac{\Delta m_{21}^{2}L}{2E_{\nu}}\right)$$

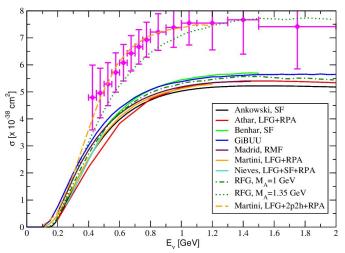


Nuclei are the active material in the detector. The energy of the incident neutrino is reconstructed from the observed final states using neutrino event generators that require theoretical cross-sections.



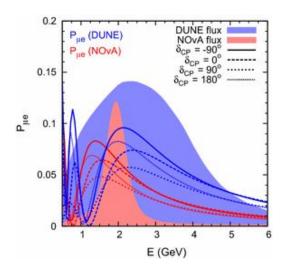
Neutrino-¹²C cross section

CCQE on ¹²C



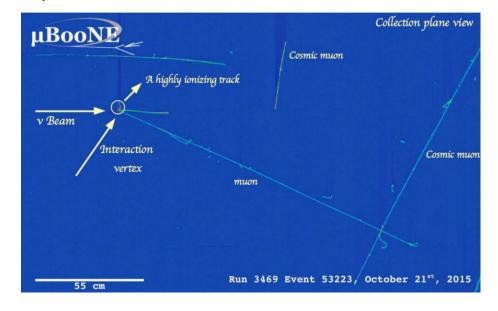
Alvarez-Ruso arXiv:1012.3871

The needs of the experimental programs

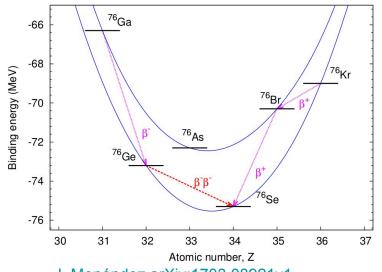


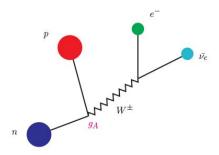
The range of challenges is extreme; ultimately we would like to be able to predict both inclusive and exclusive cross sections across a wide range of kinematics.

The experimental neutrino program is in need of accurate **theoretical calculations of neutrino-nucleus cross-sections with quantified theoretical errors** to ensure a robust implementation of interaction models in experiments



Single and Double Beta Decays







Maria Goeppert-Mayer

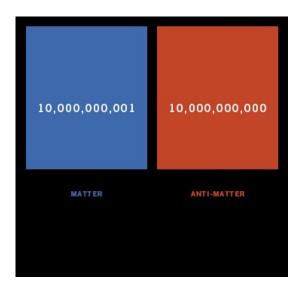
J. Menéndez arXiv:1703.08921v1

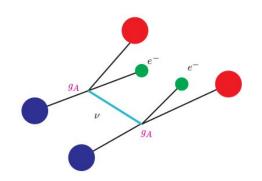
$$(\mathbf{Z}, N) \rightarrow (\mathbf{Z} + 1, N - 1) + e + \bar{\mathbf{v}}_e$$

Double beta decay
$$(\mathbf{Z},N)
ightarrow (\mathbf{Z}+\mathbf{2},N-\mathbf{2}) + 2e + 2ar{v}_e$$

Here the lepton number is conserved

Neutrinoless double beta decay





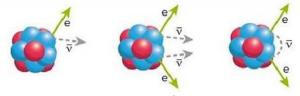


Ettore Majorana

$$(\mathbf{Z}, \mathbf{N}) \rightarrow (\mathbf{Z} + \mathbf{2}, \mathbf{N} - \mathbf{2}) + 2e$$

Hitoshi Murayama

Here the lepton number is not conserved

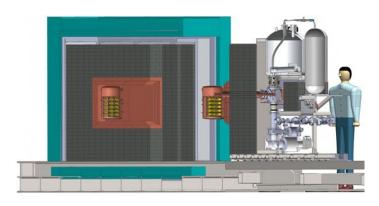


2015 Long Range Plan for Nuclear Physics

Nuclear Physics for Neutrinoless Double Beta Programs



EXO-200 Collaboration



Majorana Demonstrator

Neutrinoless double beta decay half-life $T_{1/2} \gtrsim 10^{25}$ years (age of the universe 1.4 x 10^{10} years) 1 ton of material is required to see few events per year

Decay Rate \propto (nuclear matrix element)² x (m₈₈)²

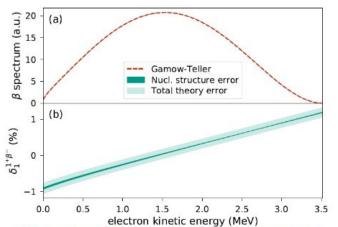
Beta decay spectrum

⁶He Beta decay spectrum for BSM searches with NCSL, He6-CRES, LPC-Caen

See Petrand Doron's talks



⁶He beta-decay spectrum from NCSM



$$\frac{d\Gamma}{d\varepsilon} = \frac{d\Gamma_0}{d\varepsilon} \times (1 + \text{corrections})$$

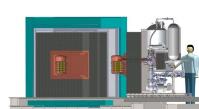
Ground States'
Electroweak Moments,
Form Factors, Radii





Neutrinoless Double Beta Decay, ____

Muon-Capture



Accelerator Neutrino
Experiments,
Lepton-Nucleus XSecs

(ω,q)~0 MeV

ω~few MeVs q~0 MeV ω~few MeVs q~10² MeV

 ω ~tens of MeVs ω ~10² MeV



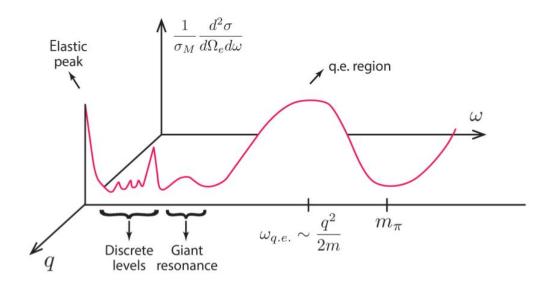
Electromagnetic
Decay, Beta Decay,
Double Beta Decay &
inverse processes



Nuclear Rates for Astrophysics



Electron-Nucleus Scattering Cross Section



Energy and momentum transferred (ω ,q)

Current and planned experimental programs rely on theoretical calculations at different kinematics

Strategy

Validate the Nuclear Model against available data for strong and electroweak observables

- Energy Spectra, Electromagnetic Form Factors, Electromagnetic Moments, ...
- Electromagnetic and Beta decay rates, ...
- Muon Capture Rates, ...
- Electron-Nucleus Scattering Cross Sections, ...

Use attained information to make (accurate) predictions for BSM searches and precision tests

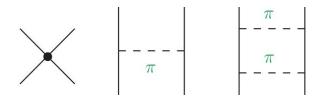
- EDMs, Hadronic PV, ...
- BSM searches with beta decay, ...
- Neutrinoless double beta decay, ...
- Neutrino-Nucleus Scattering Cross Sections, ...
- ..

Many-body Nuclear Interactions

Many-body Nuclear Hamiltonian

$$H = T + V = \sum_{i=1}^{A} t_i + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk} + \dots$$

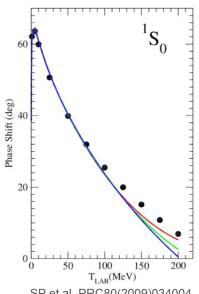
 v_{ij} and V_{ijk} are two- and three-nucleon operators based on experimental data fitting; fitted parameters subsume underlying QCD dynamics



Contact term: short-range

Two-pion range: intermediate-range $r \propto (2 m_{\pi})^{-1}$

One-pion range: long-range $r \propto m_\pi^{-1}$



SP et al. PRC80(2009)034004

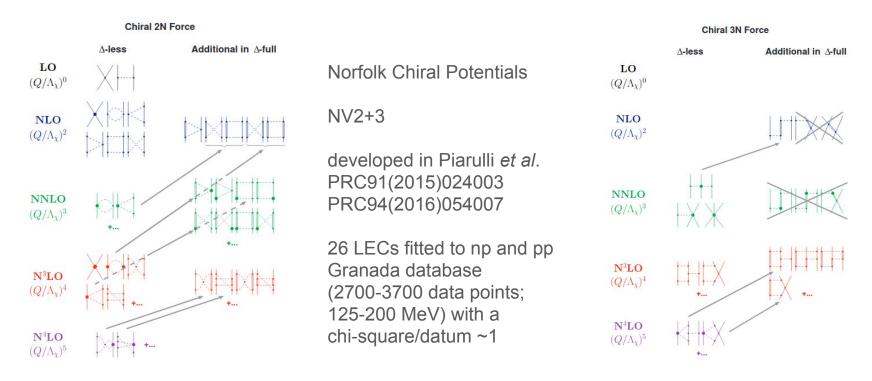


Hideki Yukawa

AV18+UIX; AV18+IL7 Wiringa, Schiavilla, Pieper et al.

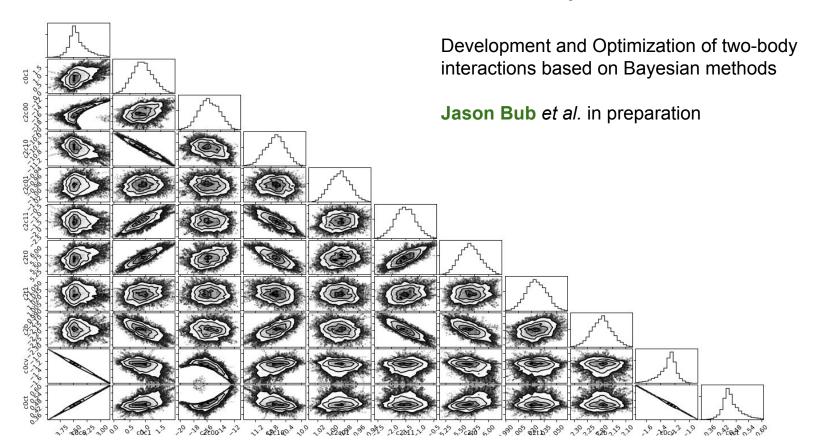
chiral πNΔ N3LO+N2LO Piarulli *et* al. Norfolk Models

Norfolk Two- and Three-body Potentials



Figs. credit Entem and Machleidt Phys.Rept.503(2011)1

Optimization of Nuclear Two-body Interactions



Quantum Monte Carlo Methods

Minimize the expectation value of the nuclear Hamiltonian: $H = T + v_{ij} + V_{ijk}$

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

using the trial wave function:

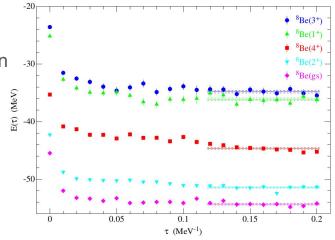
$$|\Psi_V\rangle = \left[\mathcal{S} \prod_{i < j} (1 + U_{ij} + \sum_{k \neq i, j} U_{ijk})\right] \left[\prod_{i < j} f_c(r_{ij})\right] |\Phi_A(JMTT_3)\rangle$$

Further improve the trial wave function by eliminating spurious contaminations via a Green's Function Monte Carlo propagation in imaginary time

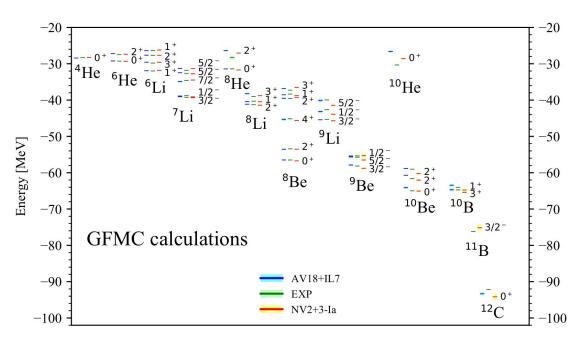
$$\Psi(\tau) = \exp[-(H - E_0)\tau]\Psi_V = \sum_n \exp[-(E_n - E_0)\tau]a_n\psi_n$$

$$\Psi(\tau \to \infty) = a_0\psi_0$$

Carlson, Wiringa, Pieper et al.

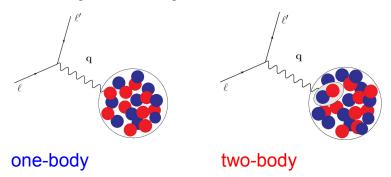


Energies



Piarulli et al. PRL120(2018)052503

Many-body Nuclear Electroweak Currents



- Two-body currents are a manifestation of two-nucleon correlations
- Electromagnetic two-body currents are required to satisfy current conservation

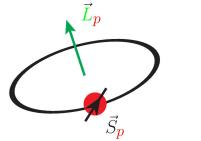
$$\mathbf{q} \cdot \mathbf{j} = [H, \rho] = [t_i + v_{ij} + V_{ijk}, \rho]$$

Nuclear Charge Operator

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

Nuclear (Vector) Current Operator

$$\mathbf{j} = \sum_{i=1}^{A} \mathbf{j}_i + \sum_{i < j} \mathbf{j}_{ij} + ...$$





Magnetic Moment: Single Particle Picture

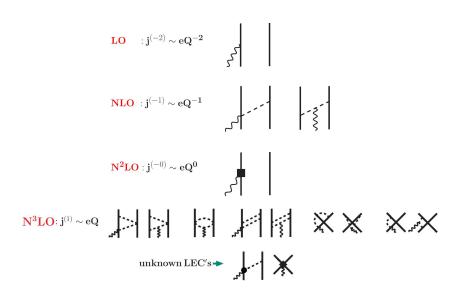
Many-body Currents

Meson Exchange Currents (MEC)

Constrain the MEC current operators by imposing that the current conservation relation is satisfied with the given two-body potential

Chiral Effective Field Theory Currents

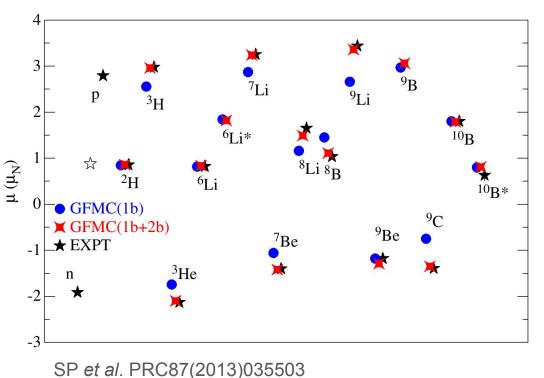
Are constructed consistently with the two-body chiral potential; Unknown parameters, or Low Energy Constants (LECs), need to be determined by either fits to experimental data or by Lattice QCD calculations



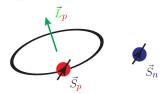
Electromagnetic Current Operator

SP et al. PRC78(2008)064002, PRC80(2009)034004, PRC84(2011)024001, PRC87(2013)014006 Park et al. NPA596(1996)515, Phillips (2005) Kölling et al. PRC80(2009)045502 & PRC84(2011)054008

Magnetic Moments of Light Nuclei



Single particle picture



$$\mu_N(1b) = \sum_i [(L_i + g_p S_i)(1 + \tau_{i,z})/2 + g_n S_i(1 - \tau_{i,z})/2]$$

Small two-body current effects



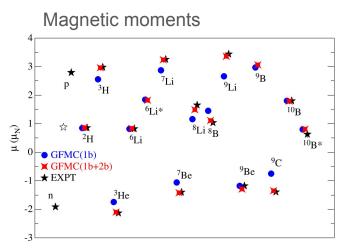
 ^{9}Be

Large two-body current effects



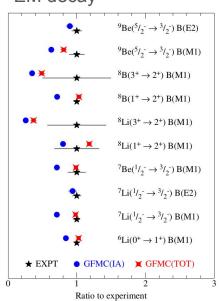
90

Electromagnetic Observables

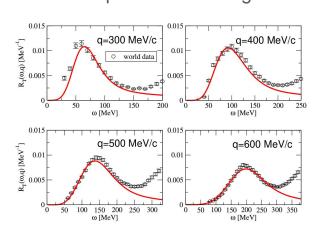


SP et al. PRC87(2013)035503, PRC101(2020)044612

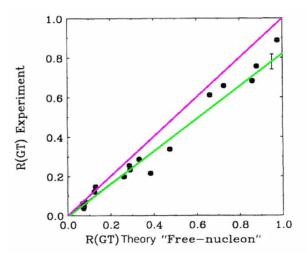




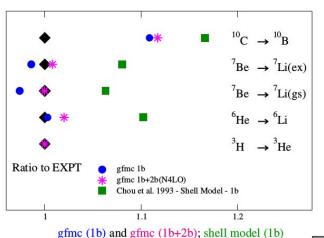
e-4He particle scattering



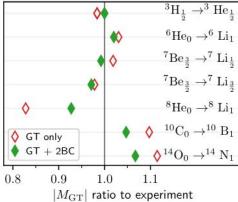
Beta decay



Chou et al. PRC47(1993)163

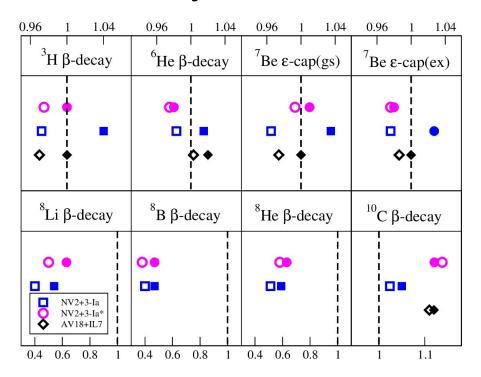


SP et al. PRC97(2018)022501



P. Gysbers Nature Phys. 15 (2019)

Beta Decay and Electron Capture in Light Nuclei



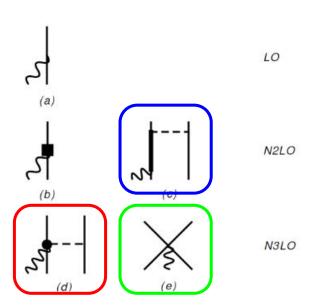
Garrett King et al. PRC102(2020)025501

Calculations based on

- chiral interactions and currents
 NV2+3-la Norfolk unstarred
 NV2+3-la* Norfolk* starred
 Piarulli et al. PRL120(2018)052503
 Baroni et al. PRC98(2018)044003
- phenomenological AV18+IL7
 potential and chiral axial currents
 (hybrid calculation)

Two-body currents are small/negligible; Results for A=6-7 are within 2% of data; Results for A=8 are off by a 30-40%; Results for A=10 are affected by the second $J^{\pi}=(1^{+})$ state in ^{10}B

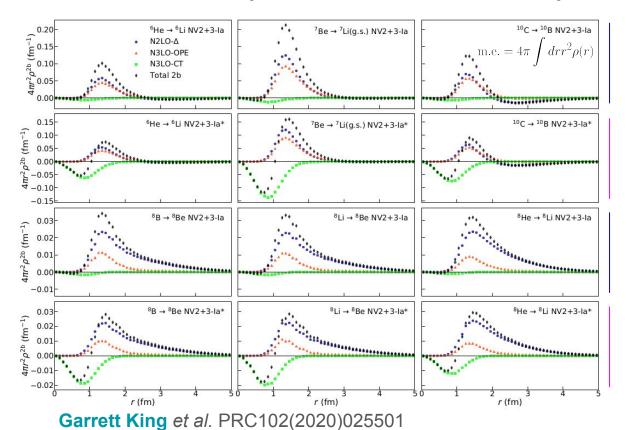
Axial currents with Δ at tree-level



Two body currents of one pion range (red and blue) with c_3 c_4 from Krebs et al. Eur.Phys.J.(2007)A32

Contact current involves the LEC c_p

Axial Two-body Transition Density



NV2+3-la; NV2+3-la*

enhanced contribution from contact current in the starred model gives rise to nodes in the two-body transition density

Two-body axial currents



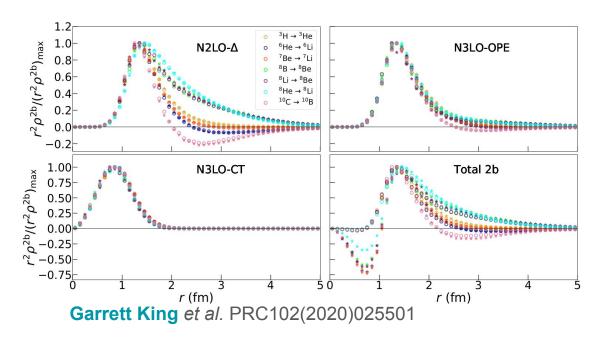


long-range at N2LO and N3LO



contact current at N3LO

Scaling & Universality of Short-Range Dynamics

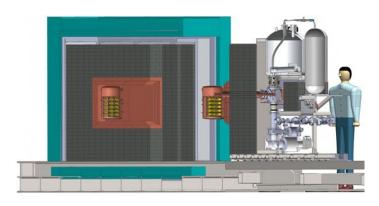


NV2+3-la empty circles; NV2+3-la* stars Different colors refer to different transitions

Nuclear Physics for Neutrinoless Double Beta Programs



EXO-200 Collaboration

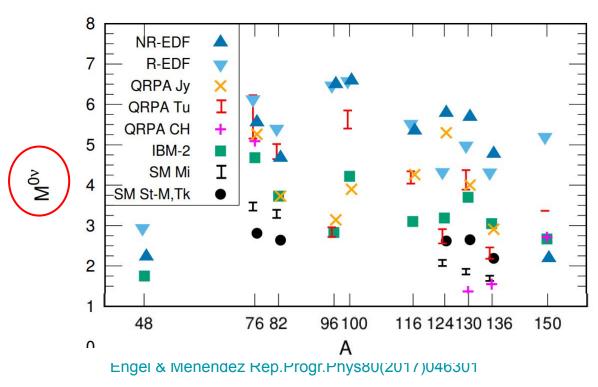


Majorana Demonstrator

Neutrinoless double beta decay half-life $T_{1/2} \gtrsim 10^{25}$ years (age of the universe 1.4 x 10^{10} years) 1 ton of material is required to see few events per year

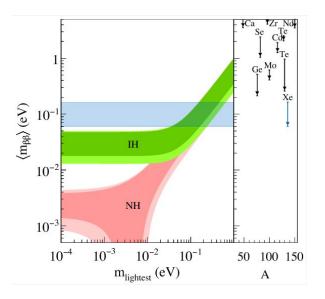
Decay Rate \propto (nuclear matrix element)² x (m₈₈)²

Neutrinoless Double Beta Decay



$$[T_{1/2}^{0\nu}]^{-1} = G_{0\nu}(Q, Z) (M_{0\nu})^2 n_{\beta\beta}^2$$

$$(Z, N) \to (Z + 2, N - 2) + 2e$$



Partial muon capture rates: VMC calculations

$$\Gamma_{VMC}(avg.) = 1495 \text{ s}^{-1} \pm 19 \text{ s}^{-1}$$

 $\Gamma_{expt} = 1496.0 \text{ s}^{-1} \pm 4.0 \text{ s}^{-1}$

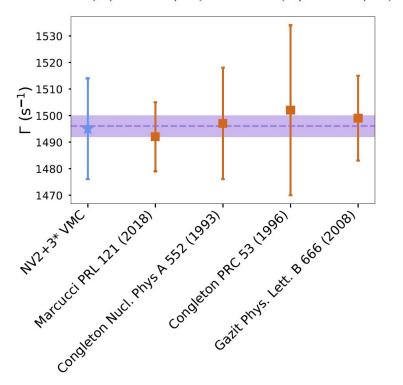
Ackerbauer et al. PLB417, 224(1998)

Momentum transfer **q**∼ 100 MeV

Two-body correction is ~8% of total rate on average for A=3

Garrett King et al. PRC2022

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



Partial muon capture rates: VMC calculations

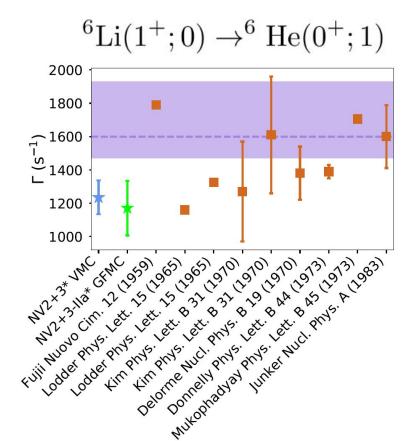
$$\Gamma_{VMC}(avg.) = 1235 \text{ s}^{-1} \pm 101 \text{ s}^{-1}$$

 $\Gamma_{GFMC}(IIa^*) = 1171 \text{ s}^{-1} \pm 164 \text{ s}^{-1}$
 $\Gamma_{expt} = 1600 \text{ s}^{-1} + 330/-129 \text{ s}^{-1}$

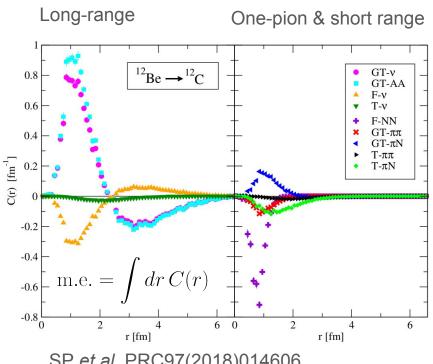
Garrett King et al. PRC2022

Deutsch et al. PLB26(1968)315

FRIB: extraction of the Gamow-Teller strength A=11, A=12 PRC2022 J. Schmitt et al.



Neutrinoless Double Beta Decay Matrix Elements



SP et al. PRC97(2018)014606





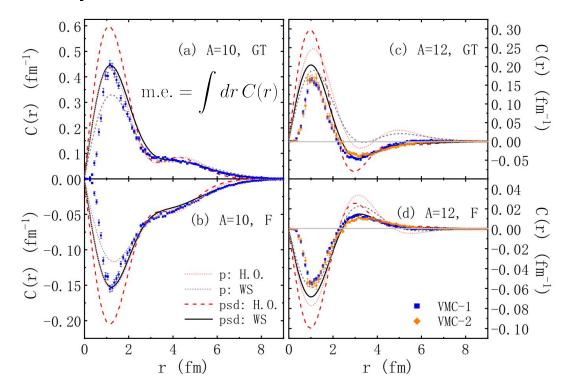




Cirigliano Dekens DeVries Graesser Mereghetti et al. PLB769(2017)460, JHEP12(2017)082, PRC97(2018)065501

- Leading operators in neutrinoless double beta decay are two-body operators
- These observables are particularly sensitive to short-range and two-body physics
- Transition densities calculated in momentum space indicate that the momentum transfer in this process is of the order of q ~ 200 MeV

Comparison with Shell-Model Calculations

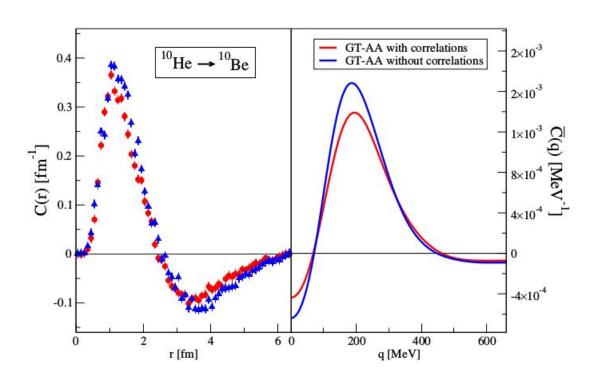


X. Wang et al. PLB798(2019)134974

Closer agreement between Shell-Model calculations with Variational Monte Carlo results is reached by

- Increasing the size of the model space
- Wood-Saxon single particle wave functions are superion in describing the tails of the densities wrt harmonic oscillator wave functions
- Phenomenological Short-Range-Correlations functions further improve the agreement

Correlations in neutrinoless double beta decay ME

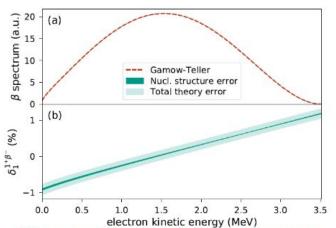


Beta decay spectrum

⁶He Beta decay spectrum for BSM searches with NCSL, He6-CRES, LPC-Caen



⁶He beta-decay spectrum from NCSM



$$\frac{d\Gamma}{d\varepsilon} = \frac{d\Gamma_0}{d\varepsilon} \times (1 + \text{corrections})$$

⁶He Beta Decay Spectrum

$$d\Gamma = \frac{2\pi}{2J_i + 1} \sum_{S_0, S_W} \sum_{M_i, M_f} |\langle f | H_W | i \rangle|^2 \delta(\Delta E) \frac{d^3 k_e}{(2\pi)^3} \frac{d^3 k_\nu}{(2\pi)^3}$$

Multipoles

$$C_{1}(q;A) = \frac{i}{\sqrt{4\pi}} \langle {}^{6}\text{Li}, 10 | \rho_{+}^{\dagger}(q\hat{\mathbf{z}};A) | {}^{6}\text{He}, 00 \rangle$$

$$C_{1}(q;A) = -i\frac{qr_{\pi}}{3} \left(C_{1}^{(1)}(A) - \frac{(qr_{\pi})^{2}}{10} C_{1}^{(3)}(A) + \mathcal{O}\left((qr_{\pi})^{4}\right) \right)$$

$$L_{1}(q;A) = \frac{i}{\sqrt{4\pi}} \langle {}^{6}\text{Li}, 10 | \hat{\mathbf{z}} \cdot \mathbf{j}_{+}^{\dagger}(q\hat{\mathbf{z}};A) | {}^{6}\text{He}, 00 \rangle$$

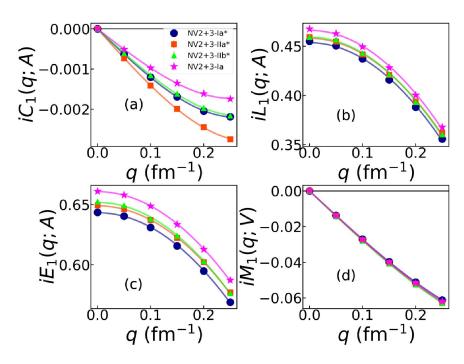
$$L_{1}(q;A) = -\frac{i}{3} \left(L_{1}^{(0)}(A) - \frac{(qr_{\pi})^{2}}{10} L_{1}^{(2)}(A) + \mathcal{O}\left((qr_{\pi})^{4}\right) \right)$$

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

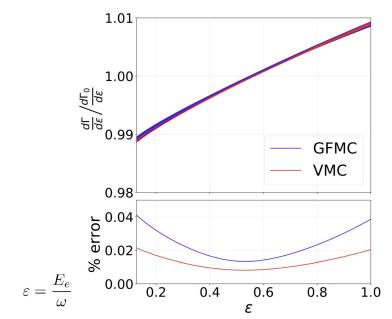
$$M_{1}(q;V) = -i\frac{qr_{\pi}}{3} \left(M_{1}^{(1)}(V) - \frac{(qr_{\pi})^{2}}{10} M_{1}^{(3)}(V) + \mathcal{O}\left((qr_{\pi})^{4}\right) \right)$$

$$M_{1}(q;V) = -\frac{i}{3} \left(E_{1}^{(0)}(A) - \frac{(qr_{\pi})^{2}}{10} E_{1}^{(2)}(A) + \mathcal{O}\left((qr_{\pi})^{4}\right) \right)$$

Beta Decay Spectrum



Dominant terms L₁₍₀₎ and E₁₍₀₎ have model dependence of ~1% to ~2%



$$\tau_{\text{GFMC}}$$
 = 808 +/- 24 ms
 $\tau_{\text{Expt.}}$ = 807.25 +/- 0.16 +/- 0.11 ms

Garrett King et al. PRC Editors' suggestion (2023)

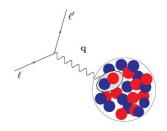
Lepton-Nucleus scattering: Inclusive Processes

Electromagnetic Nuclear Response Functions

$$R_{\alpha}(q,\omega) = \sum_{f} \delta\left(\omega + E_0 - E_f\right) |\langle f|O_{\alpha}(\mathbf{q})|0\rangle|^2$$

Longitudinal response induced by the charge operator $O_L = \rho$ Transverse response induced by the current operator $O_T = \mathbf{j}$ 5 Responses in neutrino-nucleus scattering

$$\frac{d^2 \sigma}{d \omega d \Omega} = \sigma_M \left[v_L R_L(\mathbf{q}, \omega) + v_T R_T(\mathbf{q}, \omega) \right]$$

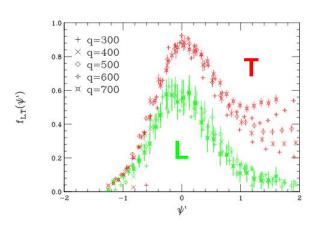


For a recent review on QMC, SF methods see Rocco *Front. In Phys.*8 (2020)116

Lepton-Nucleus scattering: Data

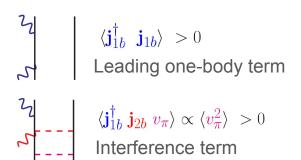
Transverse Sum Rule

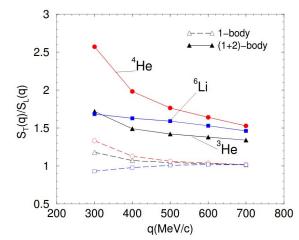
$$S_T(q) \propto \langle 0|\mathbf{j}^{\dagger}|\mathbf{j}|0\rangle \propto \langle 0|\mathbf{j}_{1b}^{\dagger}|\mathbf{j}_{1b}|0\rangle + \langle 0|\mathbf{j}_{1b}^{\dagger}|\mathbf{j}_{2b}|0\rangle + \dots$$



⁴He Electromagnetic Data Carlson *et al.* PRC65(2002)024002

Observed transverse enhancement explained by the combined effect of two-body correlations and currents in the interference term



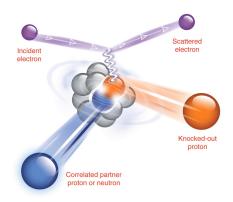


Transverse/Longitudinal Sum Rule Carlson *et al.* PRC65(2002)024002

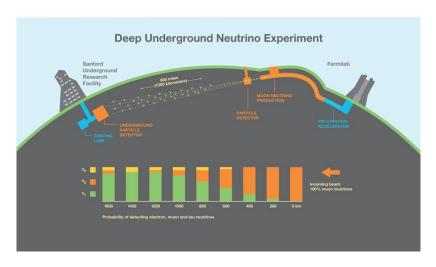
Beyond Inclusive: Short-Time-Approximation

Short-Time-Approximation Goals:

- Describe electroweak scattering from A
 12 without losing two-body physics
- Account for exclusive processes
- Incorporate relativistic effects



Subedi et al. Science320(2008)1475



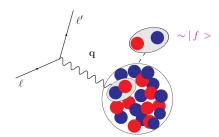
Stanford Lab article



Short-Time-Approximation

Short-Time-Approximation:

- Based on Factorization
- Retains two-body physics
- Response functions are given by the scattering from pairs of fully interacting nucleons that propagate into a correlated pair of nucleons
- Allows to retain both two-body correlations and currents at the vertex
- Provides "more" exclusive information in terms of nucleon-pair kinematics via the Response Densities



Response Functions ∝ Cross Sections

$$R_{\alpha}(q,\omega) = \sum_{f} \delta\left(\omega + E_0 - E_f\right) |\langle f|O_{\alpha}(\mathbf{q})|0\rangle|^2$$

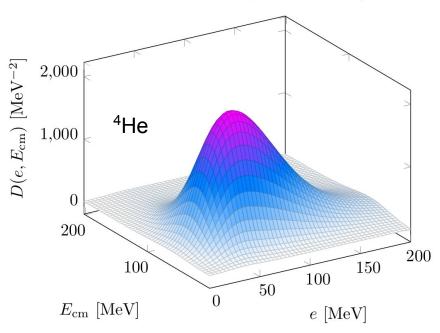
Response **Densities**

$$R(q,\omega) \sim \int \delta \left(\omega + E_0 - E_f\right) dP' dp' \mathcal{D}(p', P'; q)$$

P' and *p'* are the CM and relative momenta of the struck nucleon pair

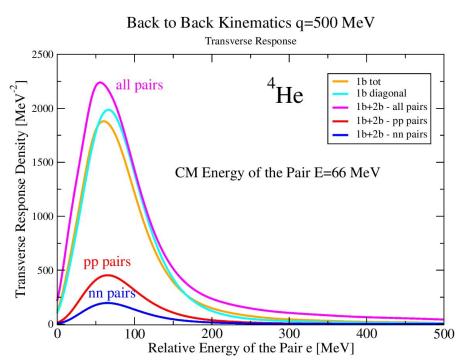
Transverse Response Density: e-4He scattering

Transverse Density q = 500 MeV/c



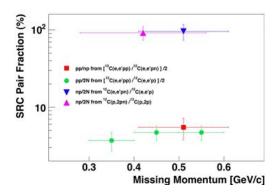
SP et al. PRC101(2020)044612

e-4He scattering in the back-to-back kinematic



SP et al. PRC101(2020)044612

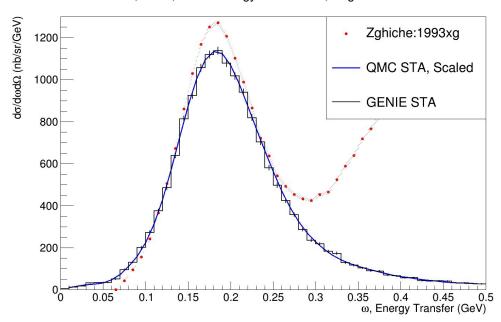
- pp pairs
- all pairs 1body
- nn pairs
- all pairs tot



Subedi et al. Science320(2008)1475

GENIE validation using e-scattering

Z = 2, A = 4, Beam Energy = 0.64 GeV, Angle = $60^{\circ} \pm 0.25^{\circ}$

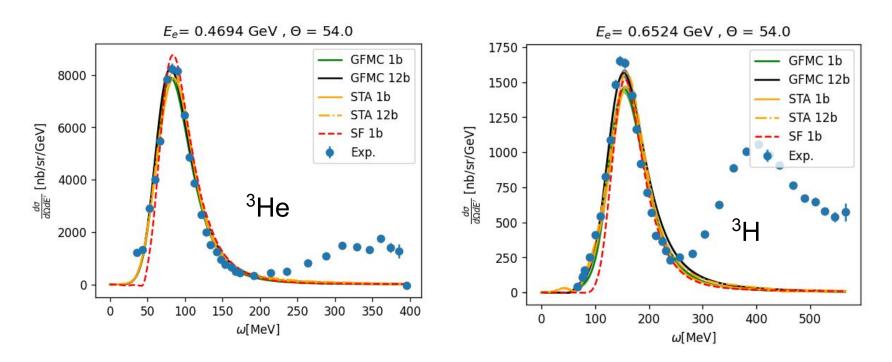


- STA responses used to build the cross sections
- Cross sections are used to generate events in GENIE (a Monte Carlo neutrino event generator)
- Here, we use electromagnetic processes (for which data are available) to validate the generator

$$\frac{d^2 \sigma}{d \omega d \Omega} = \sigma_M \left[v_L R_L(\mathbf{q}, \omega) + v_T R_T(\mathbf{q}, \omega) \right]$$

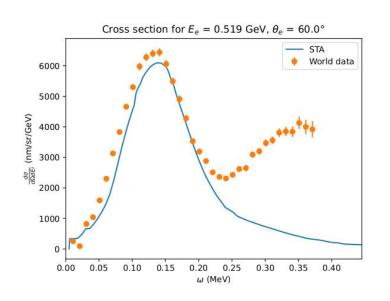
Barrow, Gardiner, SP et al. PRD 103 (2021) 5, 052001

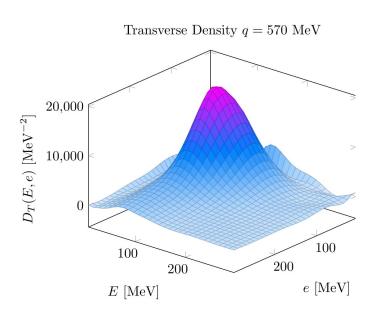
GFMC SF STA: Benchmark & error estimate



Lorenzo Andreoli, et al. PRC 2021

STA for Carbon 12: Preliminary results

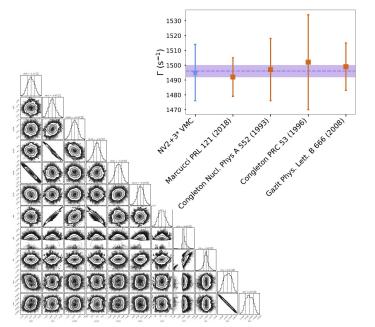


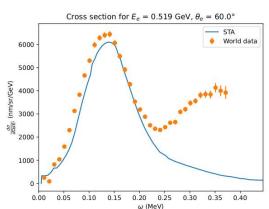


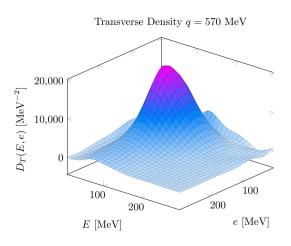
Lorenzo Andreoli et al. in preparation

Summary

Ab initio calculations of light nuclei yield a picture of nuclear structure and dynamics where many-body effects play an essential role to explain available data.







NP, LQCD, Pheno, Hep,
Comp, Expt, ...
are required to progress
e.g., NP is represented in the
Snowmass process

It's a very exciting time!

Collaborators

WashU: Andreoli Bub King Piarulli

LANL: Baroni Carlson Cirigliano Gandolfi Hayes Mereghetti

JLab+ODU: Schiavilla

ANL: Lovato Rocco Wiringa

UCSD/UW: Dekens

Pisa U/INFN: Kievsky Marcucci Viviani

Salento U: Girlanda Huzhou U: Dong Wang

Fermilab: Gardiner Betancourt

MIT: Barrow





Theory Alliance FACILITY FOR RARE ISOTOPE BEAMS















Quantum Monte Carlo group



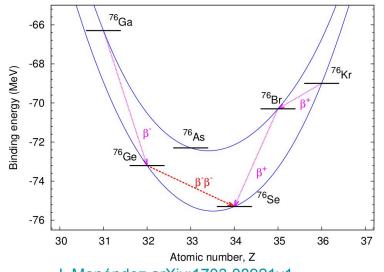


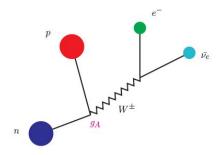




webpage: Quantum Monte Carlo group

Single and Double Beta Decays







Maria Goeppert-Mayer

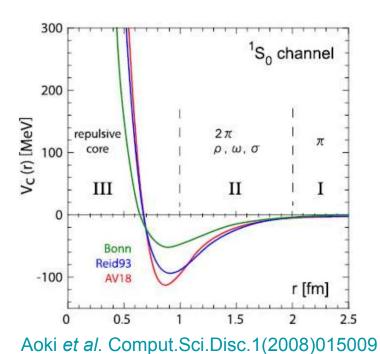
J. Menéndez arXiv:1703.08921v1

$$(\mathbf{Z}, N) \rightarrow (\mathbf{Z} + 1, N - 1) + e + \bar{\mathbf{v}}_e$$

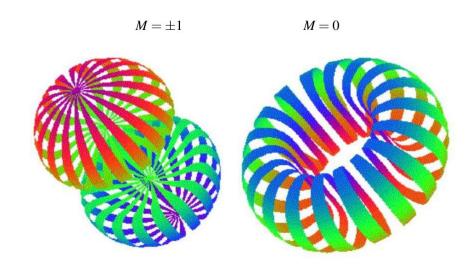
Double beta decay
$$(\mathbf{Z},N)
ightarrow (\mathbf{Z}+\mathbf{2},N-\mathbf{2}) + 2e + 2ar{v}_e$$

Here the lepton number is conserved

Nucleon-Nucleon Potential



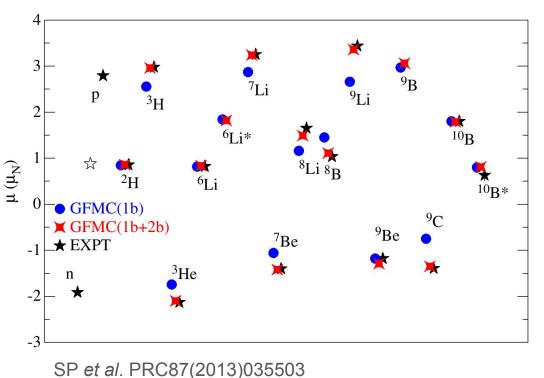
The Deuteron



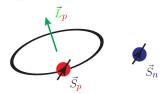
Constant density surfaces for a polarized deuteron in the $M=\pm 1$ (left) and M=0 (right) states

Carlson and Schiavilla Rev.Mod.Phys.70(1998)743

Magnetic Moments of Light Nuclei



Single particle picture



$$\mu_N(1b) = \sum_i [(L_i + g_p S_i)(1 + \tau_{i,z})/2 + g_n S_i(1 - \tau_{i,z})/2]$$

Small two-body current effects



 ^{9}Be

Large two-body current effects



90

Correlations in neutrinoless double beta decay ME

