Fundamental Physics with Nuclei

S@INT Seminar

2 June 2022
Saori Pastore

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

Quantum Monte Carlo Group @ WashU
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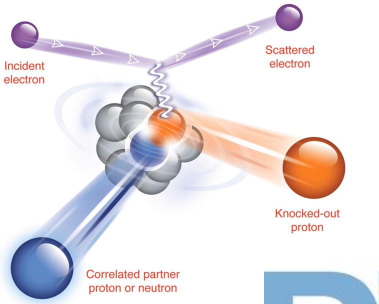
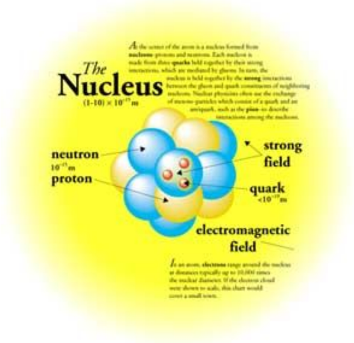
Computational Resources awarded by the DOE ALCC and INCITE programs

Fundamental Physics with Nuclei

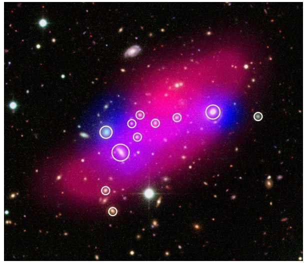
FRIB

Jefferson Lab



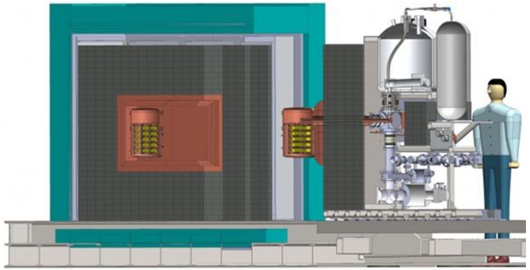


DUNE

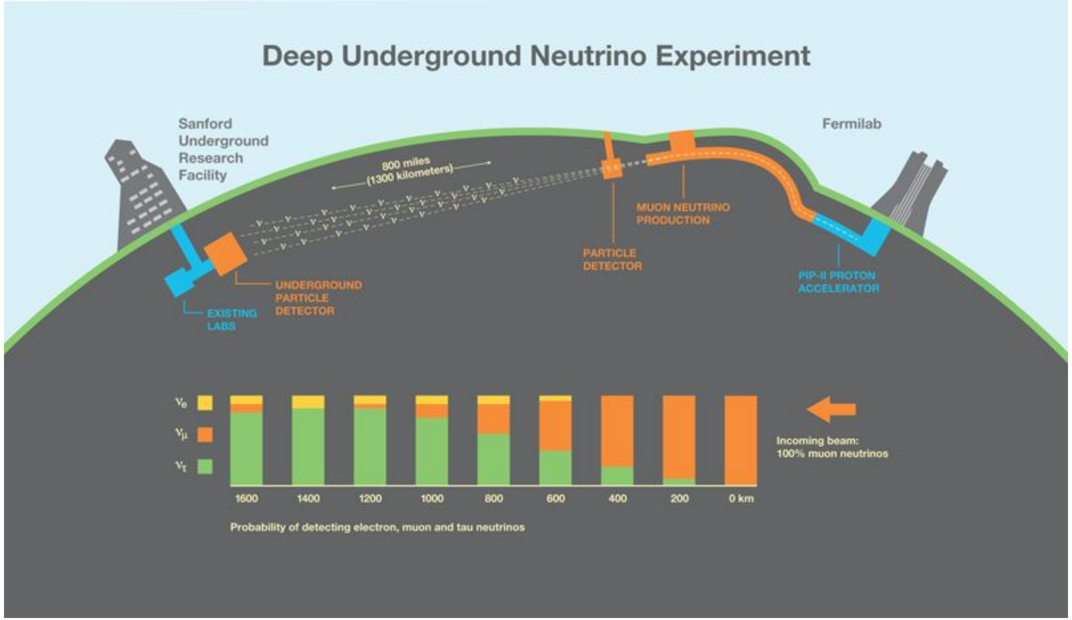


ESA, XMM-Newton, Gastaldello, CFHTL

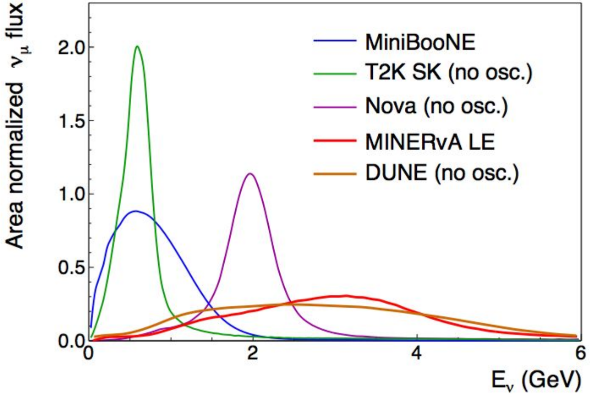
T2K



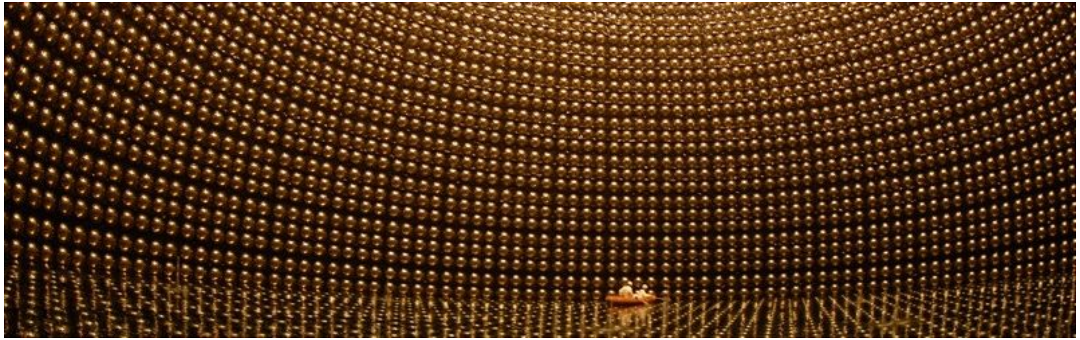
Accelerator Neutrinos’ Experiments



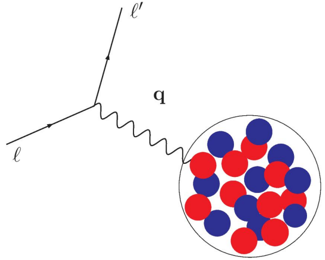
DUNE - Fermilab



Nuclei for Neutrino Oscillations’ Experiments

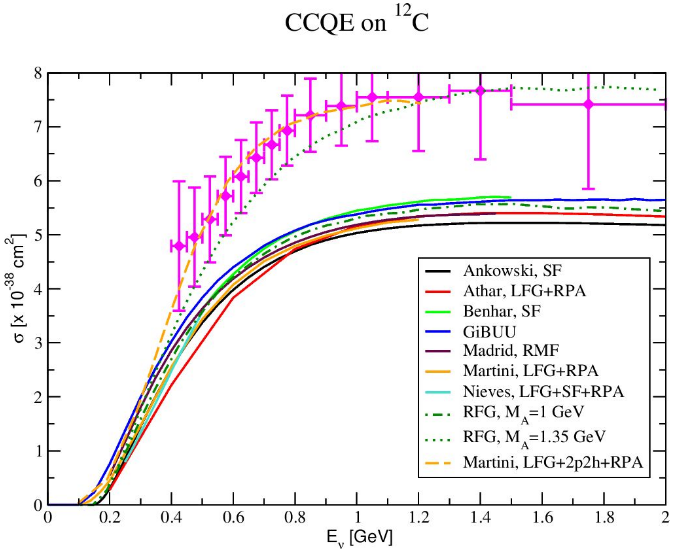


$$P(\nu_\mu \to \nu_e) = \sin^2 2\theta \sin^2\left(\frac{\Delta m^2_{21} L}{2E_\nu}\right)$$



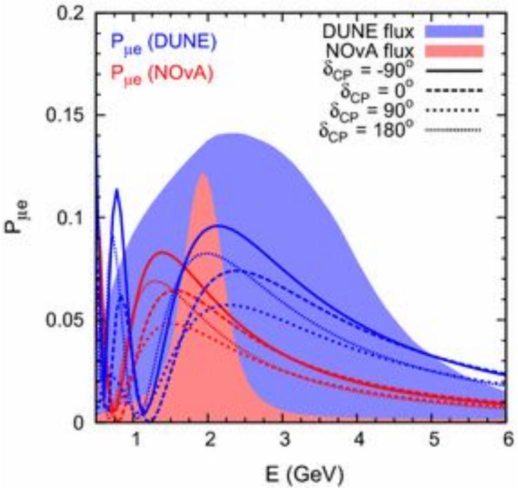
Nuclei are the active material in the detector. The energy of the incident neutrino is reconstructed from the observed final states using **neutrino event generators** that require **theoretical cross-sections**.

Neutrino-^{12}C cross section

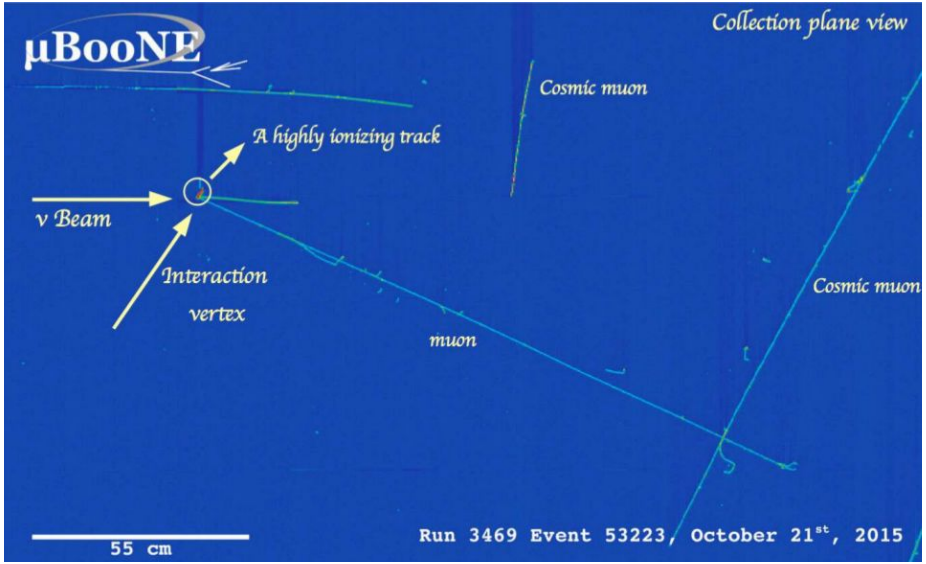


Alvarez-Ruso arXiv:1012.3871

The needs of the experimental programs

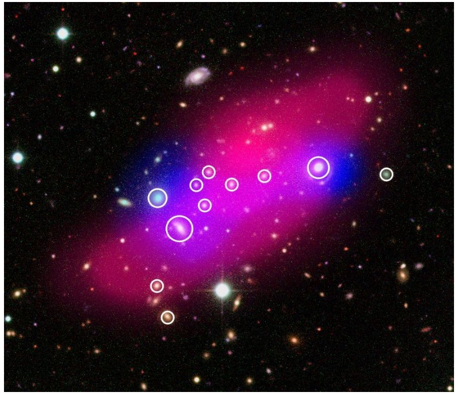


The experimental neutrino program is in need of accurate **theoretical calculations of neutrino-nucleus cross-sections with quantified theoretical errors** to ensure a robust implementation of interaction models in experiments



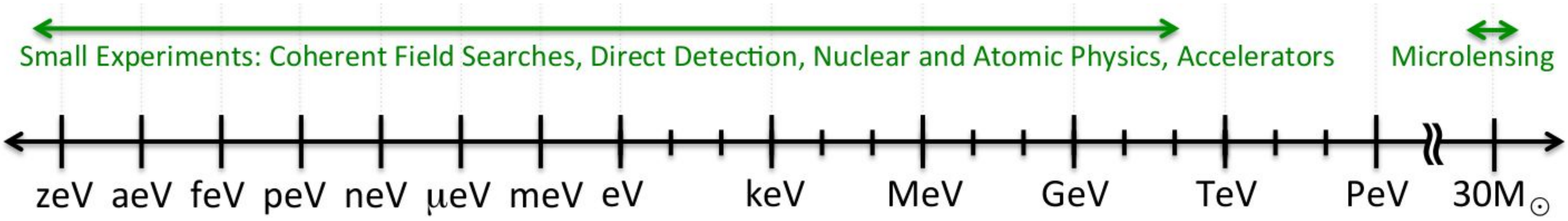
The range of challenges is extreme; ultimately we would like to be able to predict both inclusive and **exclusive cross sections across a wide range of kinematics**.

Dark Matter



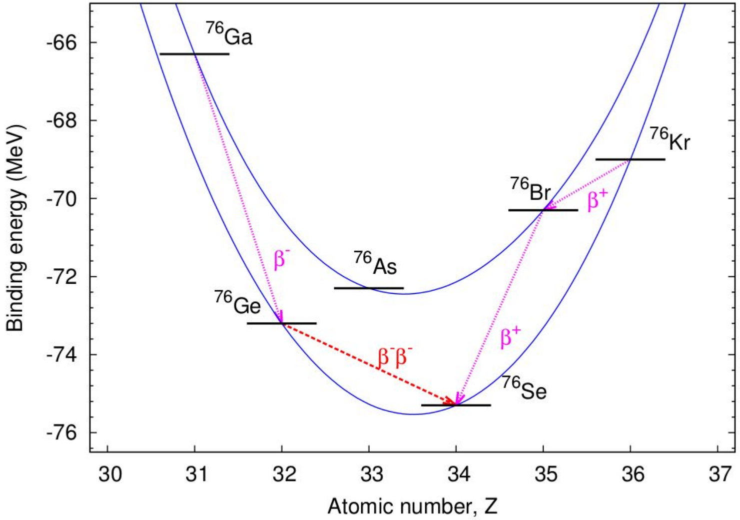
ESA, XMM-Newton, Gastaldello, CFHTL

Candidates

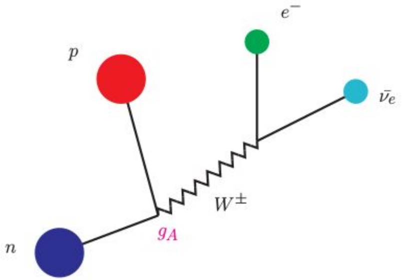


US cosmic vision 2017

Single and Double Beta Decays



J. Menéndez arXiv:1703.08921v1



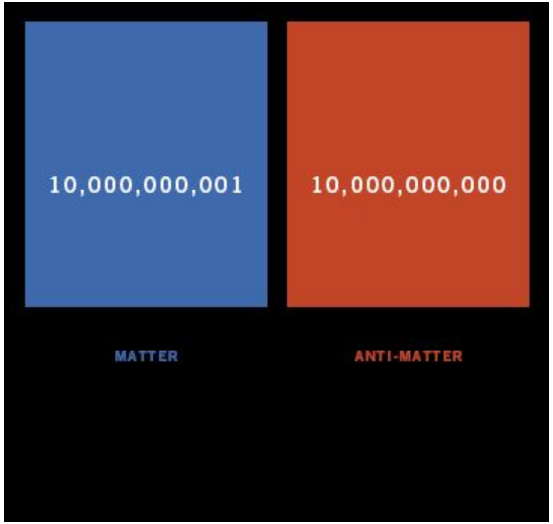
Maria Goeppert-Mayer

Single beta decay $(Z, N) \rightarrow (Z+1, N-1) + e + \bar{\nu}_e$

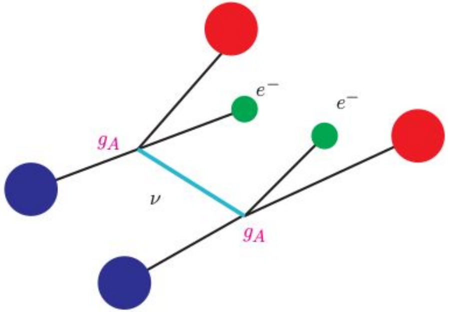
Double beta decay $(Z, N) \rightarrow (Z+2, N-2) + 2e + 2\bar{\nu}_e$

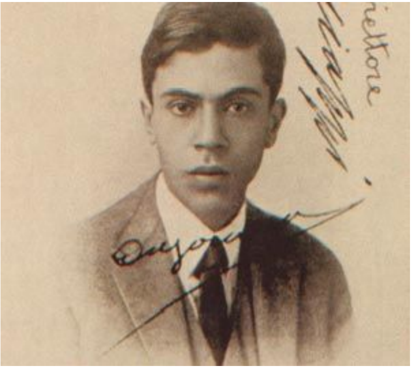
Here the lepton number is conserved

Neutrinoless double beta decay



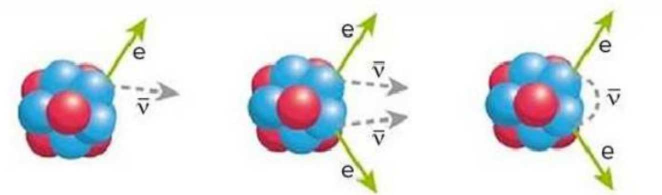
Hitoshi Murayama





Ettore Majorana

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

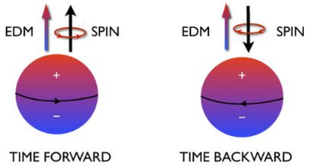


2015 Long Range Plan for Nuclear Physics

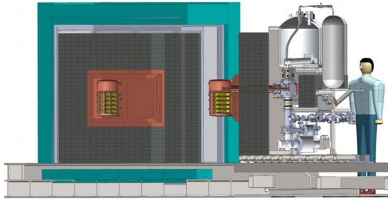
Lepton number is not conserved

Decay Rate ∝ (**nuclear matrix element**)^2 x ($m_{\beta\beta}$)^2

Ground States' Electroweak Moments, Form Factors, Radii



Neutrinoless Double Beta Decay, Muon-Capture



Accelerator Neutrino Experiments, Lepton-Nucleus XSecs

$(\omega,q)\sim0$ MeV

$\omega\sim$few MeVs
$q\sim0$ MeV

$\omega\sim$few MeVs
$q\sim10^2$ MeV

$\omega\sim$tens of MeVs

$\omega\sim10^2$ MeV

FRIB

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

JINA-CEE

Nuclear Rates for Astrophysics

DUNE

Jefferson Lab

Strategy

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

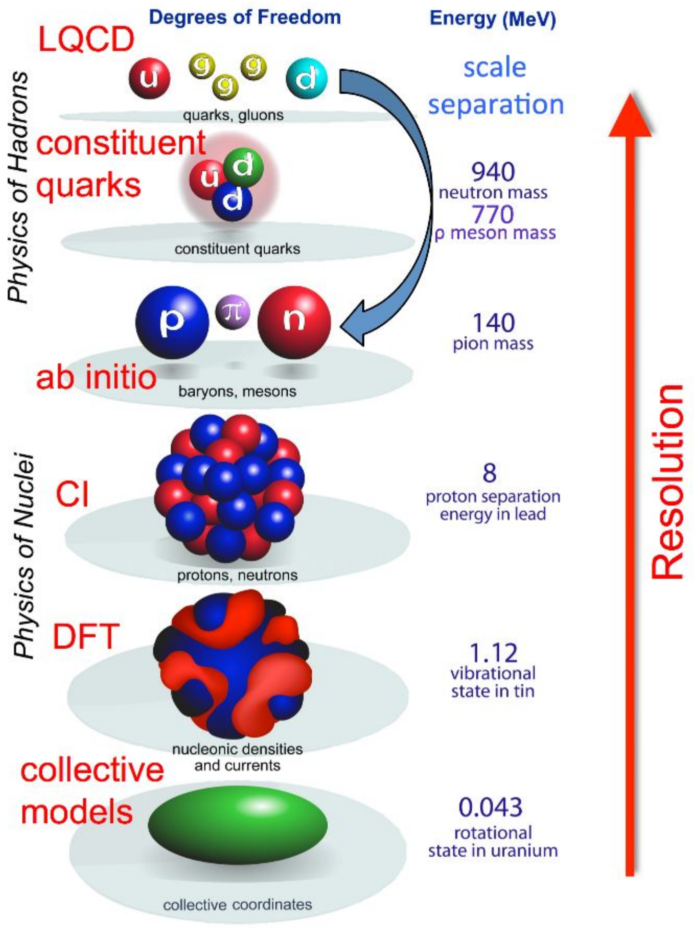
- Energy Spectra, Electromagnetic Form Factors, Electromagnetic Moments, ...
- Electromagnetic and Beta decay rates, ...
- Muon Capture Rates, ...
- Electron-Nucleus Scattering Cross Sections, ...

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, ...
- ...

From Quarks to Nuclei

- Nuclei are complex systems made of interacting protons and neutrons, which in turns are composite objects made of interacting constituent quarks.
- All fundamental forces are at play in nuclei.
- **EFTs** low-energy approximations of QCD whose d.o.f. are bound states of QCD (e.g., protons, neutrons, pions, …)
- **EFTs** are used to construct many-nucleon interactions and currents

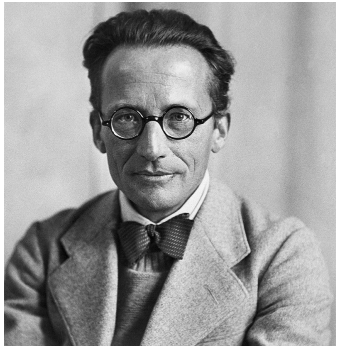


Microscopic (or *ab initio*) Description of Nuclei

Comprehensive theory that describes quantitatively and predictably nuclear structure and reactions

Requirements:

- Accurate understanding of the interactions/correlations between nucleons in **paris**, **triplets**, ... (**two- and three-nucleon forces**)
- Accurate understanding of the electroweak interactions of external probes (electrons, neutrinos, photons) with nucleons, correlated nucleon-pairs, … (**one- and two-body electroweak currents**)
- **Computational methods** to solve the many-body nuclear problem of strongly interacting particles



Erwin Schrödinger

$$H\Psi = E\Psi$$

Many-body Nuclear Problem

Nuclear Many-body Hamiltonian

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

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A, s_1, s_2, \dots, s_A, t_1, t_2, \dots, t_A)$$

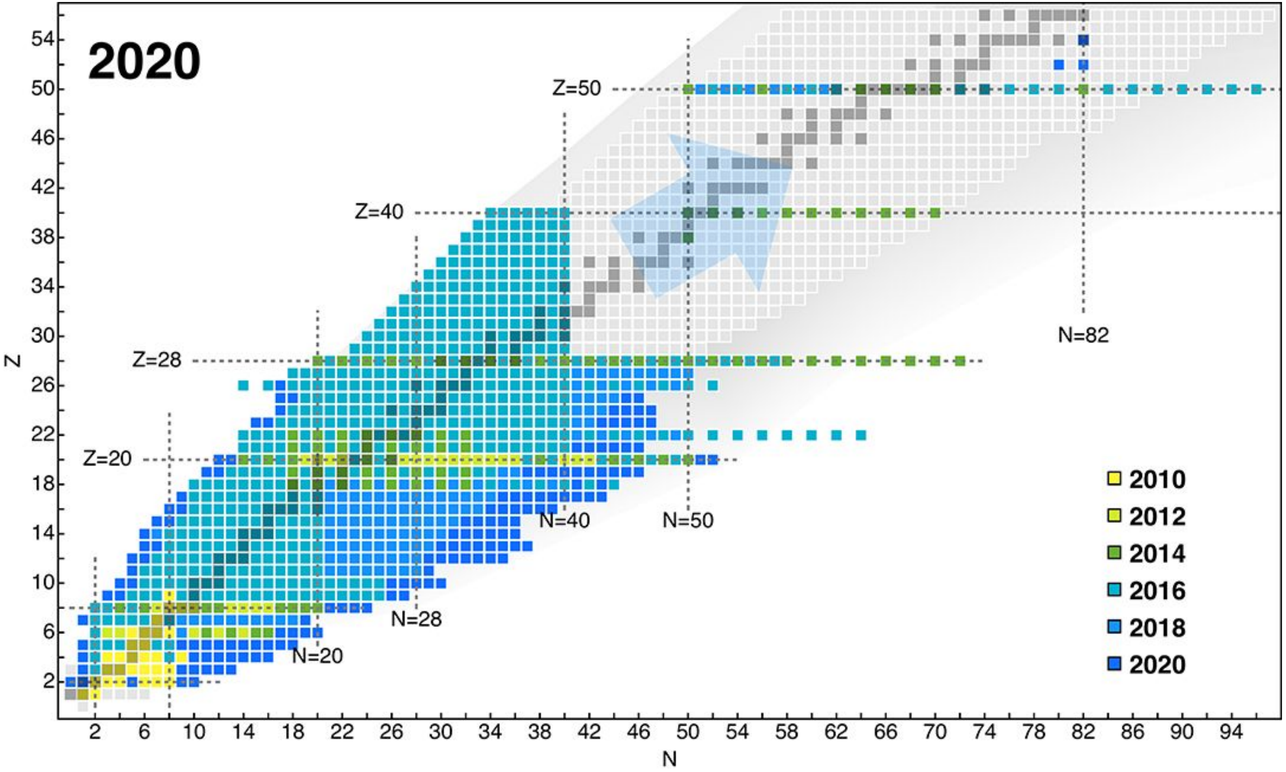
http://exascaleage.org/np/

Ψ are spin-isospin vectors in 3A dimensions with $2^A \times \frac{A!}{Z!(A-Z)!}$ components

^{4}He : 96
^{6}Li : 1280
^{8}Li : 14336
^{12}C : 540572

Develop Computational Methods to solve (numerically) exactly or within approximations that are under control the many-body nuclear problem

Current Status



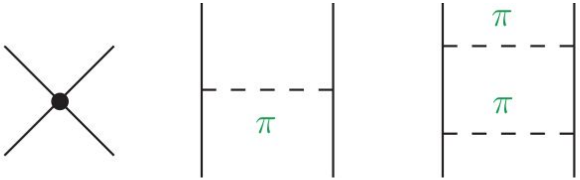
H. Hergert
Front. Phys.
07 October 2020

Many-body Nuclear Interactions

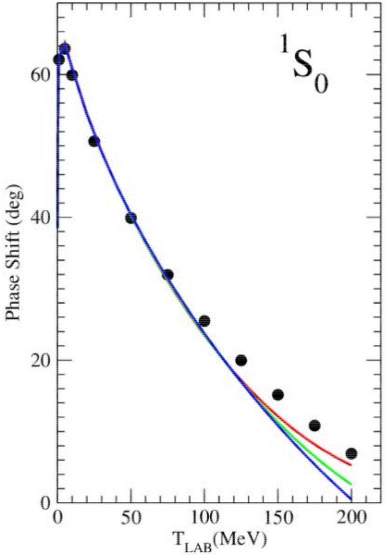
Many-body Nuclear Hamiltonian

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

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 $r \propto m_\pi^{-1}$



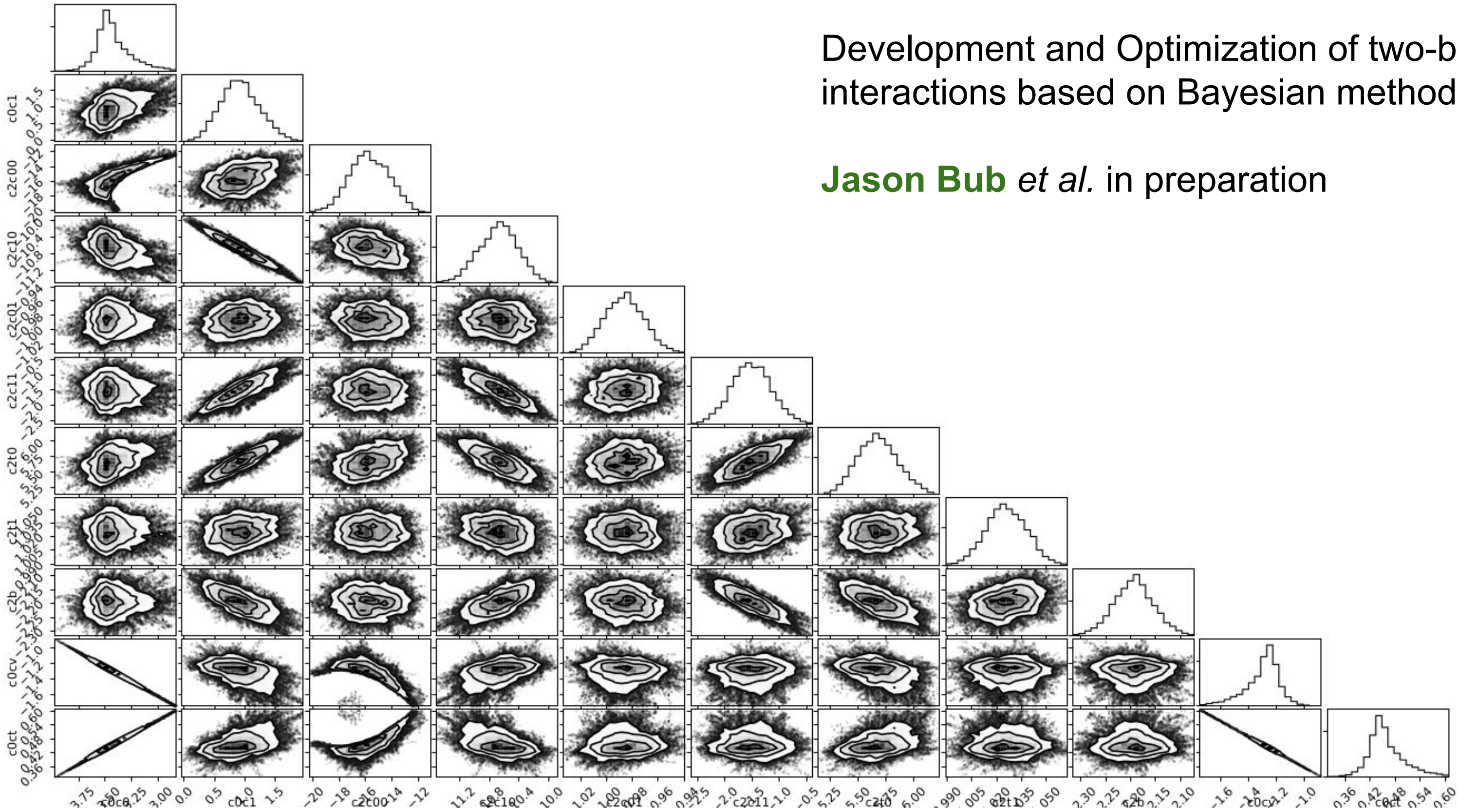
SP et al. PRC80(2009)034004

Hideki Yukawa

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

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

Optimization of Nuclear Two-body Interactions



Development and Optimization of two-body interactions based on Bayesian methods

Jason Bub *et al.* in preparation

Quantum Monte Carlo Methods

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

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

using the trial wave function:

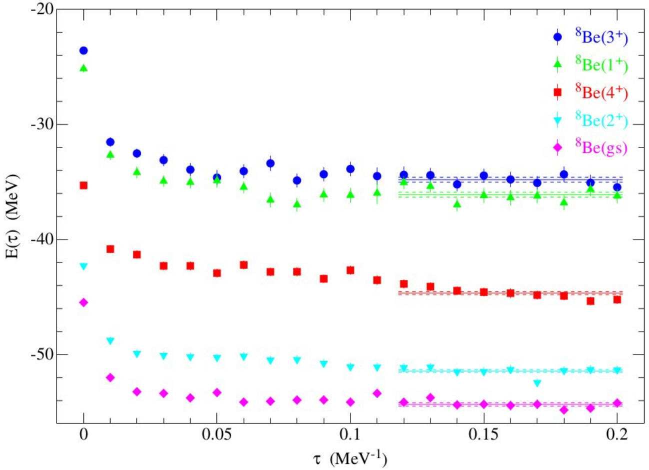
$$|\Psi_V\rangle = \left[\mathcal{S} \prod_{i<j} (1 + U_{ij} + \sum_{k \neq i,j} U_{ijk}) \right] \left[\prod_{i<j} f_c(r_{ij}) \right] |\Phi_A(JMTT_3)\rangle$$

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

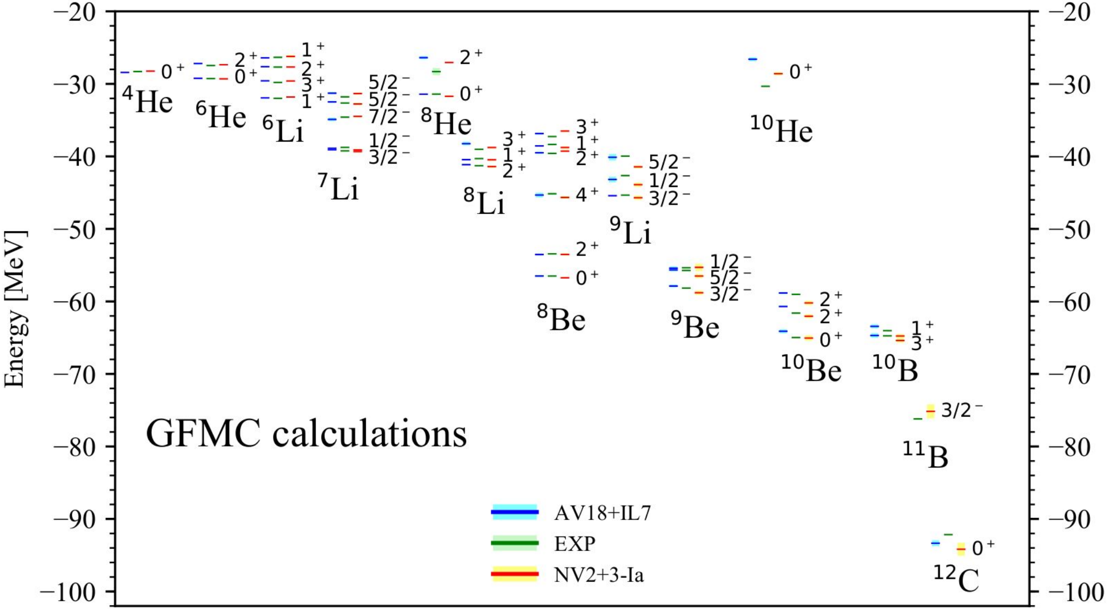
$$\Psi(\tau) = \exp[-(H - E_0)\tau]\Psi_V = \sum_n \exp[-(E_n - E_0)\tau] a_n \psi_n$$

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

Carlson, Wiringa, Pieper *et al.*

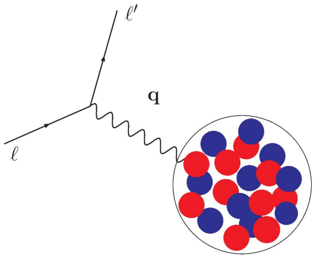


Energies

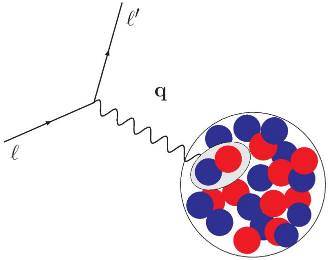


Piarulli *et al.* PRL120(2018)052503

Many-body Nuclear Electroweak Currents



one-body



two-body

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

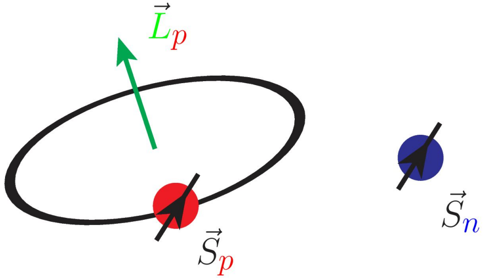
$$\mathbf{q}\cdot\mathbf{j} = [\,H,\,\rho\,] = [t_i + v_{ij} + V_{ijk},\,\rho\,]$$

Nuclear Charge Operator

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

Nuclear (Vector) Current Operator

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



Magnetic Moment: Single Particle Picture

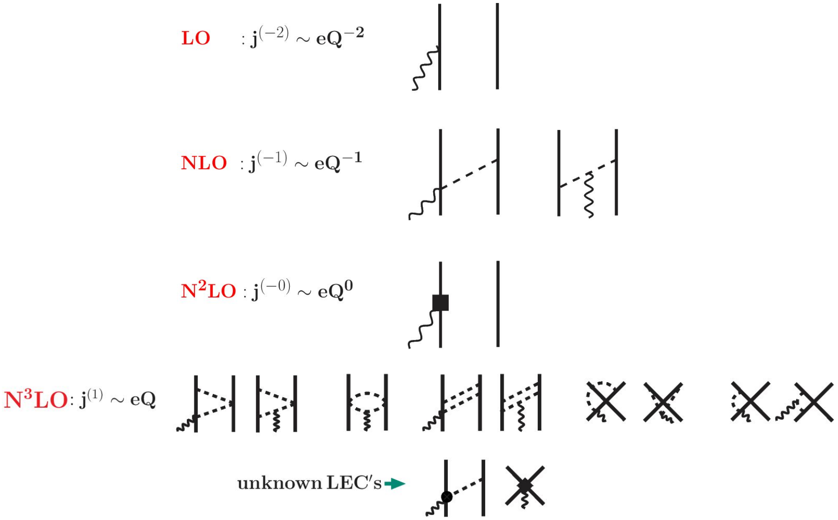
Many-body Currents

- **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**

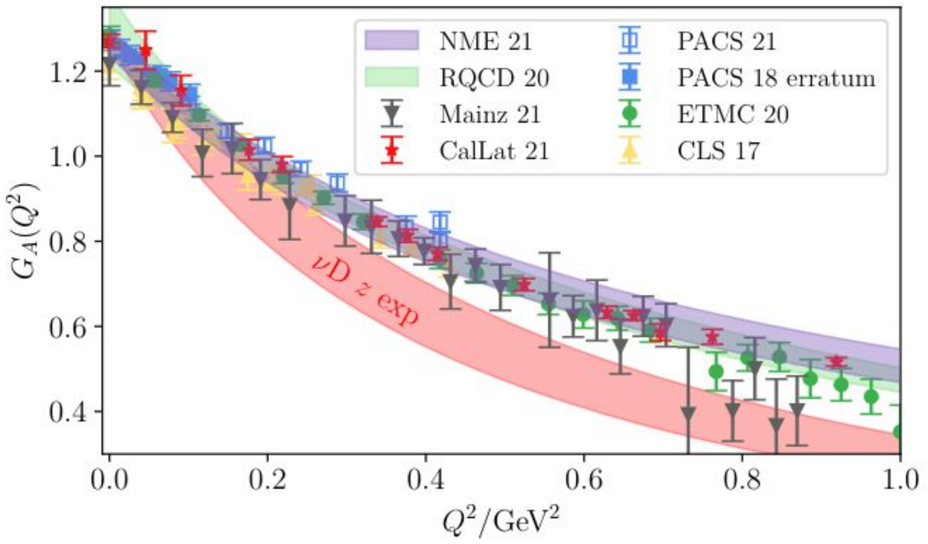
Are constructed consistently with the two-body chiral potential; Unknown parameters, or Low Energy Constants (**LECs**), need to be **determined by either fits to experimental data or by Lattice QCD calculations**



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

LCQD inputs for neutrino-nucleus scattering



Snowmass WP: Theoretical tools for neutrino scattering: interplay between lattice QCD, EFTs, nuclear physics, phenomenology, and neutrino event generators; arXiv:2203.09030

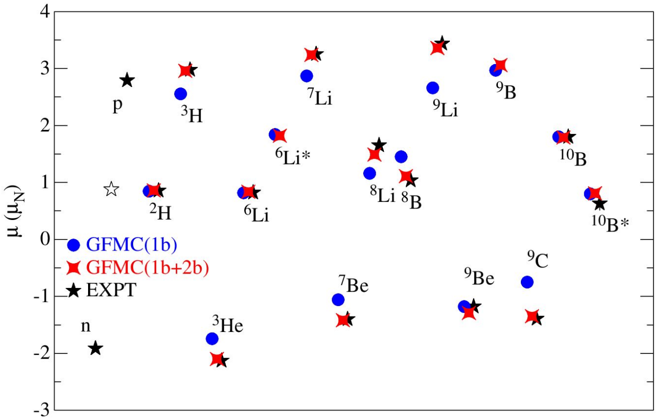
Building blocks of ab initio nuclear approaches:

Nucleonic form factors
Transition form factors
Pion production amplitudes
Two-nucleon couplings (strong and EW)
…

Taken from data where available, or from theory

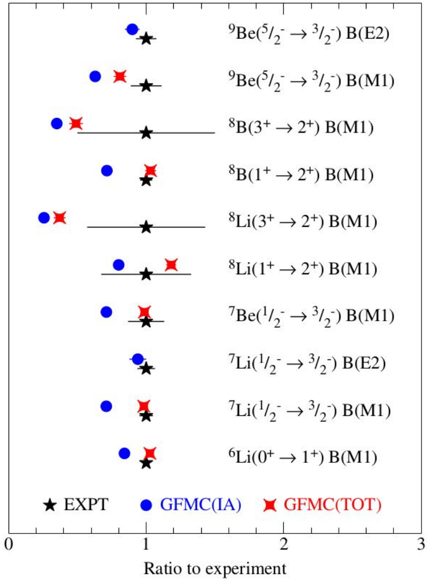
Electromagnetic Observables

Magnetic moments

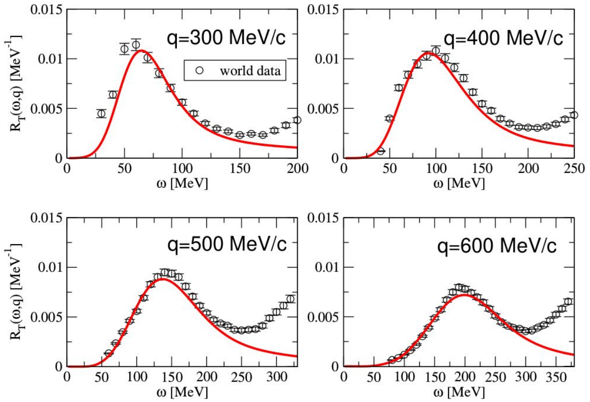


SP *et al*. PRC87(2013)035503, PRC101(2020)044612

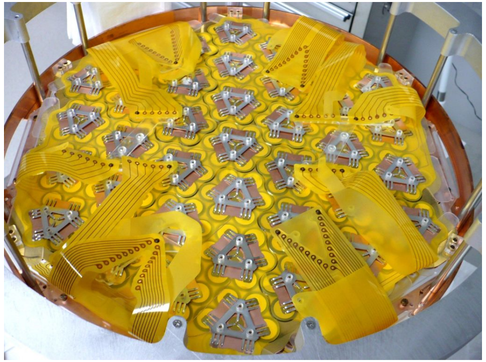
EM decay



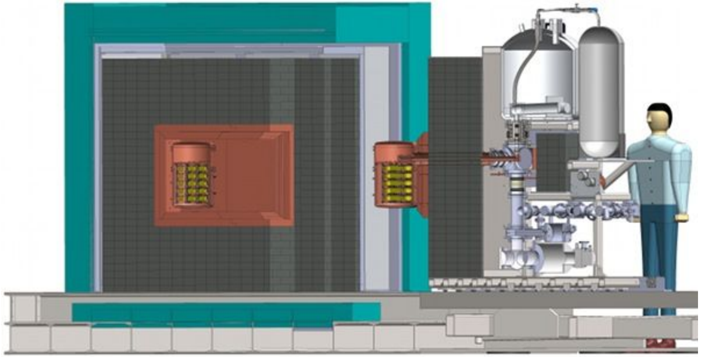
e-^{4}He particle scattering



Nuclear Physics for Neutrinoless Double Beta Programs



EXO-200 Collaboration

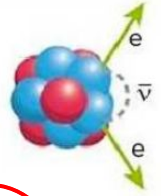


Majorana Demonstrator

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

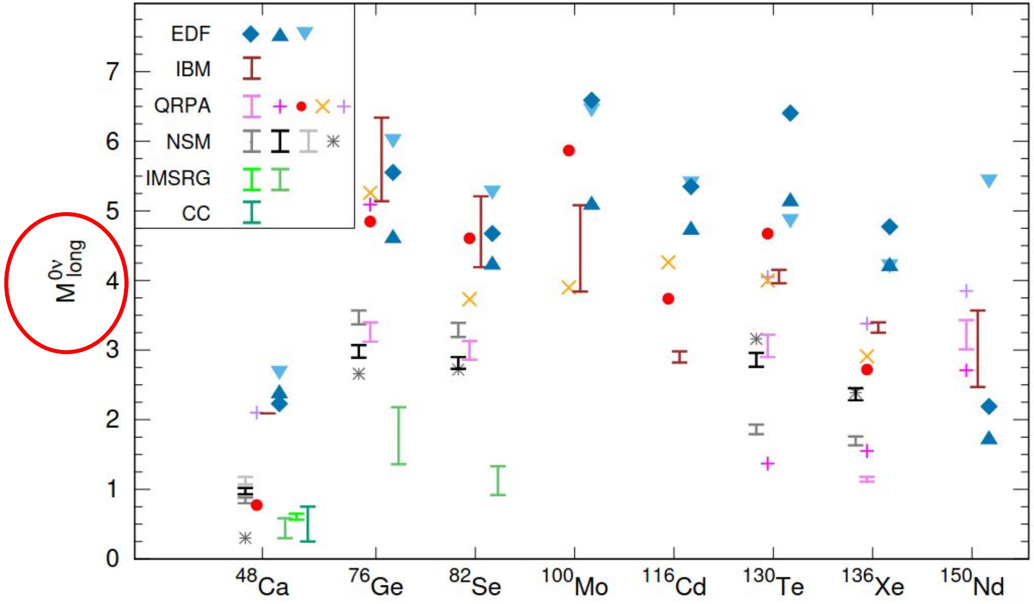
Decay Rate $\propto$ (**nuclear matrix element**)^2 x ($m_{\beta\beta}$)^2

Neutrinoless Double Beta Decay

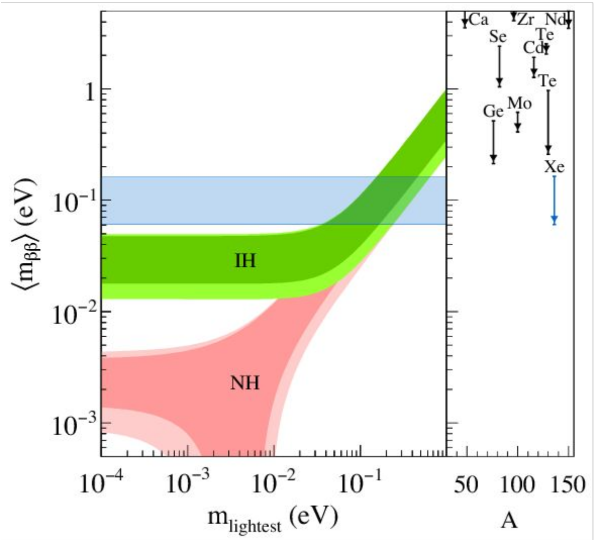


$$[T^{0\nu}_{1/2}]^{-1} = G_{0\nu}(Q,Z)\boxed{|M_{0\nu}|^2} m^2_{\beta\beta}$$

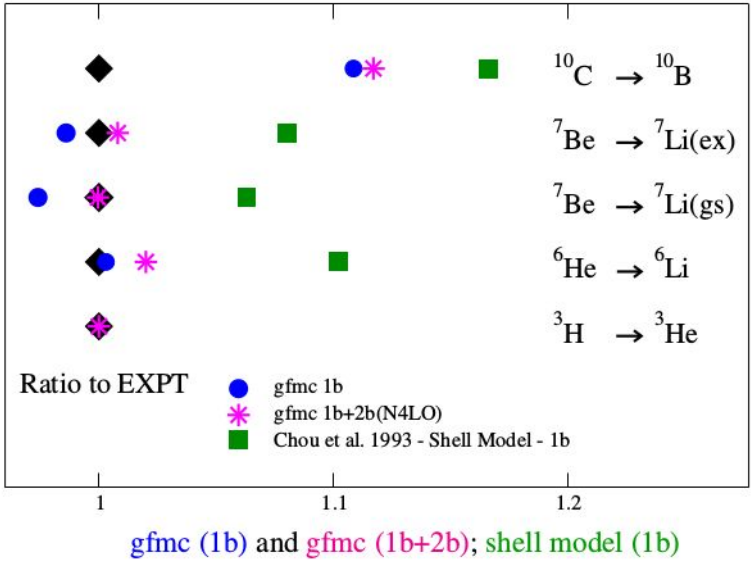
$$(Z,N) \rightarrow (Z+2,N-2)+2e$$



Agostini, Menendez et al, arXiv:2202.01787 (2022)

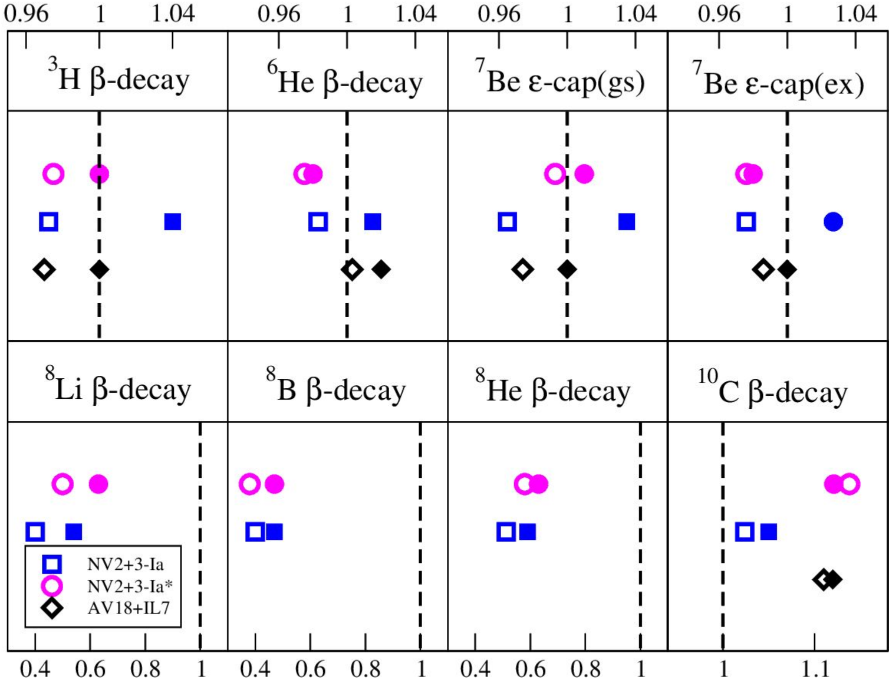


Beta decay



SP *et al*. PRC97(2018)022501

Beta Decay and Electron Capture in Light Nuclei



Garrett King *et al.* PRC102(2020)025501

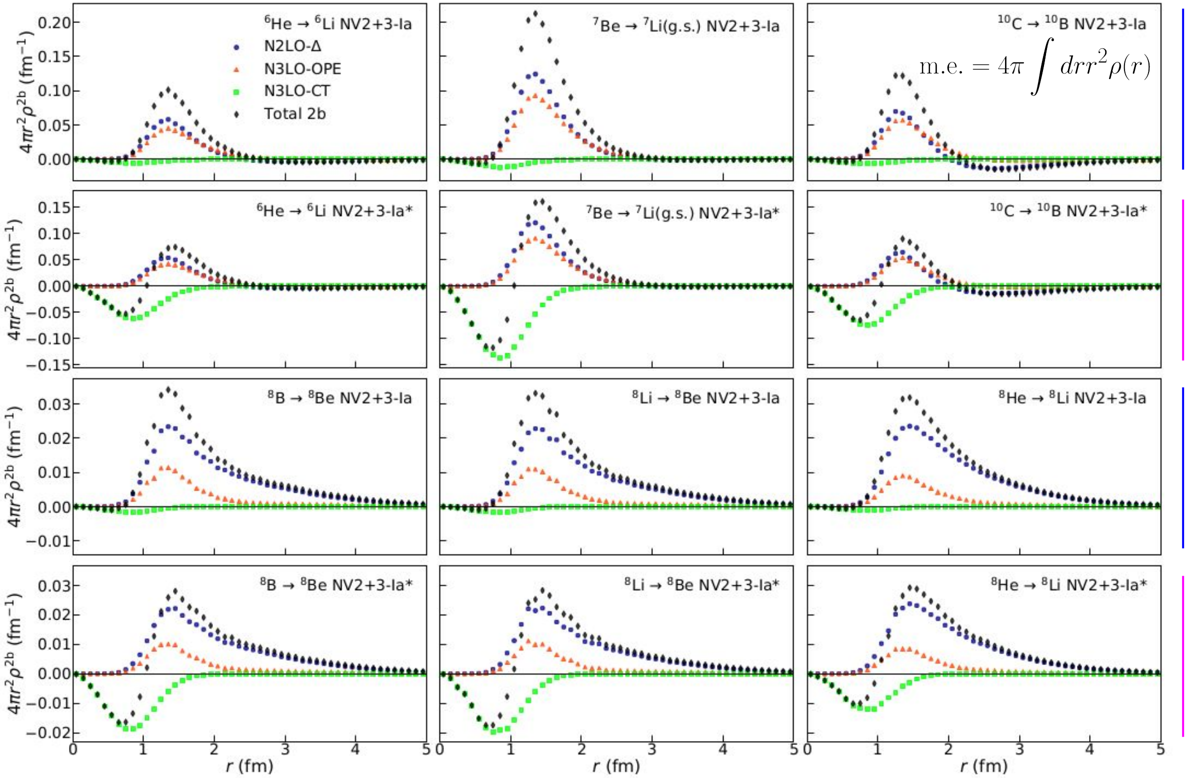
Calculations based on

- chiral interactions and currents
  NV2+3-Ia Norfolk unstarred
  NV2+3-Ia* 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 Two-body Transition Density



Garrett King *et al.* PRC102(2020)025501

NV2+3-Ia ; **NV2+3-Ia***

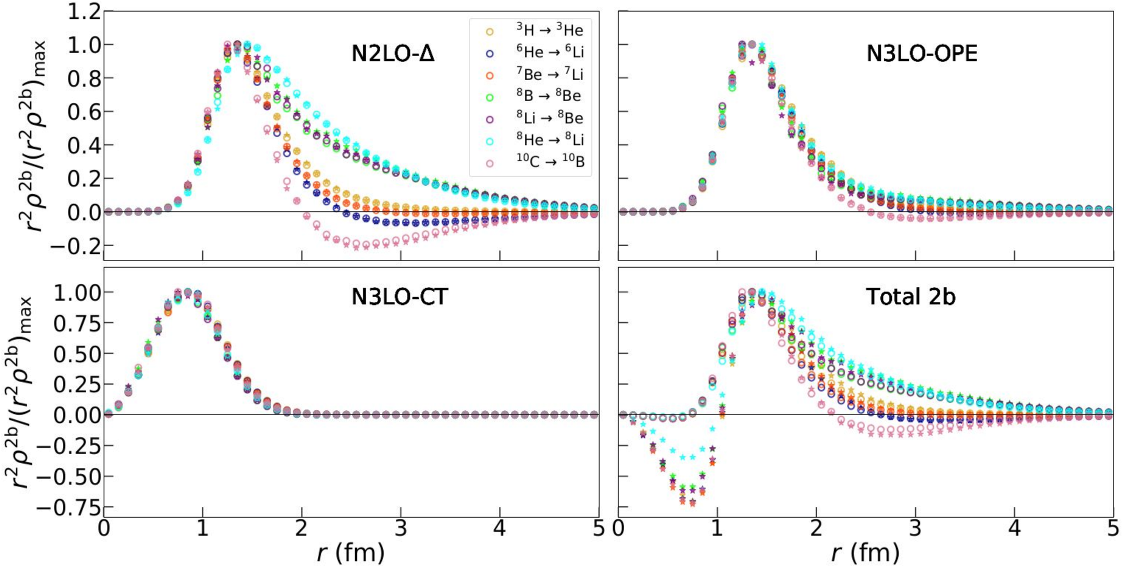
enhanced contribution from contact current in the starred model gives rise to nodes in the two-body transition density

Two-body axial currents

long-range at N2LO and N3LO

contact current at N3LO

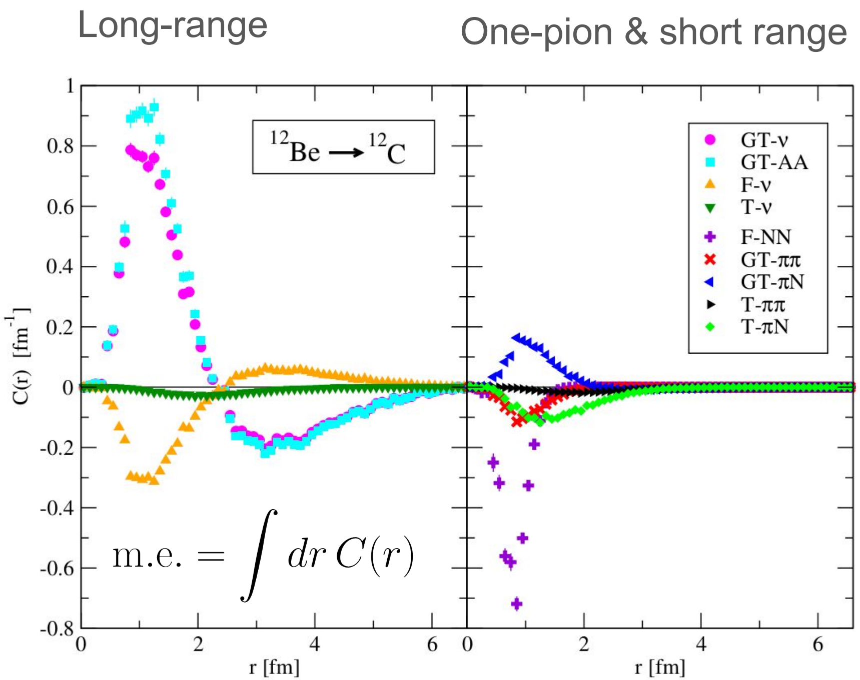
Scaling & Universality of Short-Range Dynamics



Garrett King *et al.* PRC102(2020)025501

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

Neutrinoless Double Beta Decay Matrix Elements

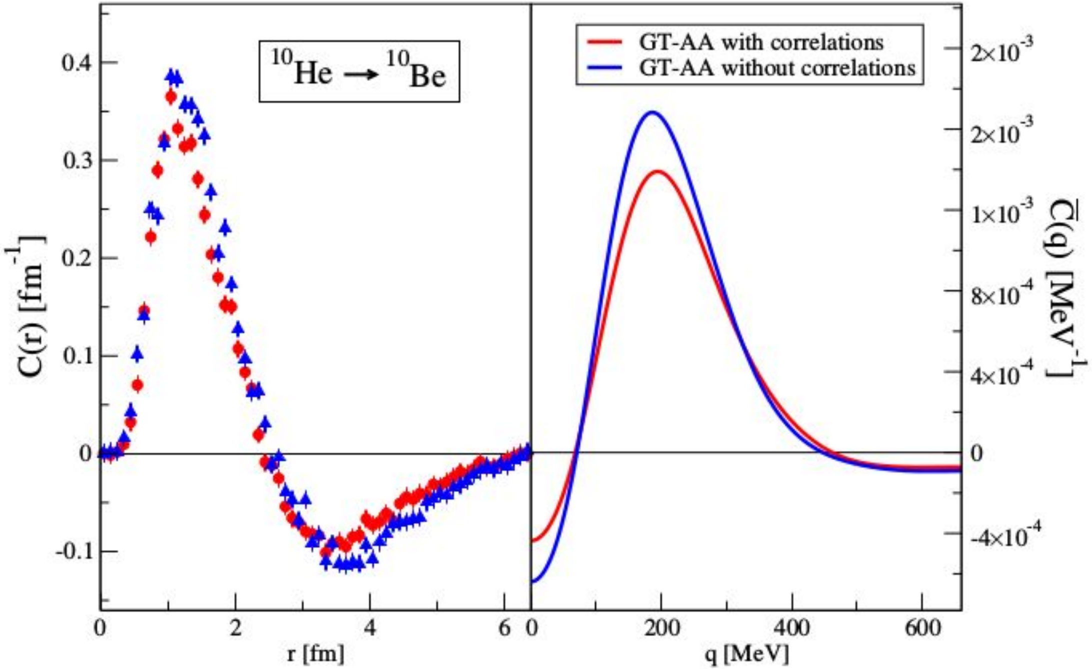


SP *et al.* PRC97(2018)014606

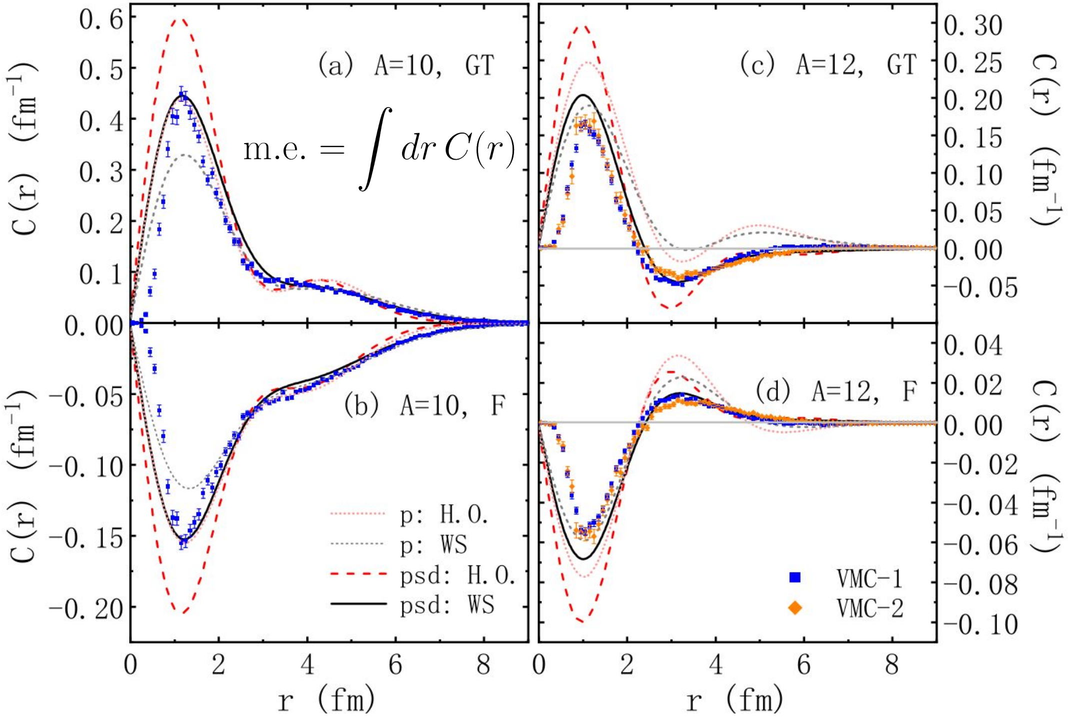
Cirigliano Dekens DeVries Graesser Mereghetti *et al.*
PLB769(2017)460, JHEP12(2017)082, PRC97(2018)065501

- 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**

Correlations in neutrinoless double beta decay ME



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

Partial muon capture rates: VMC calculations

Γ_{VMC}(avg.) = 1495 s^{-1} ± 19 s^{-1}

Γ_{expt} = 1496.0 s^{-1} ± 4.0 s^{-1}

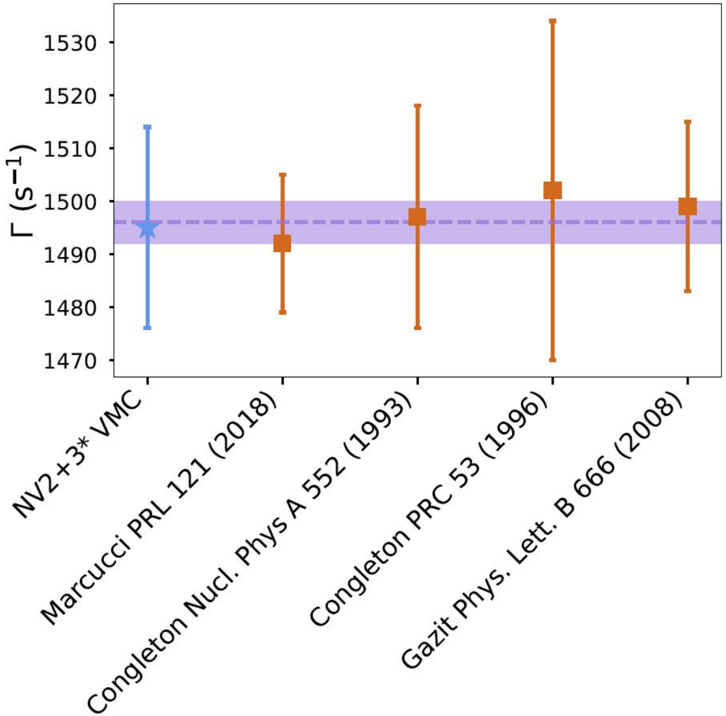
Ackerbauer *et al.* PLB417, 224(1998)

Momentum transfer **q~ 100 MeV**

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

Garrett King *et al.* PRC2022

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



Partial muon capture rates: VMC calculations

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

$\Gamma_{\mathrm{GFMC}}(\mathrm{IIa^*}) = 1171\ \mathrm{s}^{-1} \pm 164\ \mathrm{s}^{-1}$

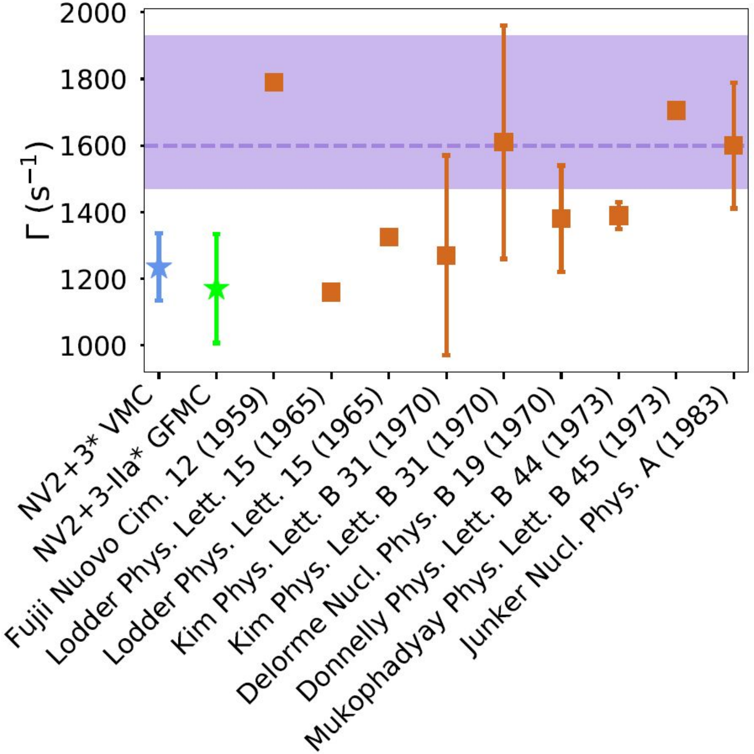
$\Gamma_{\mathrm{expt}} = 1600\ \mathrm{s}^{-1}\ +330/-129\ \mathrm{s}^{-1}$

Deutsch *et al.* PLB26(1968)315

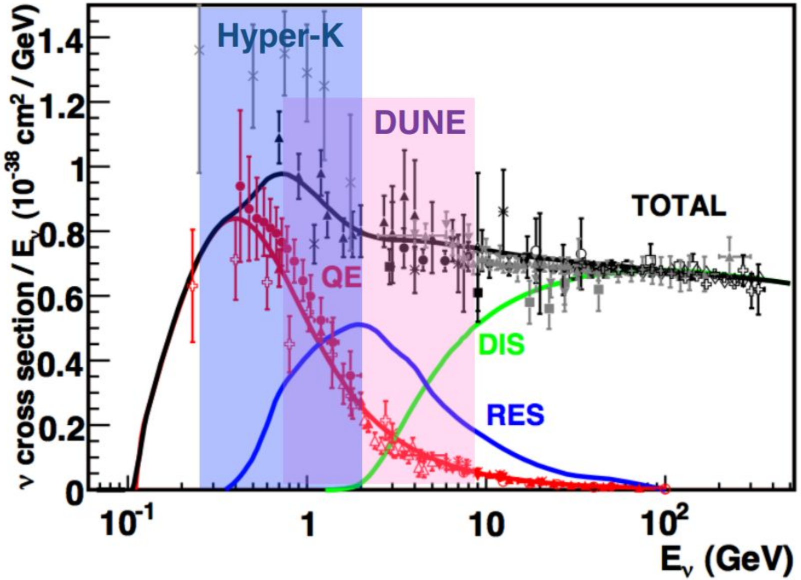
Garrett King *et al.* PRC2022

Outlook at FRIB: extraction of the Gamow-Teller strength A=11, A=12

$$^{6}\mathrm{Li}(1^+;0) \rightarrow {}^{6}\mathrm{He}(0^+;1)$$



Neutrino cross section anatomy



Formaggio & Zeller

Quasi-elastic: dominated by single-nucleon knockout

Resonance: excitation to nucleonic resonant states which decay into mesons

Deep-inelastic scattering: where the neutrino resolves the nucleonic quark content

Each of these regimes requires knowledge of both the **nuclear ground state** and the **electroweak coupling** and **propagation of the struck nucleons, hadrons, or partons**

A challenge for achieving precise neutrino-nucleus cross-section is **reliably bridging the transition regions which use different degrees of freedom**

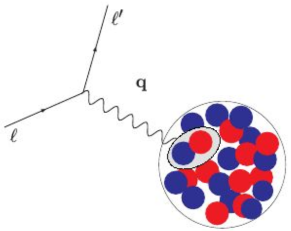
Lepton-Nucleus scattering: Inclusive Processes

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 $O_T = \boldsymbol{j}$
5 Responses in neutrino-nucleus scattering

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

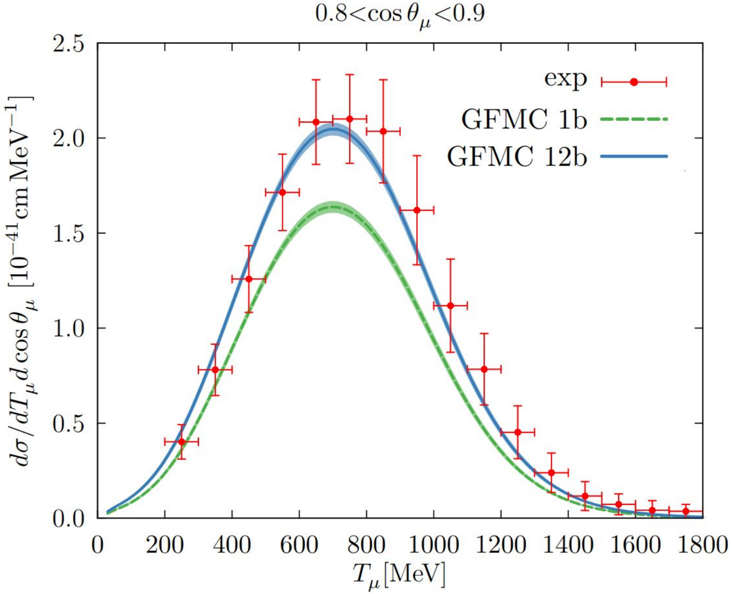


For a recent review on QMC, SF methods see
Rocco *Front. In Phys.*8 (2020)116

Inclusive Cross Sections with Integral Transforms

Exploit integral properties of the response functions and closure to avoid explicit calculation of the final states (Lorentz Integral Transform **LIT**, **Euclidean**, …)

$$\int_0^\infty \mathrm{d}\omega\, \mathrm{e}^{-\tau\omega}\, R_{\alpha\beta}(q,\omega) = \langle i|\, j_\alpha^\dagger(\mathbf{q})\, \mathrm{e}^{-\tau(H-E_i)}\, j_\beta(\mathbf{q})\, |i\rangle$$

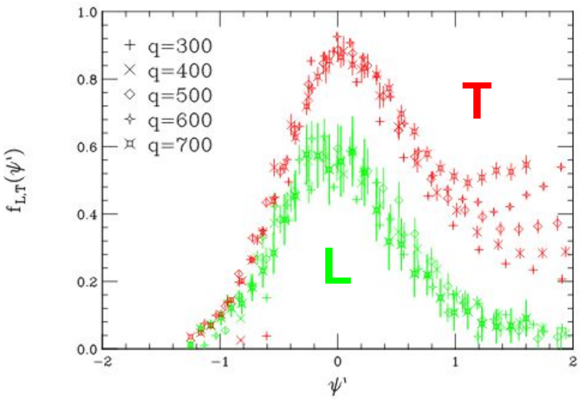


Lovato et al. PRX10 (2020)

Lepton-Nucleus scattering: Data

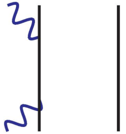
Transverse Sum Rule

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



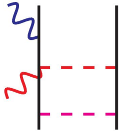
^{4}He Electromagnetic Data
Carlson *et al.* PRC65(2002)024002

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



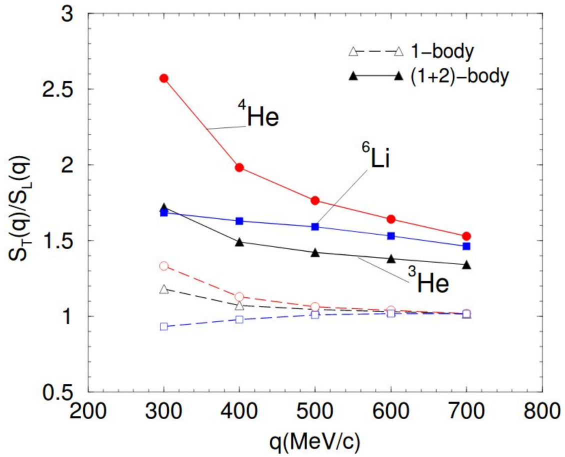
$$\langle \mathbf{j}_{1b}^\dagger\ \ \mathbf{j}_{1b}\rangle\ > 0$$

Leading one-body term



$$\langle \mathbf{j}_{1b}^\dagger\ \mathbf{j}_{2b}\ v_\pi\rangle \propto \langle v_\pi^2\rangle\ > 0$$

Interference term

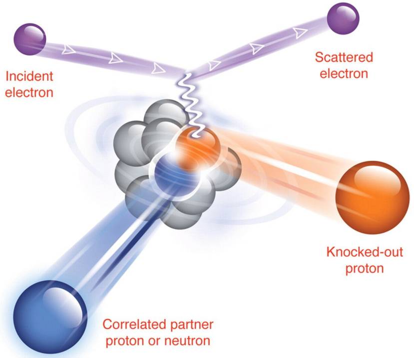


Transverse/Longitudinal Sum Rule
Carlson *et al.* PRC65(2002)024002

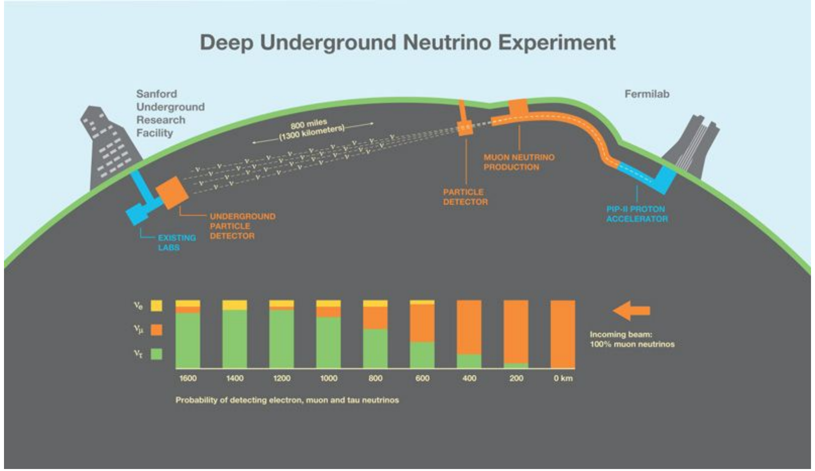
Beyond Inclusive: Short-Time-Approximation

Short-Time-Approximation Goals:

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



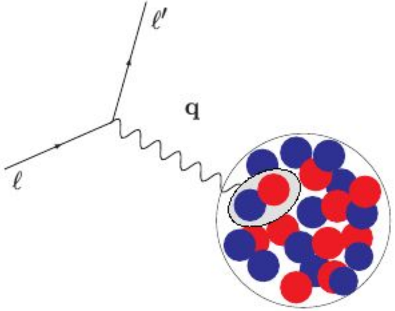
Subedi et al. Science320(2008)1475



Stanford Lab article

e4u collaboration

Short-Time-Approximation



Short-Time-Approximation:

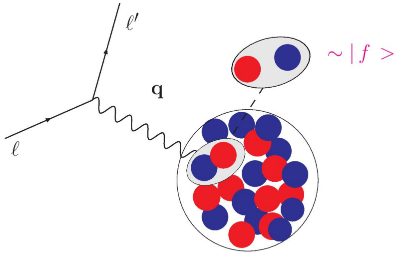
- Based on Factorization
- Retain two-body physics
- Correctly accounts for interference

$$R(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} \mathrm{e}^{i(\omega+E_0)t} \langle 0|O^\dagger \mathrm{e}^{-iHt} O|0\rangle$$

$$O_i^\dagger \mathrm{e}^{-iHt} O_i + O_i^\dagger \mathrm{e}^{-iHt} O_j + O_i^\dagger \mathrm{e}^{-iHt} O_{ij} + O_{ij}^\dagger \mathrm{e}^{-iHt} O_{ij}$$

$$H \sim \sum_i t_i + \sum_{i<j} v_{ij}$$

Factorization Schemes



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

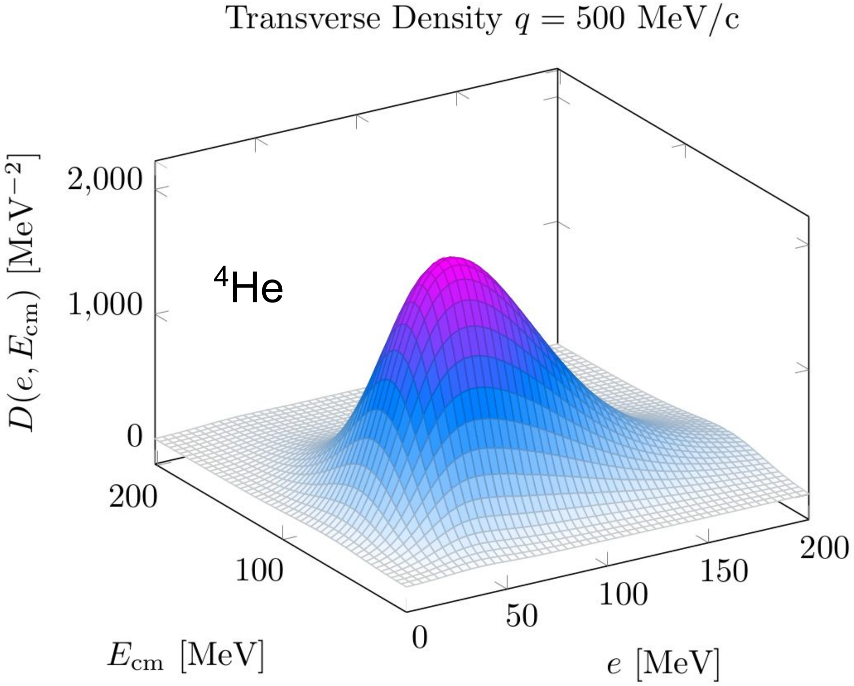
$$R_\alpha(q,\omega) = \sum_f \delta\left(\omega + E_0 - E_f\right) |\langle f|O_\alpha(\mathbf{q})|0\rangle|^2$$

Response ***Densities***

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

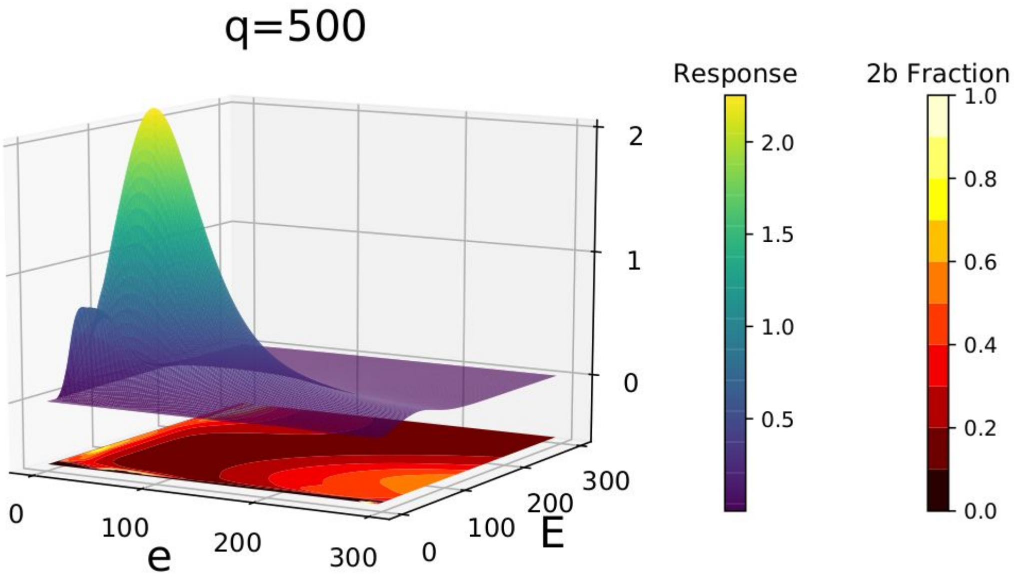
P' and *p'* are the CM and relative momenta of the struck nucleon pair

Transverse Response Density: *e*-^{4}He scattering

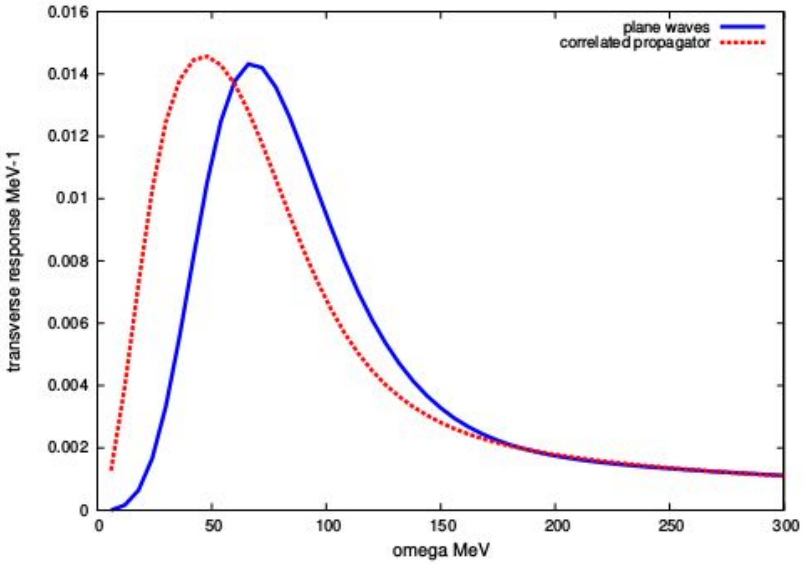


SP *et al.* PRC101(2020)044612

Transverse Response Density: two-body physics

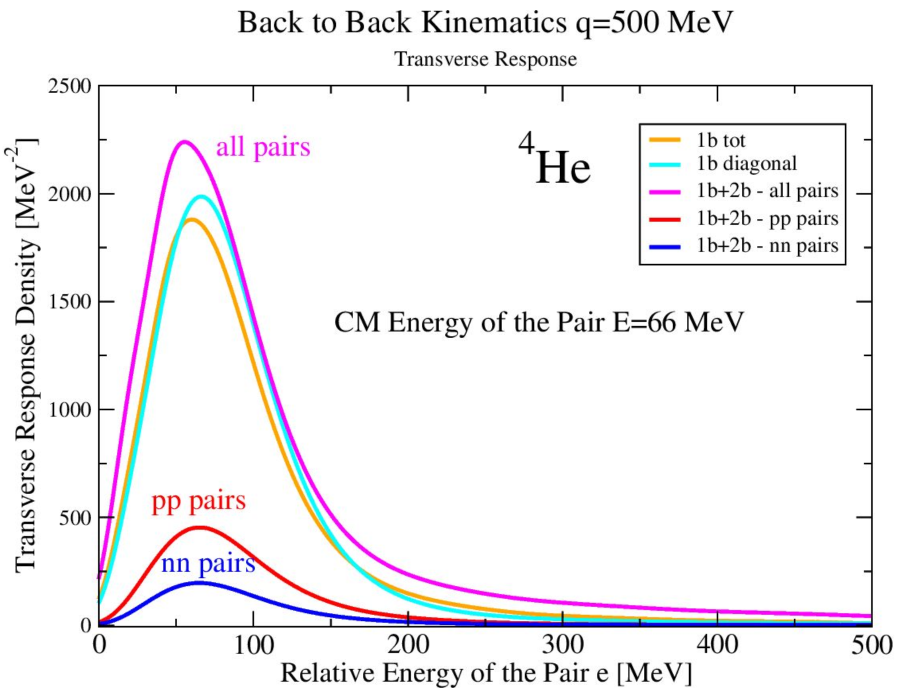


Correlated pairs vs uncorrelated pairs



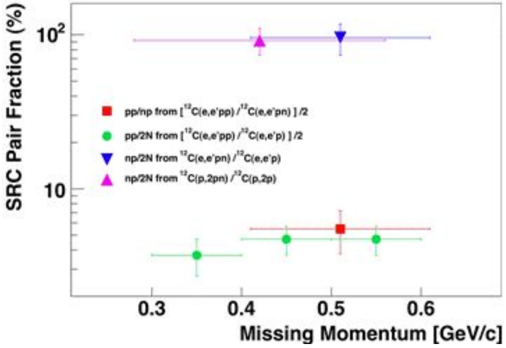
Scattering from uncorrelated vs correlated nucleon pairs

e-^{4}He scattering in the back-to-back kinematic



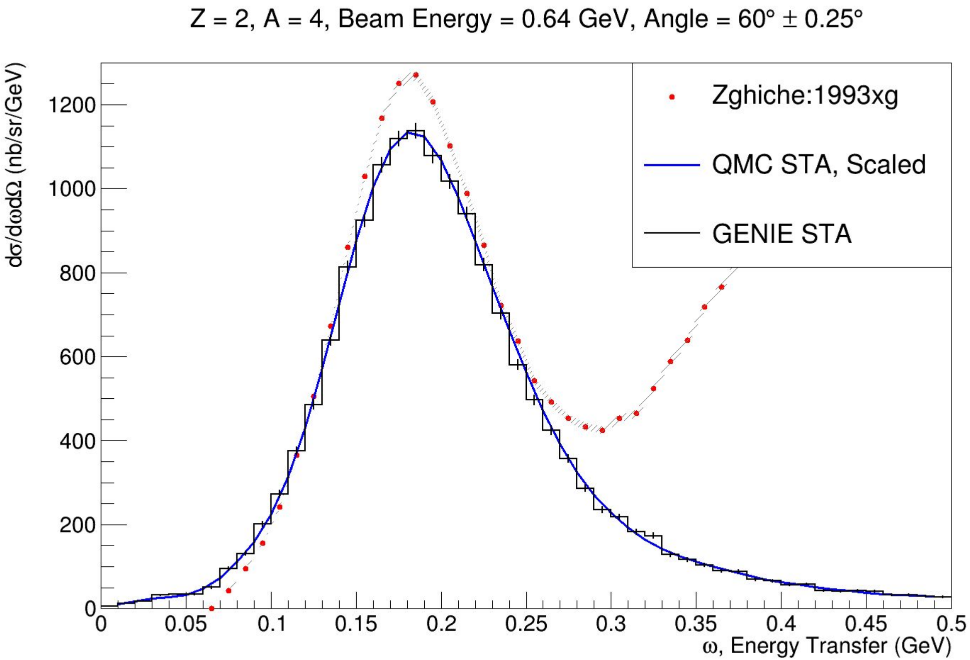
SP *et al.* PRC101(2020)044612

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



Subedi et al. Science320(2008)1475

GENIE validation using e-scattering



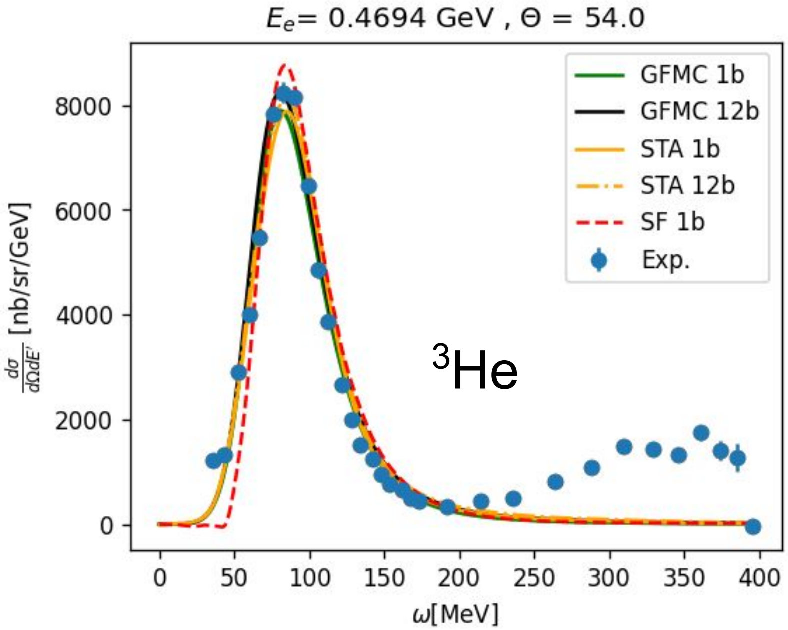
Barrow Gardiner Betancourt SP *et al.*
PRD 103 (2021) 5, 052001

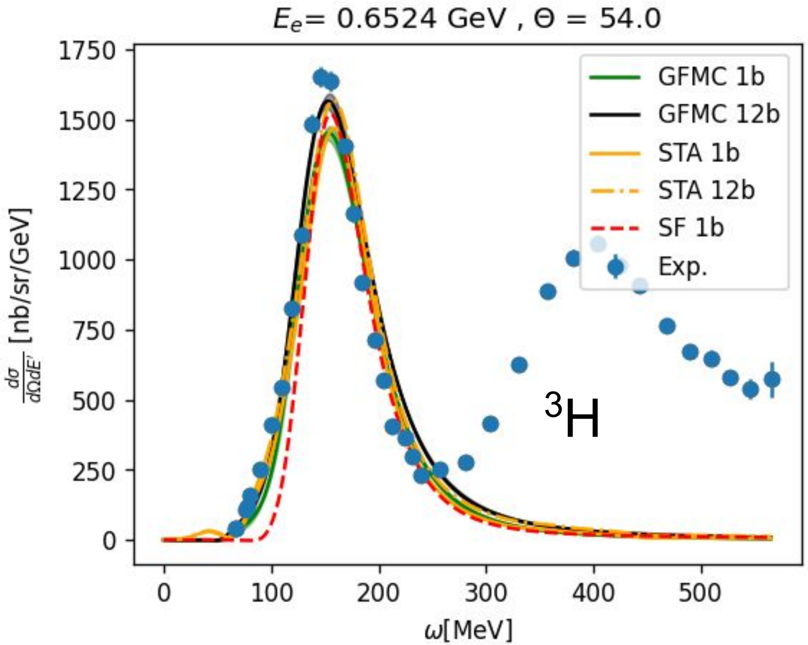
Ongoing work

- Implementation of moment-morphin interpolation techniques
- Implementations of response ***Densities*** in GENIE
- ^{12}C response densities with Lorenzo Andreoli

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

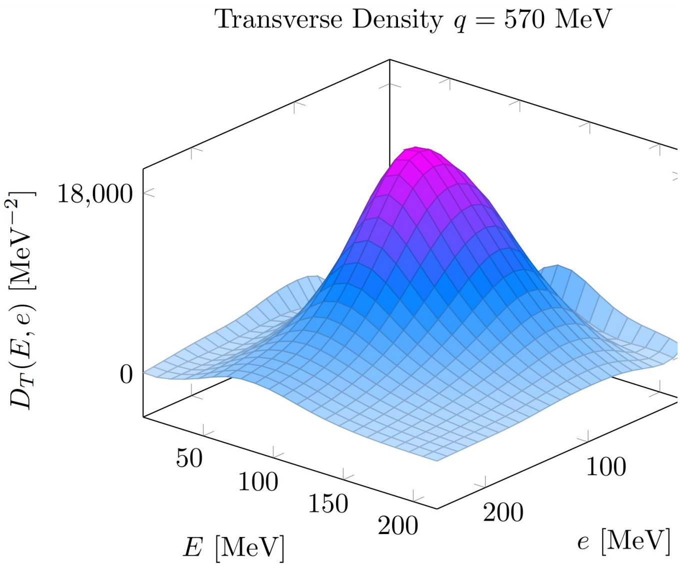
GFMC SF STA: Benchmark & error estimate

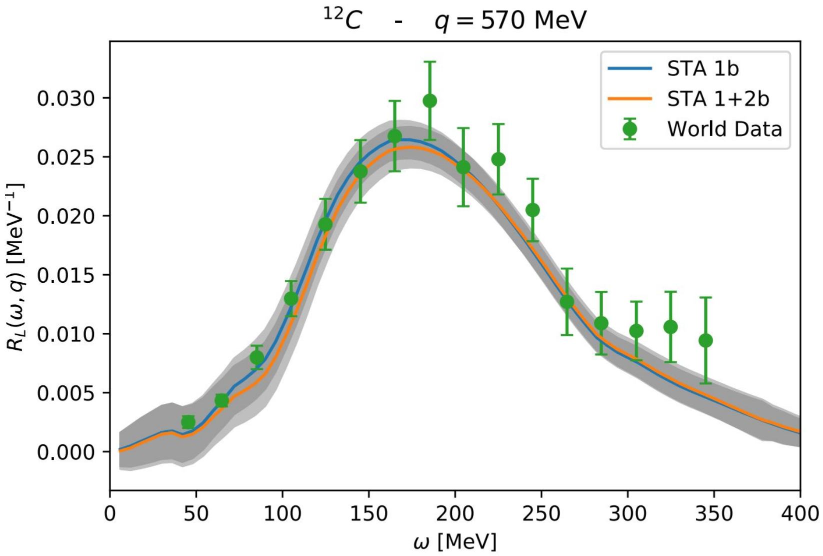




Andreoli, Rocco *et al.* submitted to PRC

STA for Carbon 12: Preliminary results

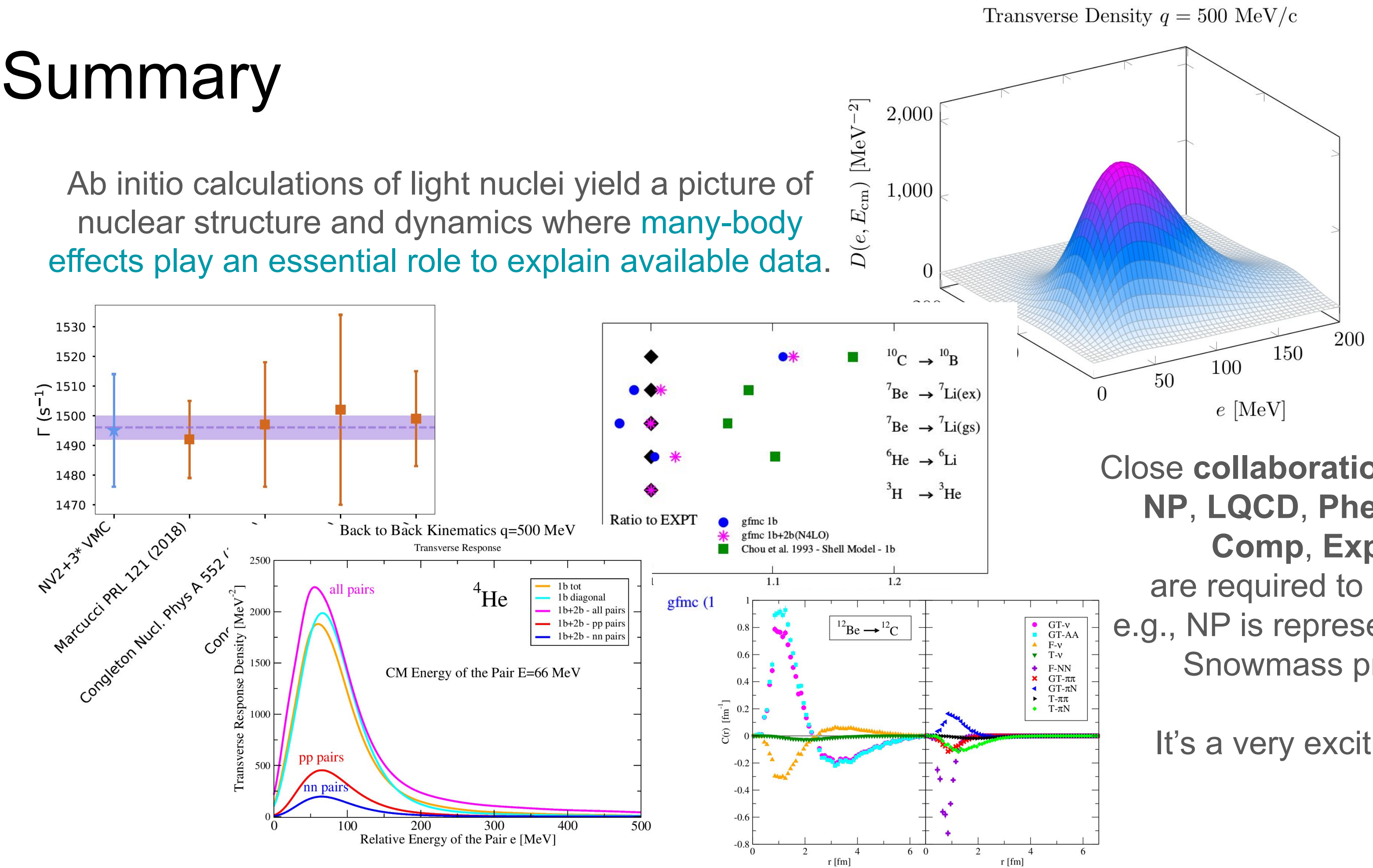




Lorenzo Andreoli *et al.* in preparation

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.



Close **collaborations** between
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

Washington University in St. Louis
Arts & Sciences

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Los Alamos
NATIONAL LABORATORY
EST. 1943

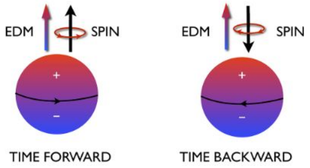
Argonne
NATIONAL LABORATORY

U.S. DEPARTMENT OF
ENERGY
Office of Science

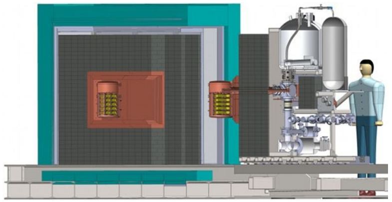
McDonnell Center
for the Space Sciences

Fermilab

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~10^2 MeV

ω~tens of MeVs

ω~10^2 MeV

FRIB

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

JINA-CEE

Nuclear Rates for Astrophysics

DUNE

Jefferson Lab