Quantum Monte Carlo calculations of lepton-nucleus interactions

Saori Pastore
Theory Seminar - Jefferson Lab
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Washington University in St. Louis
Arts & Sciences

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Collaborators:
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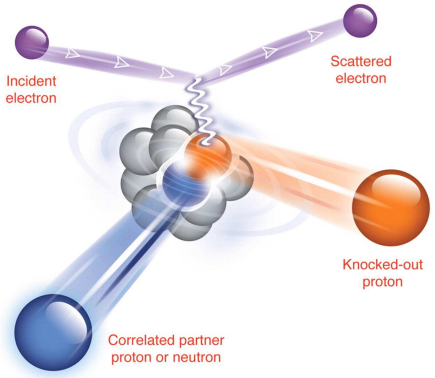
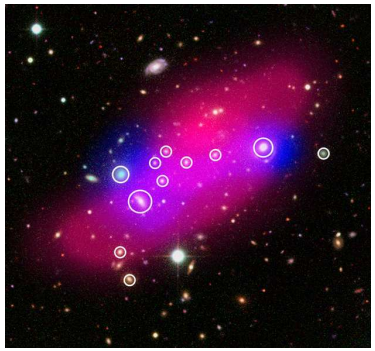
Baroni (USC) Girlanda (Salento U.) Marcucci & Viviani (Pisa U/INFN)
Mereghetti & Dekens & Cirigliano & Graesser (LANL)
de Vries (UMass-Amherst) van Kolck (AU+CNRS/IN2P3)

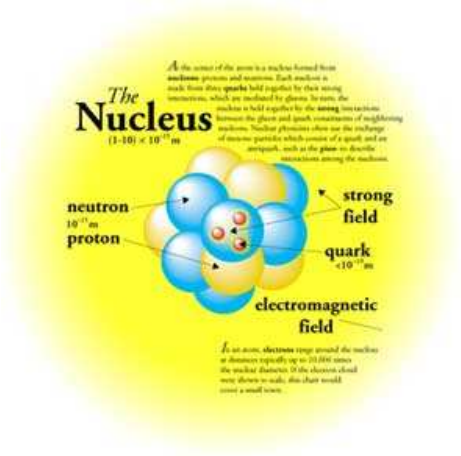
Resources: DOE-ALCC 0.39 MNH for "Low Energy Neutrino-Nucleus Interactions", SP *et al.* 2019

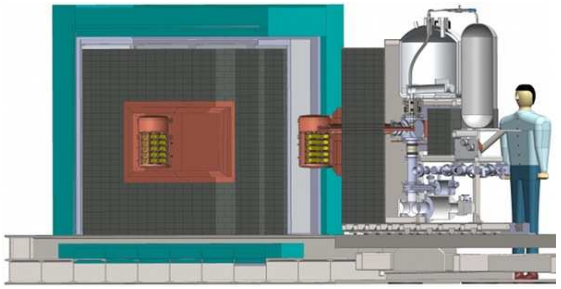
FRIB



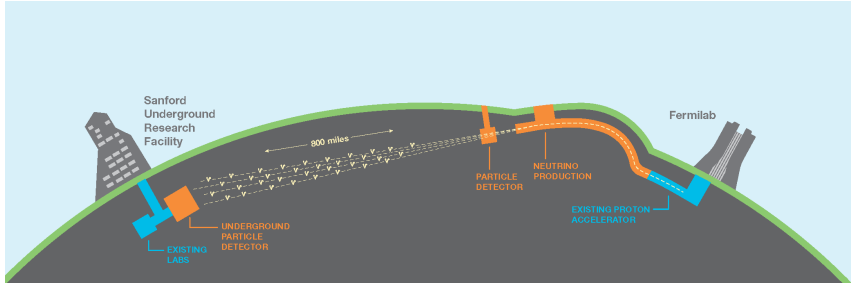


ESA, XMM-Newton, Gastaldello, CFHTL



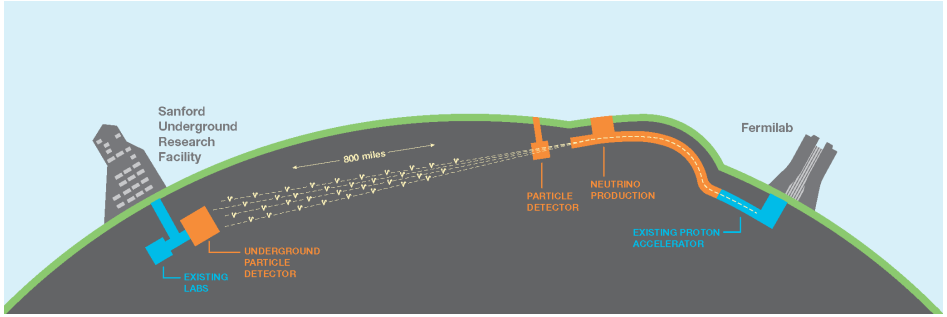


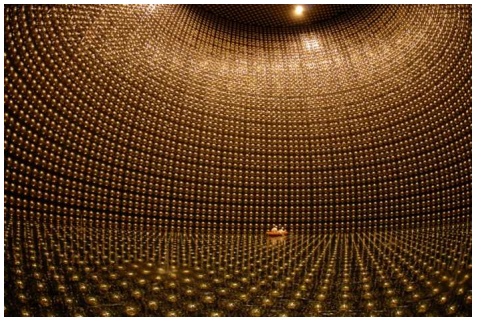
Majorana Demonstrator



LBNF

Nuclei for Accelerator Neutrinos' Experiments

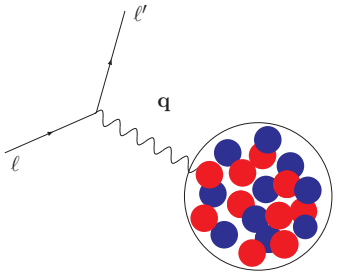




LBNF

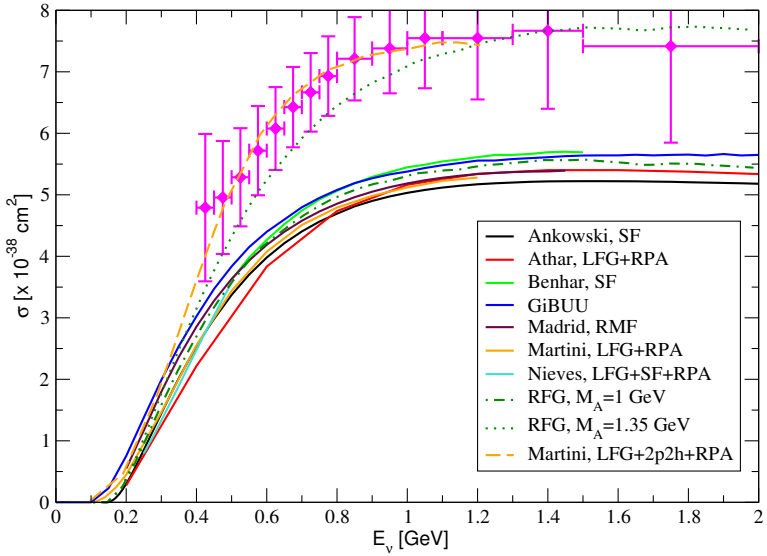
T2K

Neutrino-Nucleus scattering



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

CCQE on ^{12}C

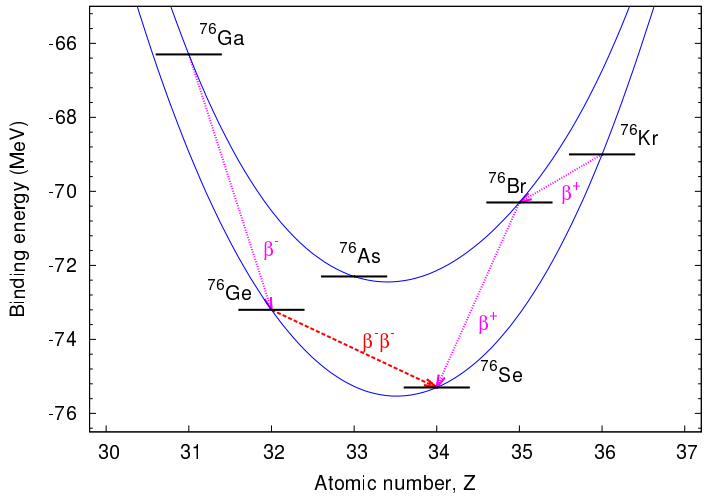


Alvarez-Ruso arXiv:1012.3871

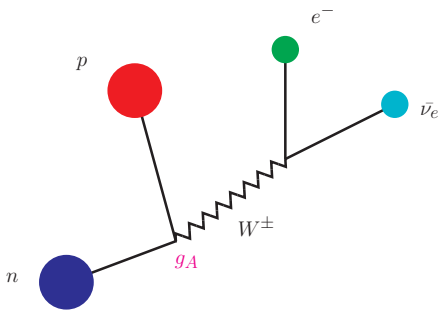
* Nuclei of ^{12}C, ^{40}Ar, ^{16}O, ^{56}Fe, ... *

are the DUNE, MiniBoone, T2K, Minerνa ... detectors' active material

Standard Single and Double Beta Decays

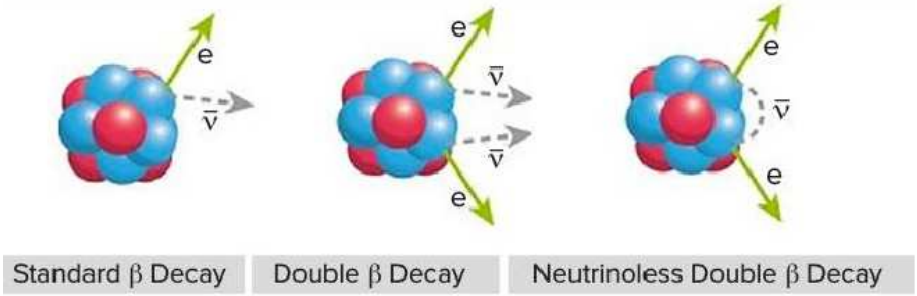


J. Menéndez - arXiv:1703.08921v1



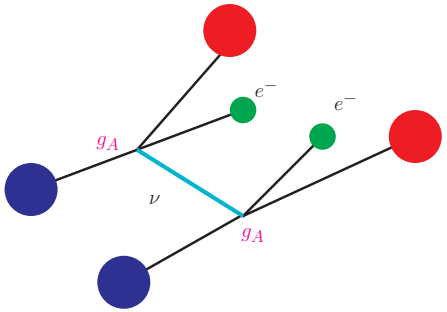
Maria Geoppert-Mayer

$$\text{single beta decay: } (Z,N) \to (Z+1, N-1) + e + \bar{\nu}_e$$
$$\text{double beta decay: } (Z,N) \to (Z+2, N-2) + 2e + 2\bar{\nu}_e$$
$$\text{lepton \# } L = l - \bar{l} \text{ is conserved}$$



Neutrinoless Double Beta Decay

H. Murayama

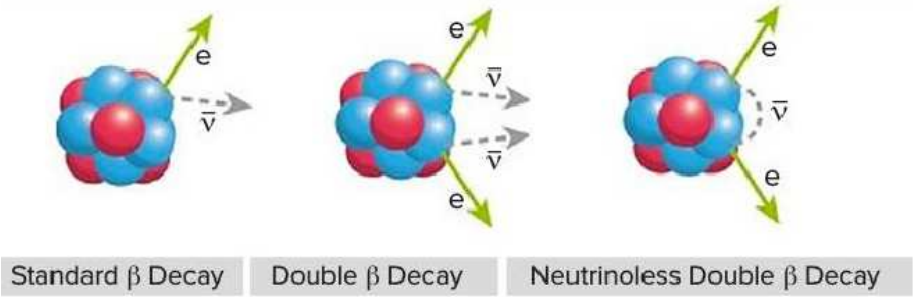


Ettore Majorana

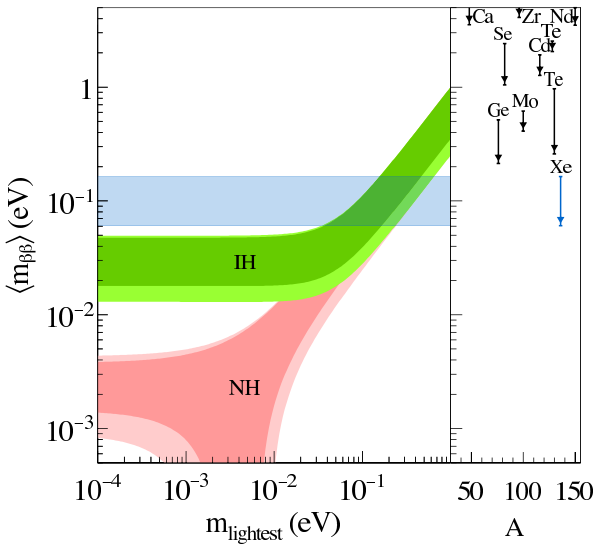
$0\nu\beta\beta$ neutrinoless double beta decay

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

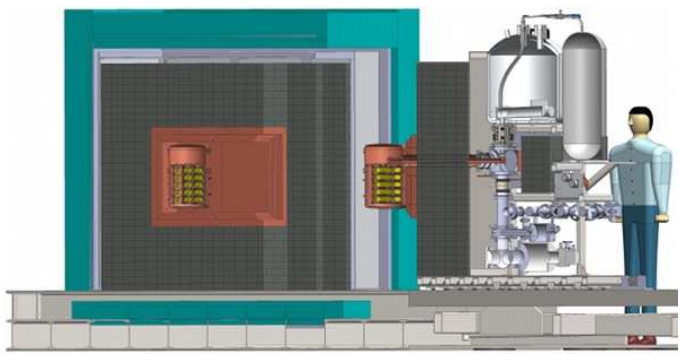
lepton # $L = l - \bar{l}$ is not conserved



Nuclear Physics for Neutrinoless Double Beta Decay Searches

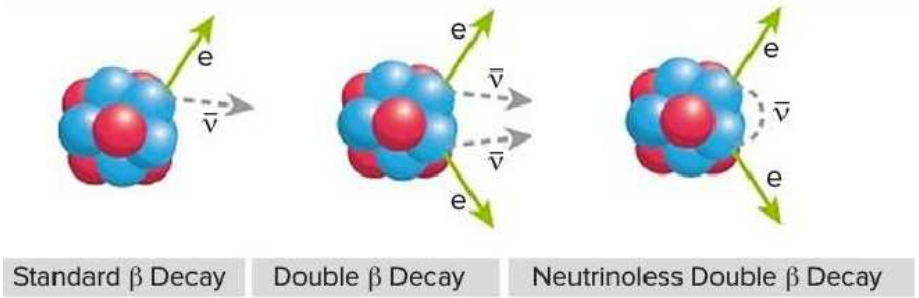


J. Engel and J. Menéndez - arXiv:1610.06548

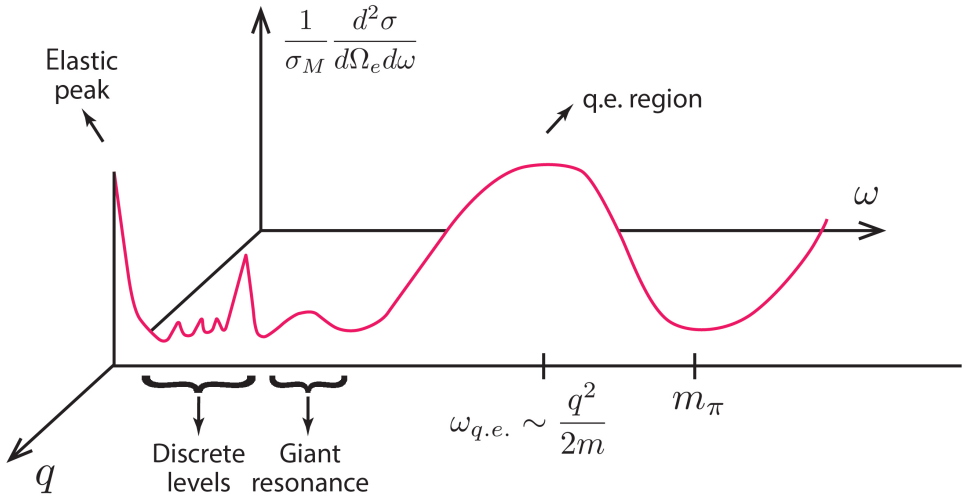


Majorana Demonstrator

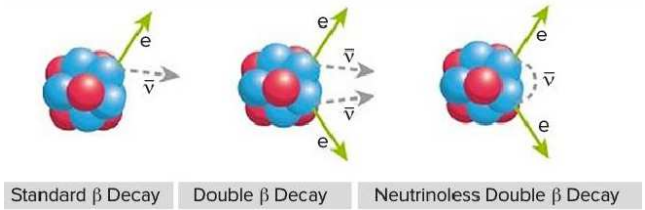
$0\nu\beta\beta$-decay $\tau_{1/2} \gtrsim 10^{25}$ years (age of the universe 1.4×10^{10} years)
need 1 ton of material to see (if any) ~ 5 decays per year
* Decay Rate $\propto$ (nuclear matrix elements)$^2 \times \langle m_{\beta\beta} \rangle^2$ *



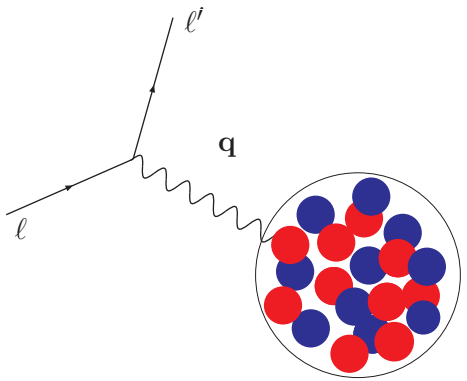
Towards a coherent and unified picture of lepton-nucleus interactions



* $\omega \sim$ few MeV, $q \sim 0$: EM-decay, β-decay, $\beta\beta$-decay
* $\omega \sim$ few MeV, $q \sim 10^2$ MeV: μ-capture, Neutrinoless $\beta\beta$-decay
* $\omega \lesssim$ tens MeV: Nuclear Rates for Astrophysics
* $\omega \sim 10^2$ MeV: Accelerator neutrinos, e- and ν-nucleus scattering



The Microscopic (or *ab initio*) Description of Nuclei



Develop a comprehensive theory that describes quantitatively and predictably all nuclear structure and reactions

* Accurate understanding of interactions between nucleons, p's and n's
* and between electrons and neutrinos with nucleons, nucleons-pairs, ...
* Electroweak Nucleonic Form Factors are inputs of the *ab initio* framework

$$H\Psi = E\Psi$$

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

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

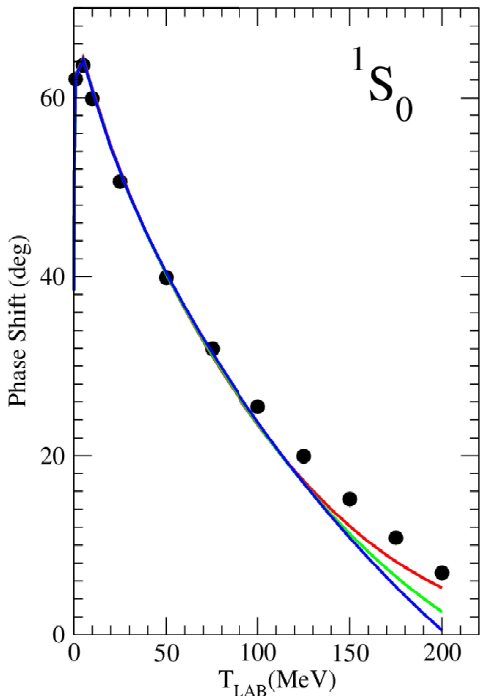
Erwin Schrödinger

Nuclear Many-Body Interactions

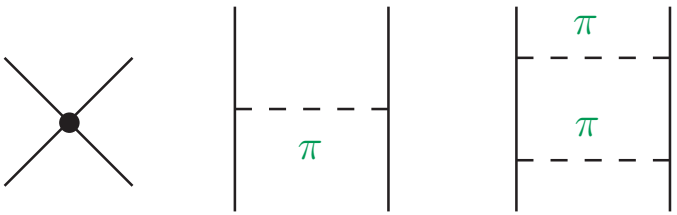
The nucleus is made of A non-relativistic interacting nucleons and its energy is

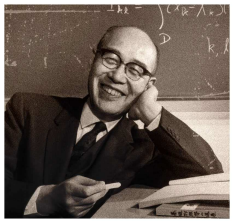
$$H = T + V = \sum_{i=1}^{A} t_i + \sum_{i<j} \upsilon_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

where υ_{ij} and V_{ijk} are two- and three-nucleon operators based on EXPT data fitting with fitted parameters subsuming underlying QCD



SP *et al.* PRC80(2009)034004





Hideki Yukawa

* Contact terms: short-range
* One-pion-exchange: range$\sim \frac{1}{m_\pi}$
* Two-pion-exchange: range$\sim \frac{1}{2m_\pi}$

Quantum Monte Carlo Methods

Minimize expectation value of H = T + υ_{ij} + V_{ijk}

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

using trial function

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

Ψ_V is further improved it by "filtering" out the remaining excited state contamination

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

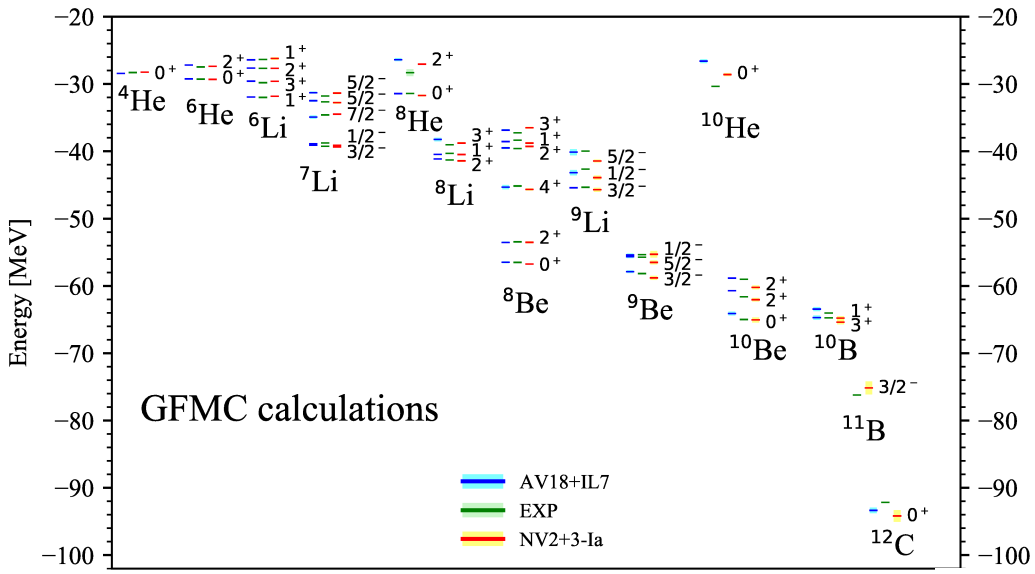
$$\Psi(\tau \to \infty) = a_0 \psi_0$$

Many-body interactions currently implemented in QMC codes:

* AV18+UIX / AV18+IL7; Wiringa+Schiavilla+Pieper *et al.*
* NN(N2LO)+3N(N2LO) (π&N); Gerzelis+Tews+Epelbaum+Gandolfi+Lynn *et al.*
* NN(N3LO)+3N(N2LO) (π&N&Δ); Piarulli *et al.*; NV2+3 Norfolk potentials

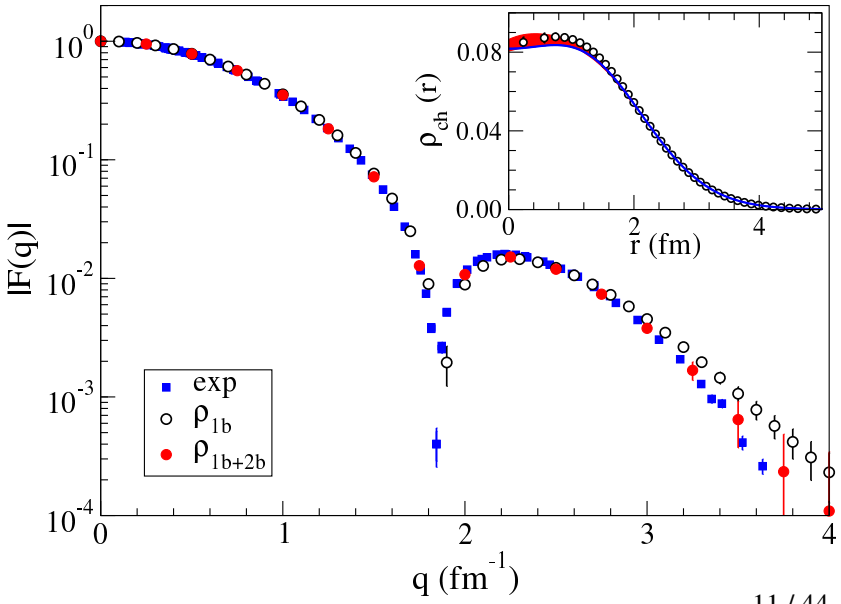
Carlson *et al.* Rev. Mod. Phys. 87(2014)1067 - Most recent review article

Energy Spectrum and Shape of Nuclei



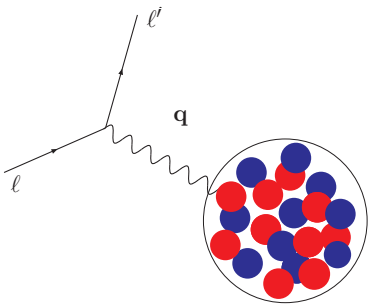
Piarulli *et al.* - PRL120(2018)052503

Lovato *et al.* PRL111(2013)092501

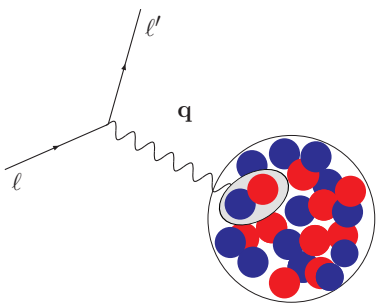


Nuclear Many-Body Currents

1b



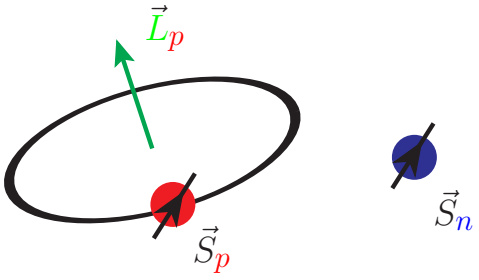
2b



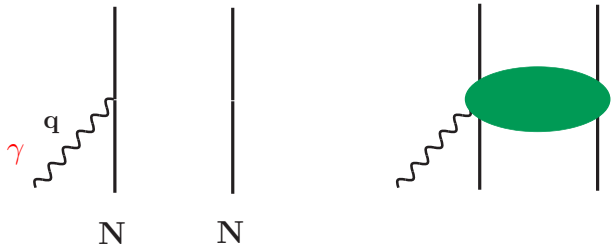
$$\rho = \sum_{i=1}^{A} \rho_i + \sum_{i<j} \rho_{ij} + \dots ,$$

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

* Nuclear currents given by the sum of p's and n's currents, one-body currents (1b)



* Two-body currents (2b) essential to satisfy current conservation
* We use Meson-Exchange Currents (MEC) or χEFT Currents

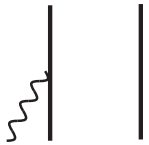


$+ \dots$

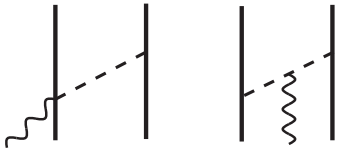
$$\mathbf{q} \cdot \mathbf{j} = [H, \rho] = [t_i + v_{ij} + V_{ijk}, \rho]$$

Electromagnetic Currents from Chiral Effective Field Theory

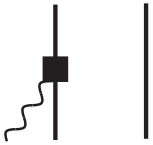
LO : $\mathbf{j}^{(-2)} \sim \mathbf{eQ^{-2}}$



NLO : $\mathbf{j}^{(-1)} \sim \mathbf{eQ^{-1}}$



N^{2}LO : $\mathbf{j}^{(-0)} \sim \mathbf{eQ^{0}}$



* 3 unknown Low Energy Constants:
fixed so as to reproduce d, ^3H, and ^{3}He magnetic moments

** also obtainable from LQCD calculations **

N^{3}LO: $\mathbf{j}^{(1)} \sim \mathbf{eQ}$

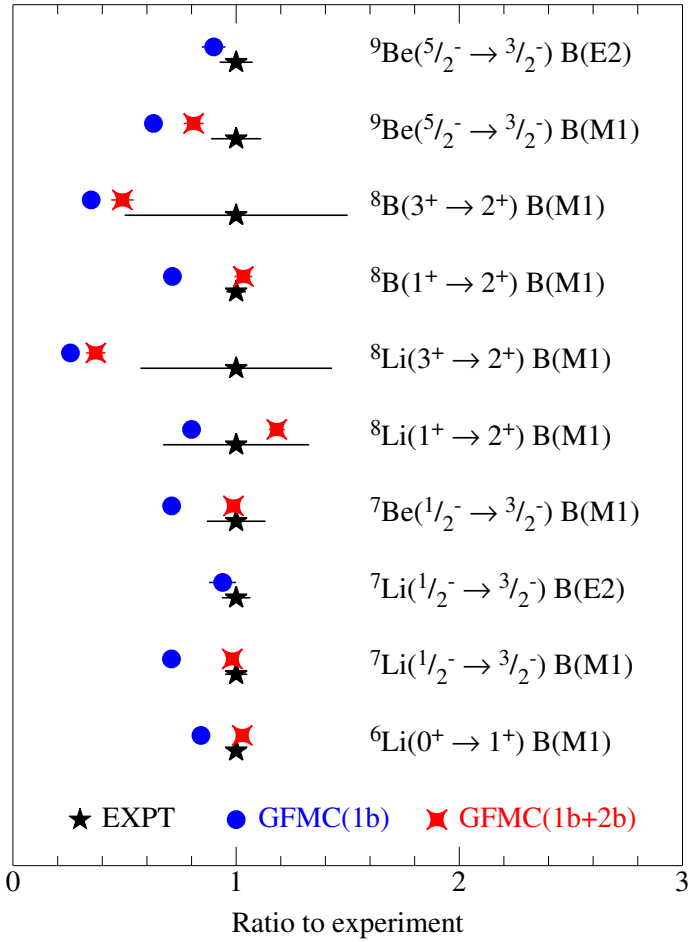
unknown LEC′s →

SP *et al.* PRC78(2008)064002 & PRC80(2009)034004 & PRC84(2011)024001 & PRCC87(2013)014006

other derivations by Park+Min+Rho NPA596(1996)515 in Covariant PT
and by Kölling+Epelbaum+Krebs+Meissner PRC80(2009)045502 & PRC84(2011)054008 with UT
Phillips development of the EM charge operator (2005)

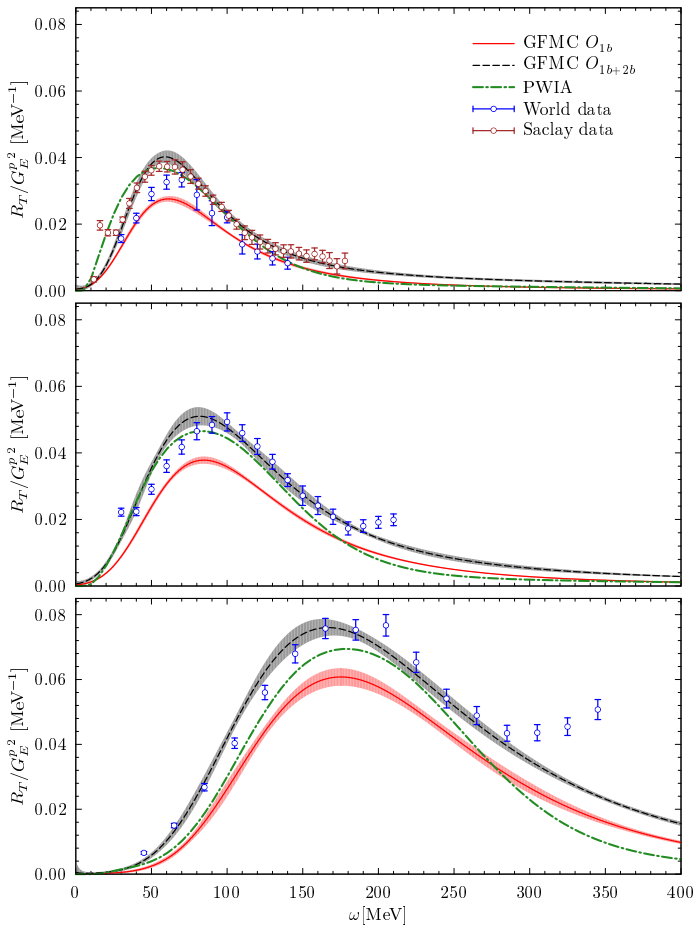
Electromagnetic Decays and *e*-scattering off nuclei

Electromagnetic Decay



SP *et al.* PRC87(2013)035503 & PRC90(2014)024321

Electromagnetic Transverse Responses

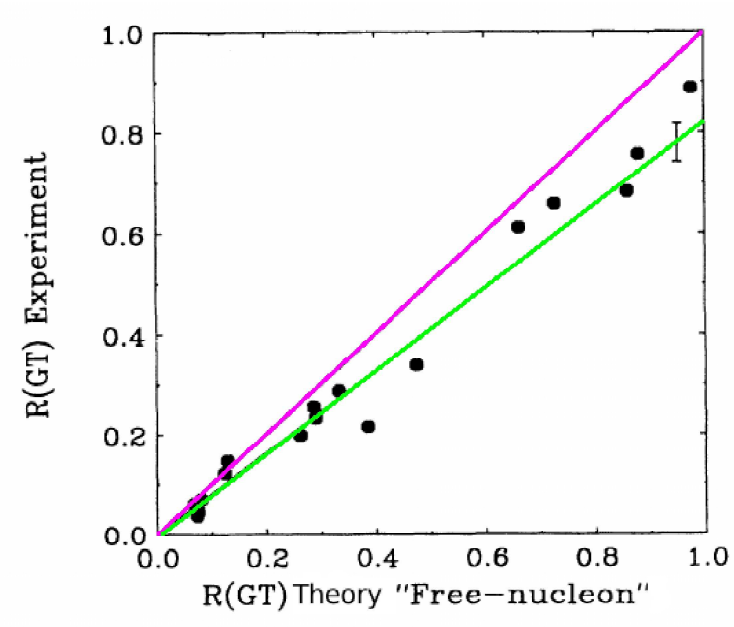


$q = [300 - 570]$ MeV

Lovato & Gandolfi *et al.* PRC91(2015)062501 & arXiv:1605.00248

Electromagnetic data are explained when
two-body correlations and currents are accounted for!

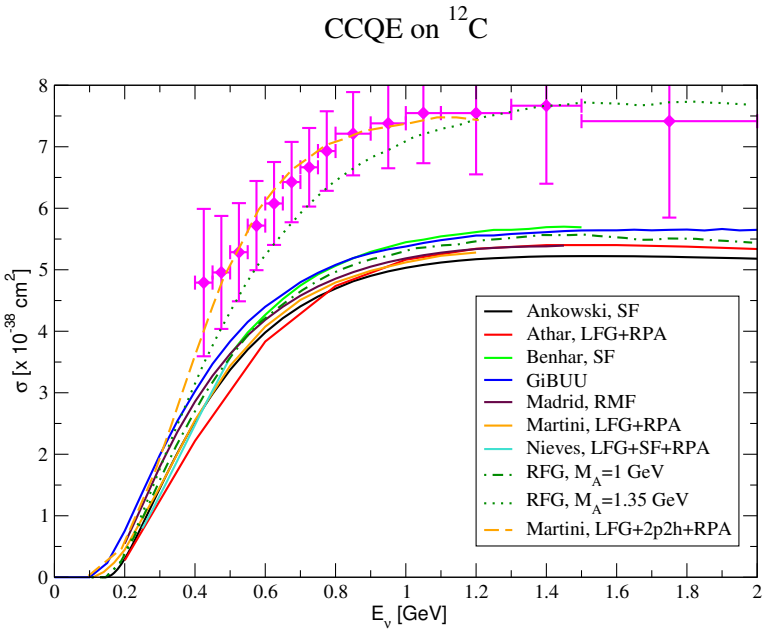
Beta Decay Rate



in $3 \leq A \leq 18 \longrightarrow g_A^{\text{eff}} \simeq 0.80\, g_A$

Chou *et al.* PRC47(1993)163

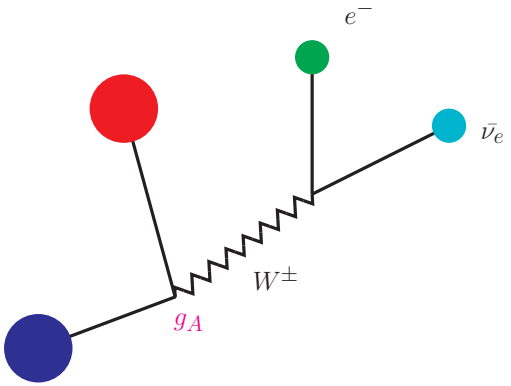
Neutrino-Nucleus Scattering



Alvarez-Ruso arXiv:1012.3871

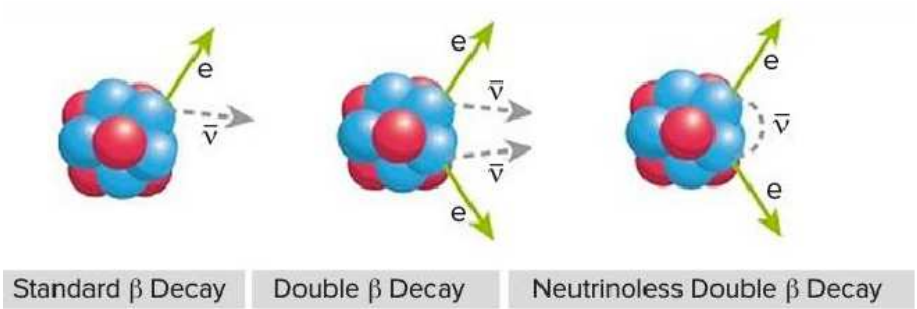
Standard Beta Decay

The "g_A problem"
and
the role of two-body correlations and two-body currents

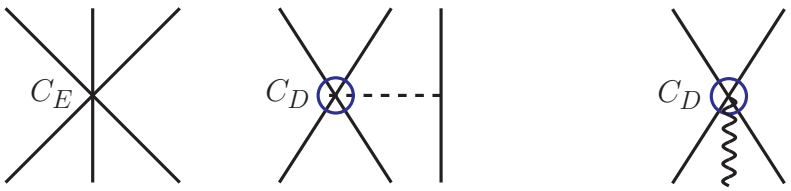


* Matrix Element $\langle \Psi_f | \mathrm{GT} | \Psi_i \rangle \propto g_A$ and Decay Rates $\propto g_A^2$ *

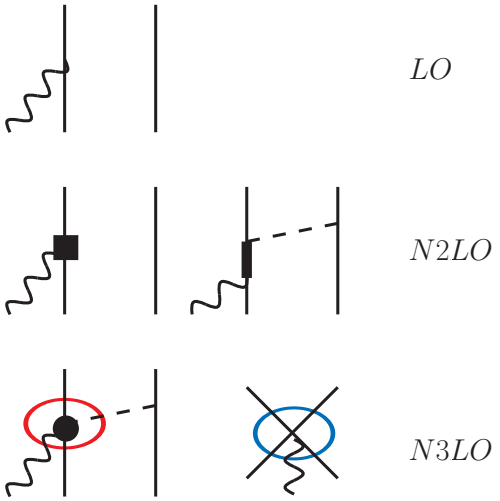
$$(Z, N) \rightarrow (Z+1, N-1) + e + \bar{\nu}_e$$



Nuclear Interactions and Axial Currents



we use
Norfolk chiral 2– and 3–body interactions by Piarulli *et al.* and
consistent axial currents up to N3LO (tree-level) by A. Baroni *et al.*



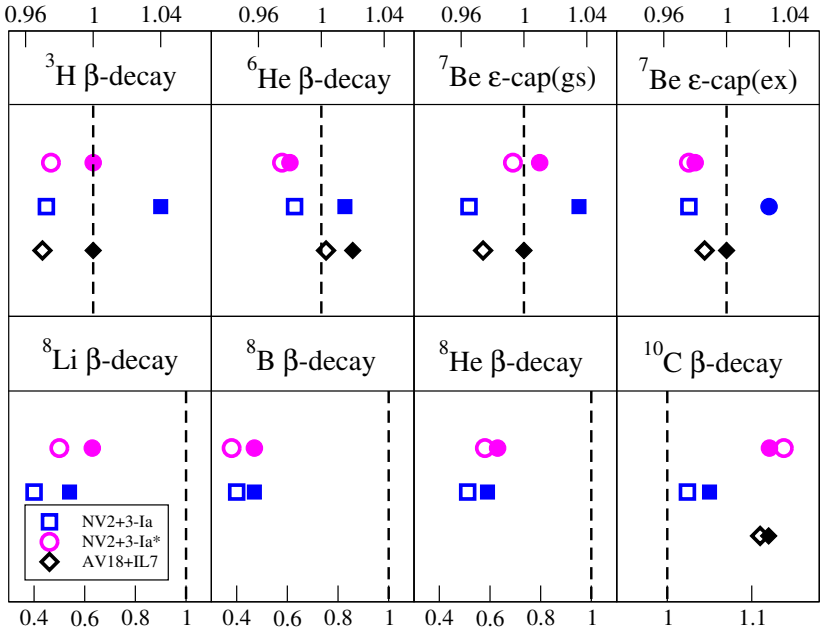
* c_3 and c_4 are taken them from Krebs *et al.* Eur.Phys.J.(2007)A32
* (c_D,c_E) fitted to:

  1. trinucleon B.E. and *nd* doublet scattering length **NV2+3 models**

     or

  2. trinucleon B.E. and GT m.e. of tritium **NV2+3* models**

Single Beta Decay Matrix Elements in $A = 6$–10



NV2+3-Ia and NV2+3-Ia*; AV18+IL7 from SP *et al.* PRC97(2018)022501

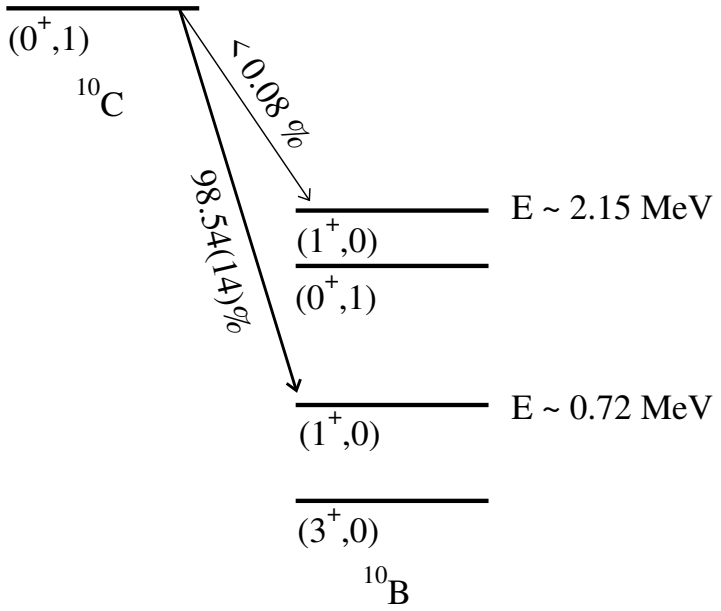
1b (empty symbols) and 2b (full symbols) GFMC predictions

King *et al.* arXiv:2004.05263

* similar results were obtained with MEC currents

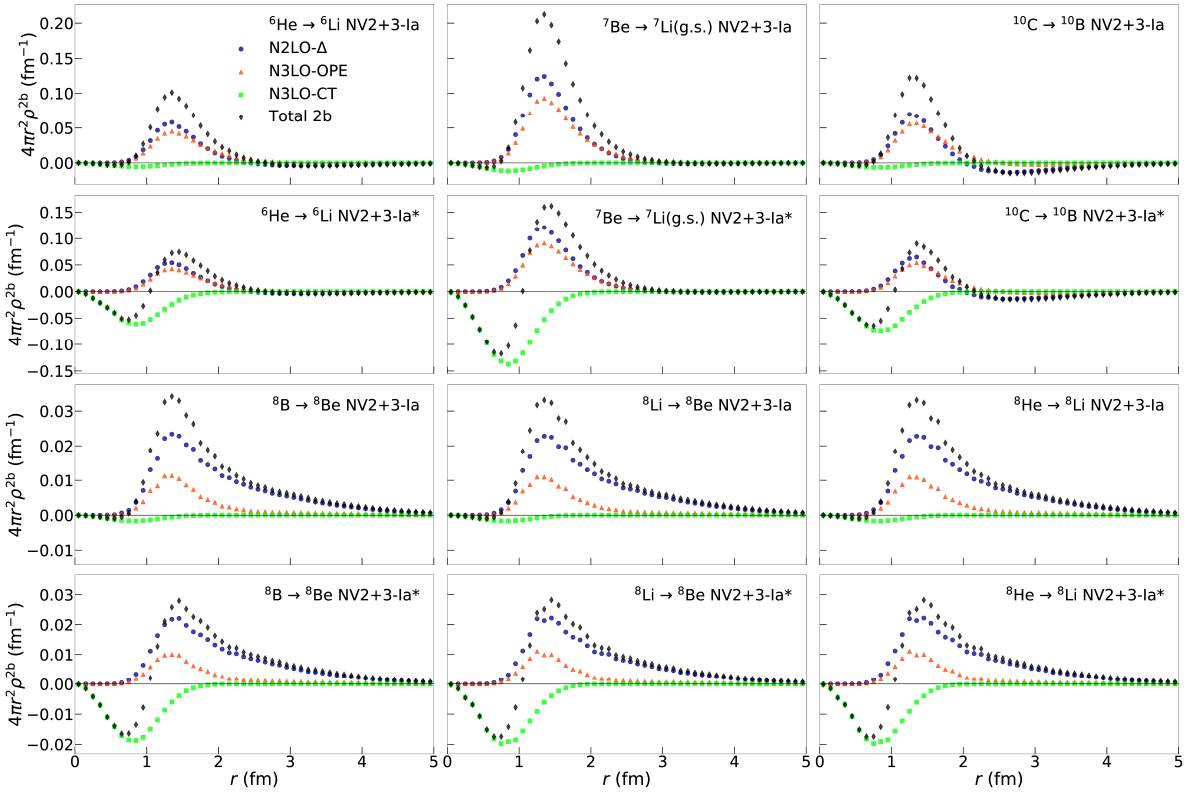
∗ data from TUNL, Suzuki *et al.* PRC67(2003)044302, Chou *et al.* PRC47(1993)163

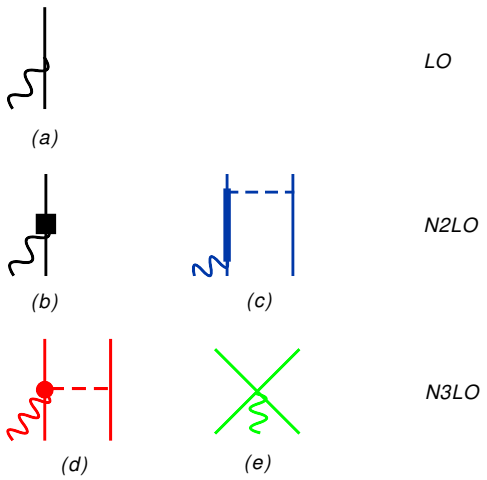
^{10}B



* In ^{10}B, ΔE with same quantum numbers ~ 1.5 MeV
* In $A = 7$, ΔE with same quantum numbers $\gtrsim 10$ MeV

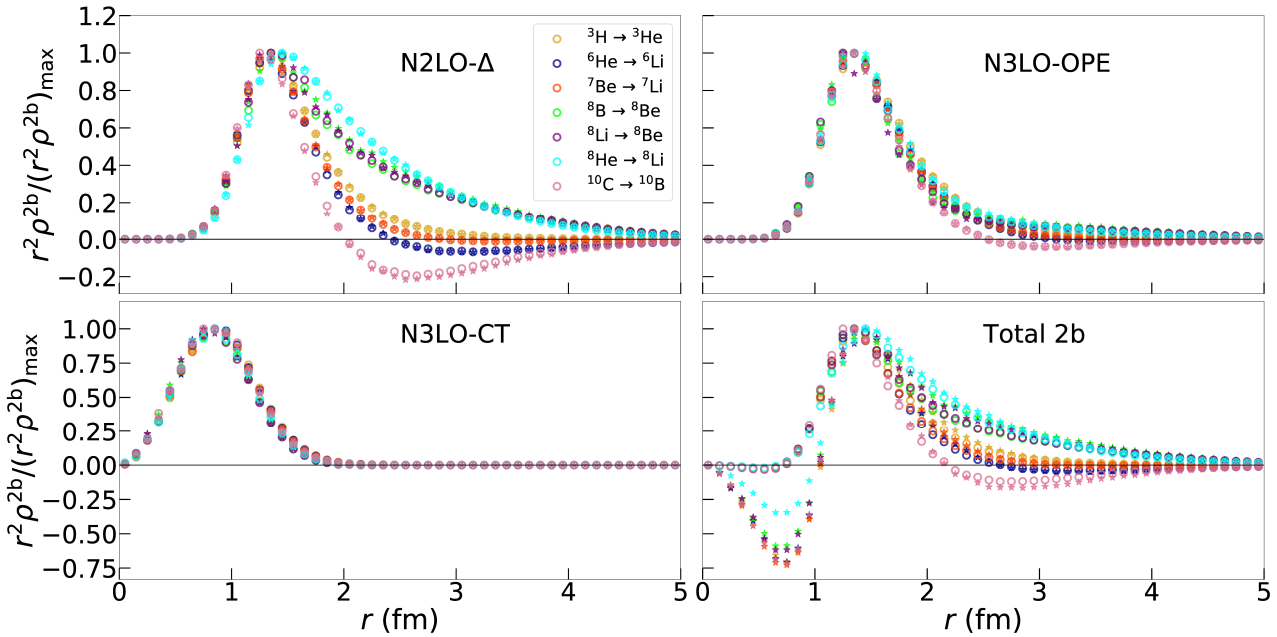
Two-body transition densities: $A = 3 - 10$





King *et al.* arXiv:2004.05263

Two-body transition densities: Scaling

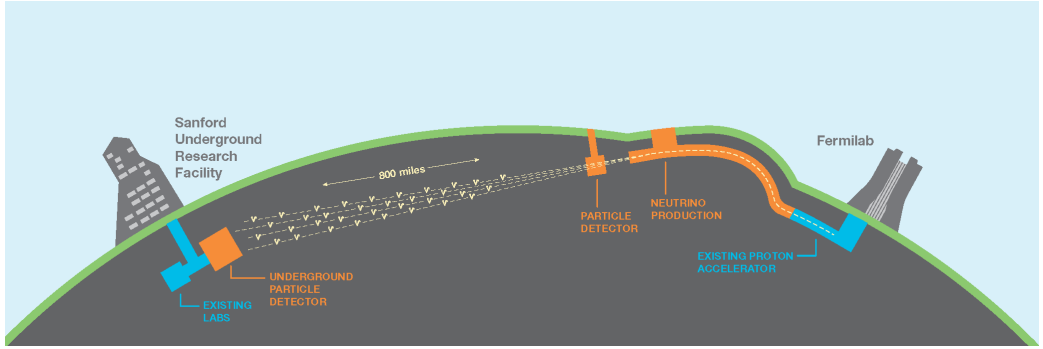


NV2+3-Ia empty circles – NV2+3-Ia* stars

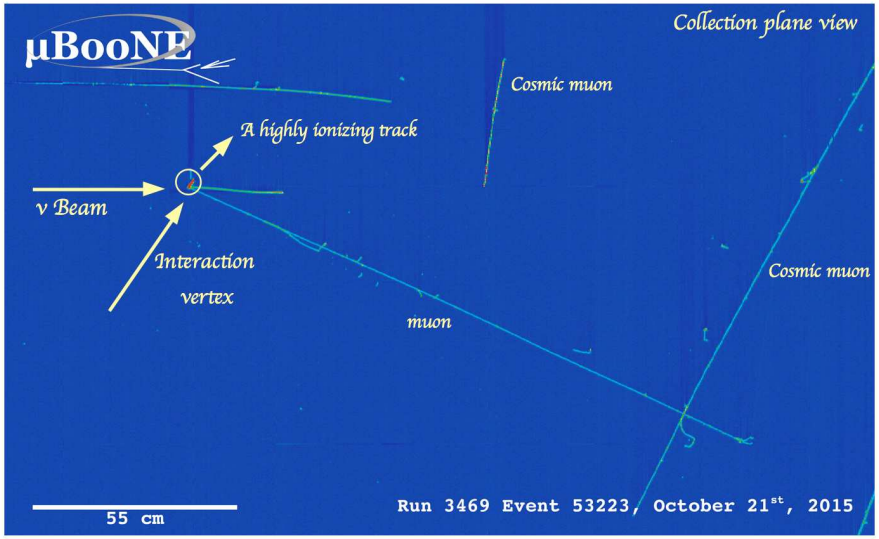
different colors refer to different transitions

King *et al.* arXiv:2004.05263

Towards a microscopic description of the ν-nucleus cross section



LBNF



μBoone

Inclusive (e,ν) scattering

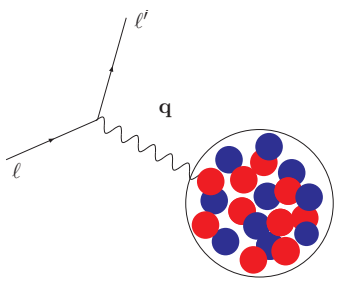
* inclusive xsecs *

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

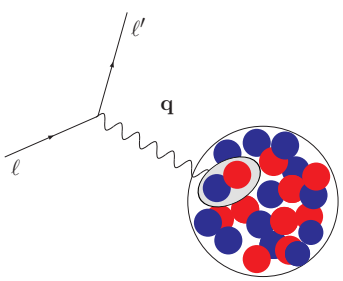
$$R_\alpha(q,\omega) = \sum_f \delta\left(\omega + E_0 - E_f\right) |\langle f | O_\alpha(\mathbf{q}) | 0 \rangle|^2$$

Longitudinal response induced by $O_L = \rho$
Transverse response induced by $O_T = \mathbf{j}$
... 5 nuclear responses in ν-scattering...

1b

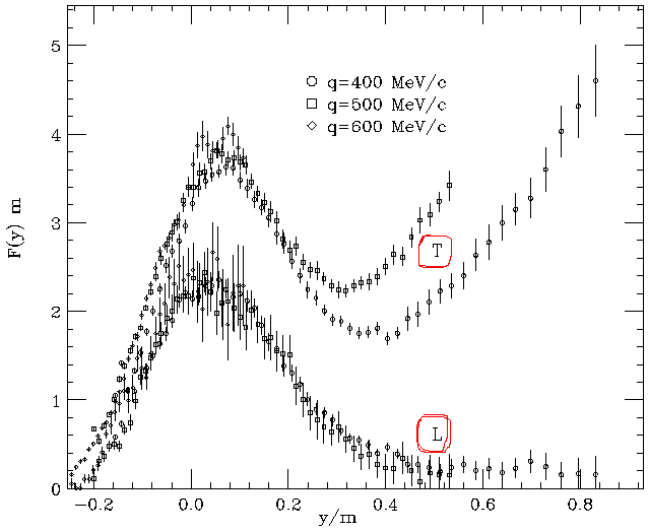


2b

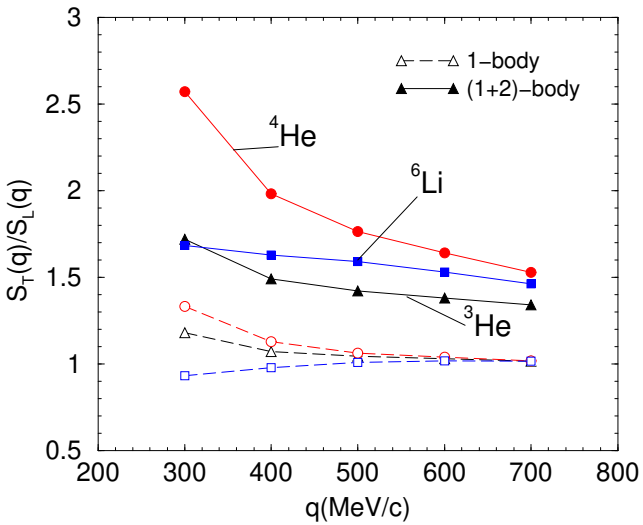


Lessons learned from exact calculations and electromagnetic data

Longitudinal and transverse responses of ^{12}C

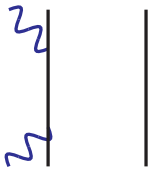


Benhar, Day, Sick Rev.Mod.Phys.80(2008)198

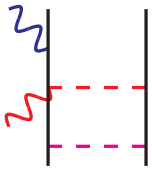


Carlson et al. PRC65(2002)024002

Fermi Gas prediction F_L=F_T



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



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

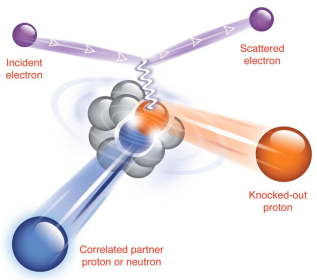
$$S_T(q) \quad \propto \quad \langle 0|\mathbf{j}^{\dagger}\,\mathbf{j}|0\rangle \propto \langle 0|\mathbf{j}_{1b}{}^{\dagger}\,\mathbf{j}_{1b}|0\rangle + \langle 0|\mathbf{j}_{1b}{}^{\dagger}\,\mathbf{j}_{2b}|0\rangle + \ldots$$

- $\mathbf{j} = \mathbf{j}_{1b} + \mathbf{j}_{2b}$

The enhancement of the transverse response is due to interference between 1b and 2b currents AND presence of two-nucleon correlations

• 2-body physics essential to explain data •

QMC Calculations of Lepton-Nucleus Scattering: Challenges and Opportunities



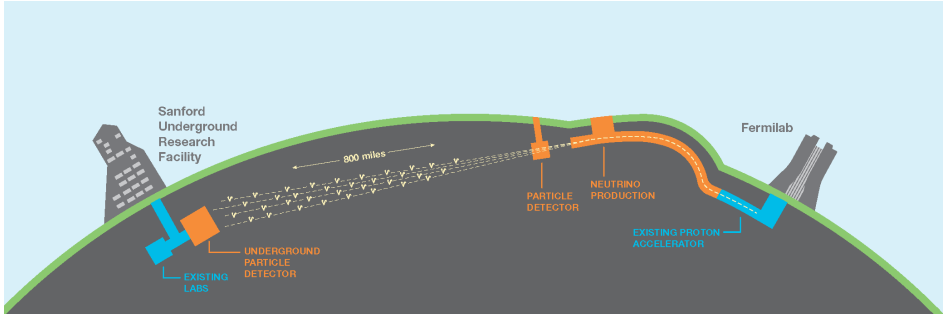
***

1. How to describe electroweak-scattering off $A > 12$ without losing two-body physics (*i.e.*, two-body correlations and currents)?

2. How to incorporate (more) exclusive processes?

3. How to incorporate relativistic effects?

***



Factorization

$$R(q,\omega) = \sum_f \delta\left(\omega + E_0 - E_f\right) \langle\, 0|O^\dagger(\mathbf{q})|f\rangle\langle f|O(\mathbf{q})|0\rangle$$

$$R(q,\omega) = \int dt \langle\, 0|O^\dagger(\mathbf{q})\, e^{i(H-\omega)t}\, O(\mathbf{q})|0\rangle$$

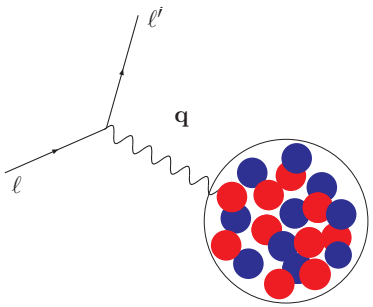
At short time, expand $P(t) = e^{i(H-\omega)t}$ and keep up to 2b-terms

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

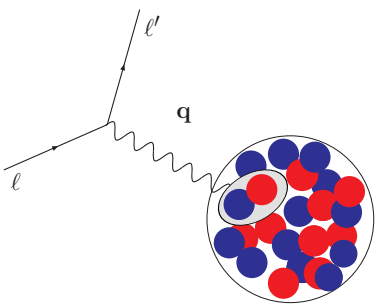
and

$$O_i^\dagger P(t) O_i + O_i^\dagger P(t) O_j + O_i^\dagger P(t) O_{ij} + O_{ij}^\dagger P(t) O_{ij}$$

1b

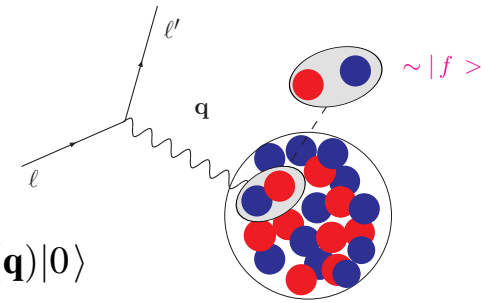


2b



The Short-Time Approximation (STA)

Response functions are given by the scattering
off pairs of fully interacting nucleons that propagate into a correlated
pair of nucleons



$$R(q,\omega) \quad = \quad \sum_f \delta\left(\omega + E_0 - E_f\right) \langle\, 0|O^\dagger(\mathbf{q})|f\rangle\langle f|O(\mathbf{q})|0\rangle$$

$$O(\mathbf{q}) \quad = \quad O^{(1)}(\mathbf{q}) + O^{(2)}(\mathbf{q}) = \text{1b} + \text{2b}$$

$$|f\rangle \quad \sim \quad |\psi_{p',P',J,M,L,S,T,M_T}(r,R)\rangle = \text{correlated two} - \text{nucleon w.f.}$$

* We retain two-body physics consistently in the nuclear interactions and electroweak currents
* $R_\alpha(q,\omega)$ requires only direct calculation of g.s. $|0\rangle$ w.f.'s *
* STA can describe pion-production induced by e and ν

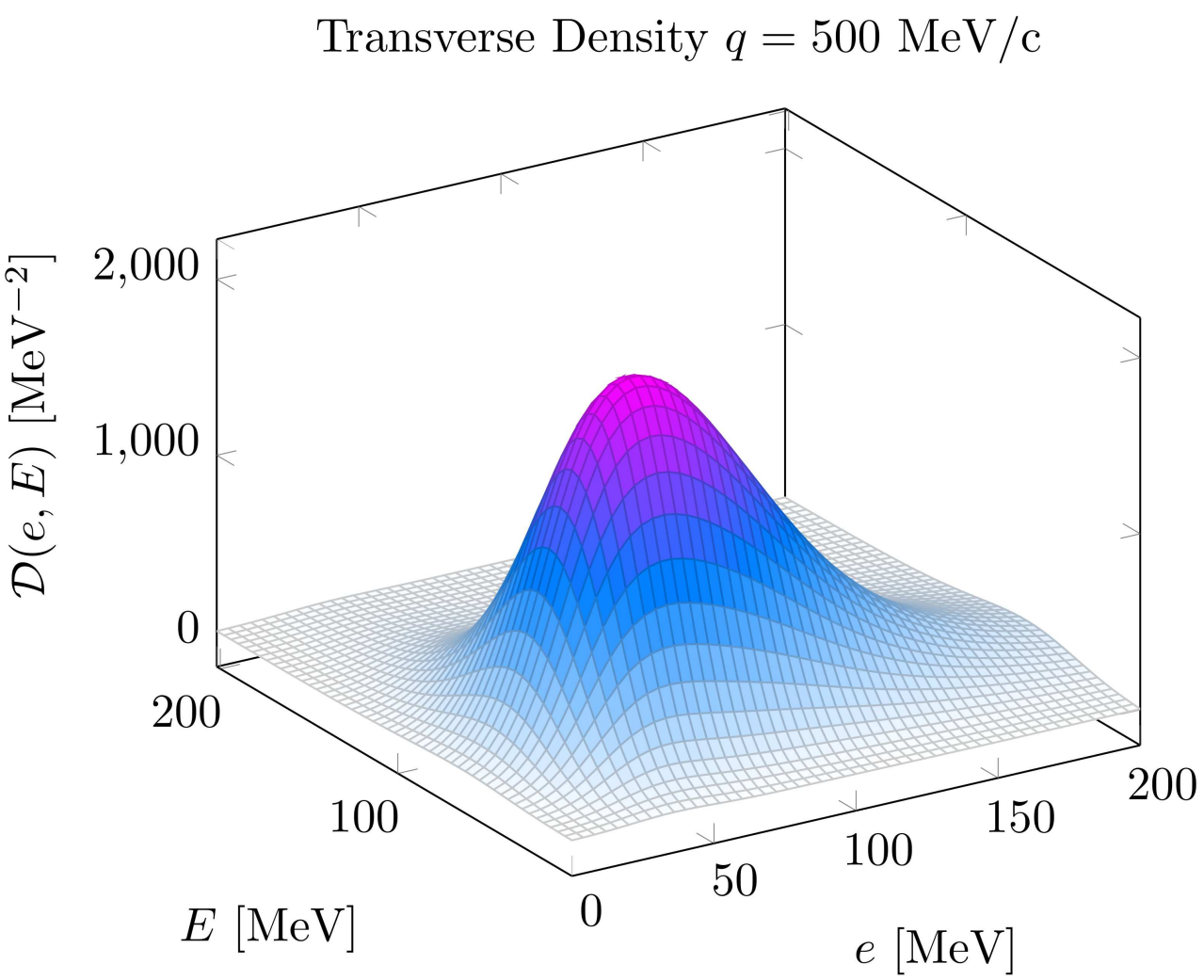
* Definition: Response Density $\mathscr{D}$ *

$$R(q,\omega) \quad \sim \quad \int \delta\left(\omega + E_0 - E_f\right) d\Omega_{P'}\, d\Omega_{p'}\, dP'\, dp' \left[p^{2\prime} P^{2\prime} \langle\, 0|O^\dagger(\mathbf{q})|\mathbf{p}',\mathbf{P}'\rangle\langle\, \mathbf{p}',\mathbf{P}'|O(\mathbf{q})|0\rangle\right]$$

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

has info on the nucleus soon after the probe interacts with the pair of nucleons;
provides more "exclusive" info in terms of nucleon-pair kinematics;
correctly accounts for interference terms

Short-Time Approximation: Response Densities

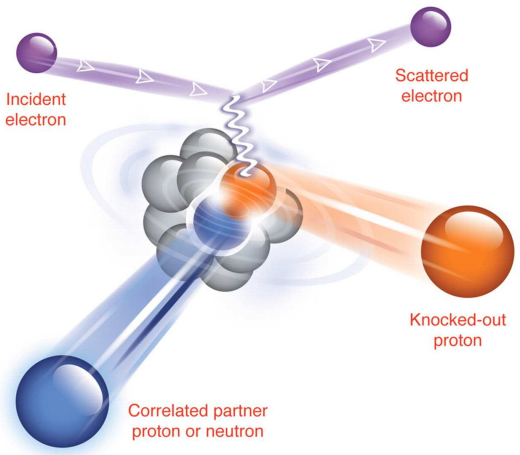


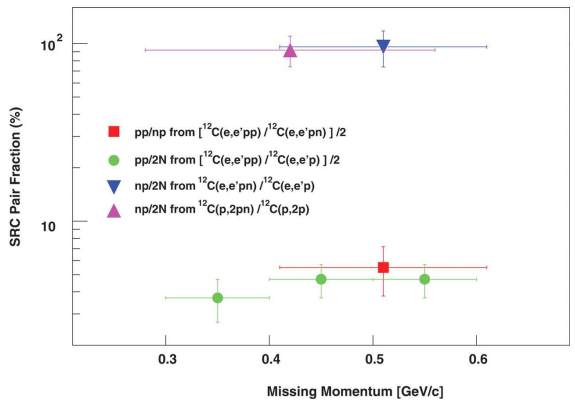
Transverse "response-density" 1b + 2b for ^4He

$\mathscr{D}(p', P'; q)$

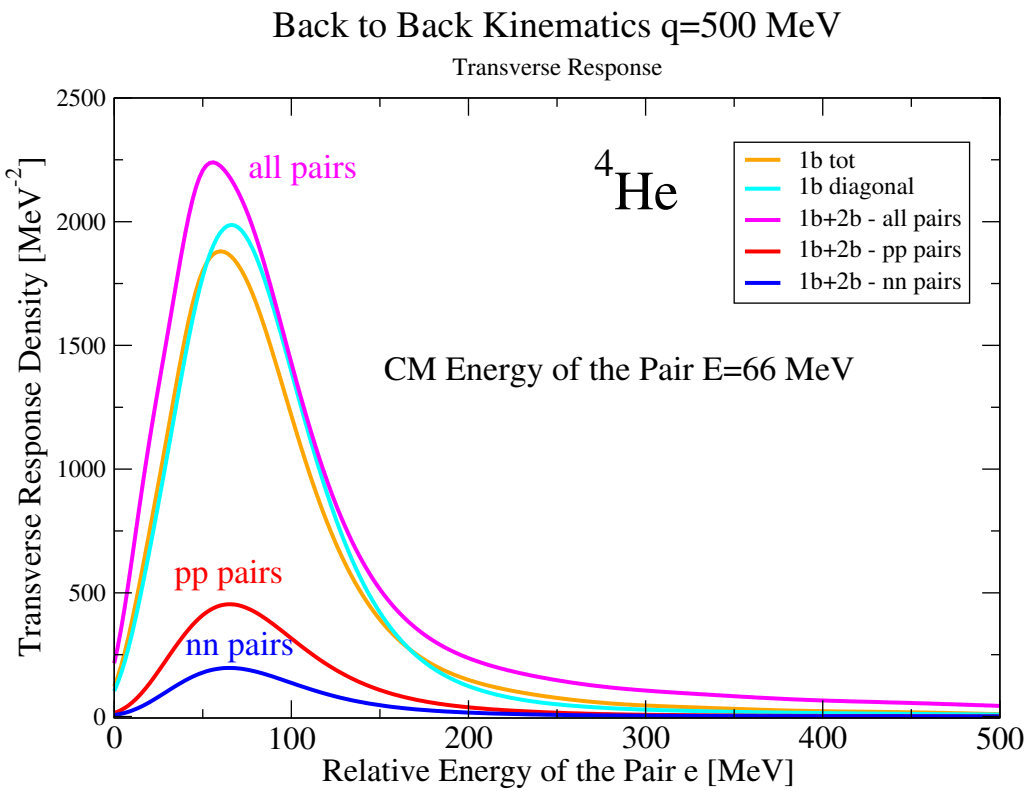
SP & Carlson *et al.* Phys.Rev.C 101 (2020) 4, 044612

Short-Time Approximation: back to back scattering



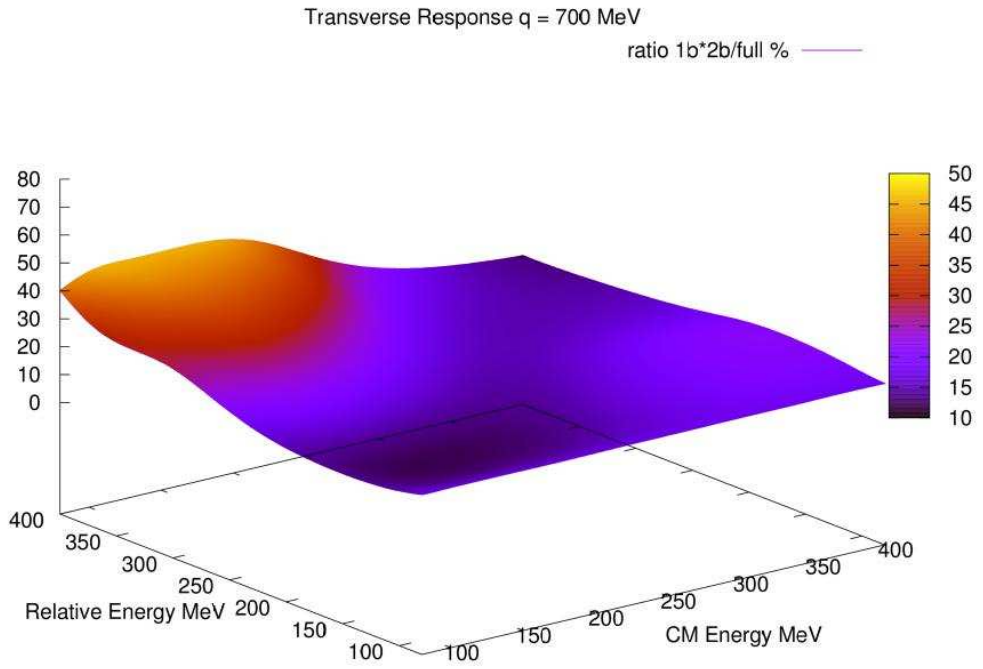


JLab. Subedi et al. Science320(2008)1475



Short-Time Approximation: Two-body Physics

^{4}He Transverse Response Density $q = 700$ MeV



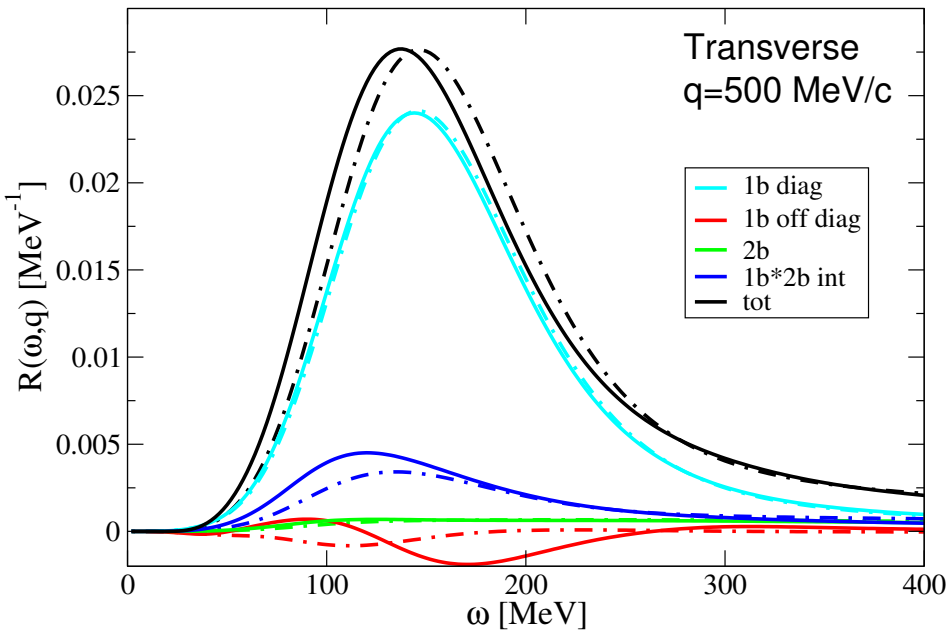
Transverse "response-density" $\mathscr{D}(p', P'; q)$

Ratio (1b$\times$2b+2b) / tot

SP & Carlson *et al.* Phys.Rev.C 101 (2020) 4, 044612

STA: The Propagator

$\dashrightarrow$ Plane Wave Propagator vs $\longrightarrow$ Correlated Propagator

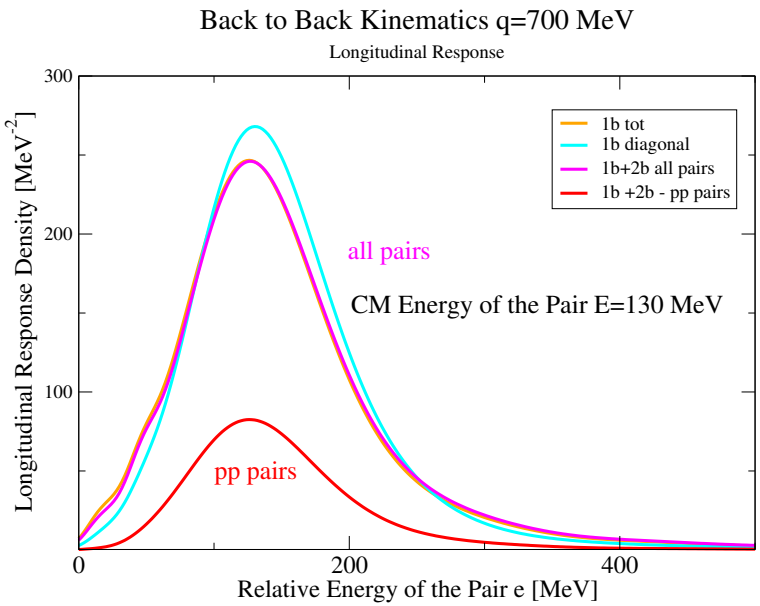


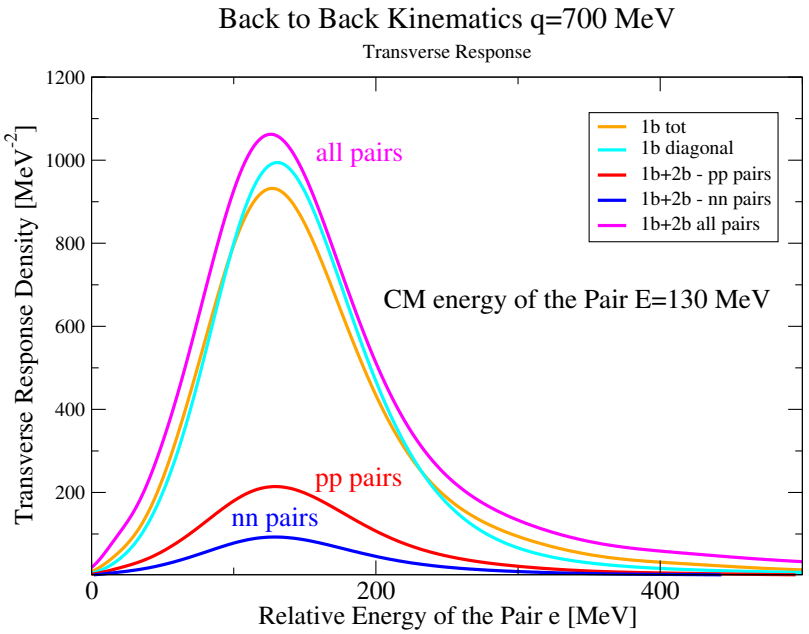
tot
one-body diagonal
one-body off-diagonal
pure two-body
interference one-body $\times$ two-body

SP & Carlson *et al.* Phys.Rev.C 101 (2020) 4, 044612

STA: Back to back scattering and particle identity

^{4}He Longitudinal and Transverse Responses, $q = 700$

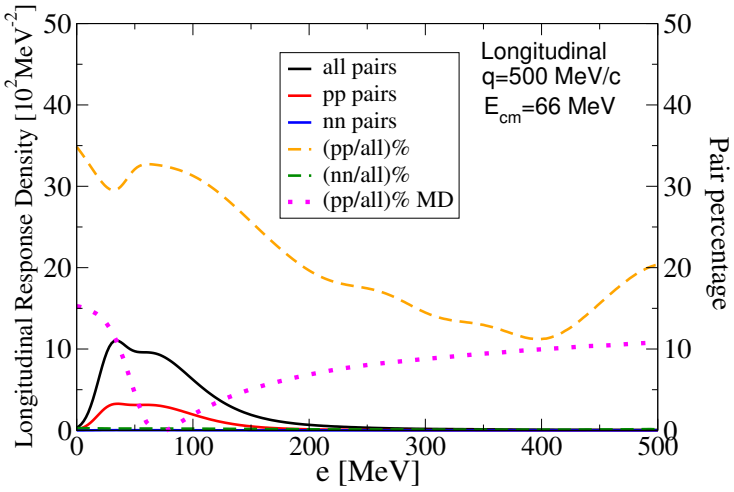


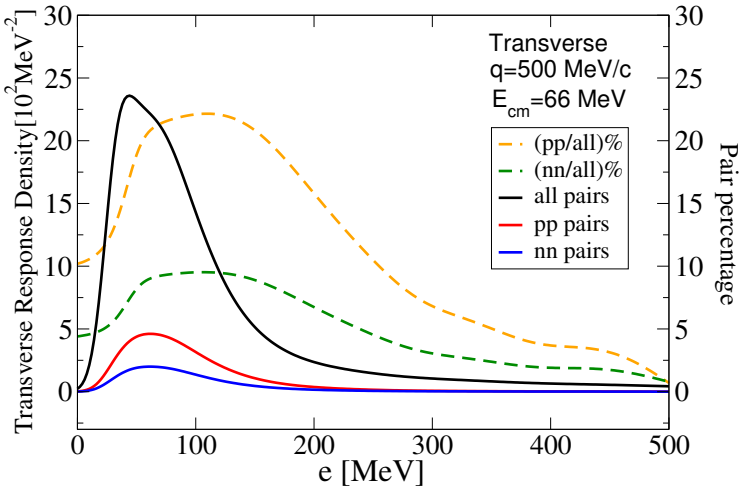


tot all pairs
tot proton-proton pairs
tot neutron-neutron pairs

STA: back to back scattering and particle identity

^{4}He Transverse Responses, $q = 500$

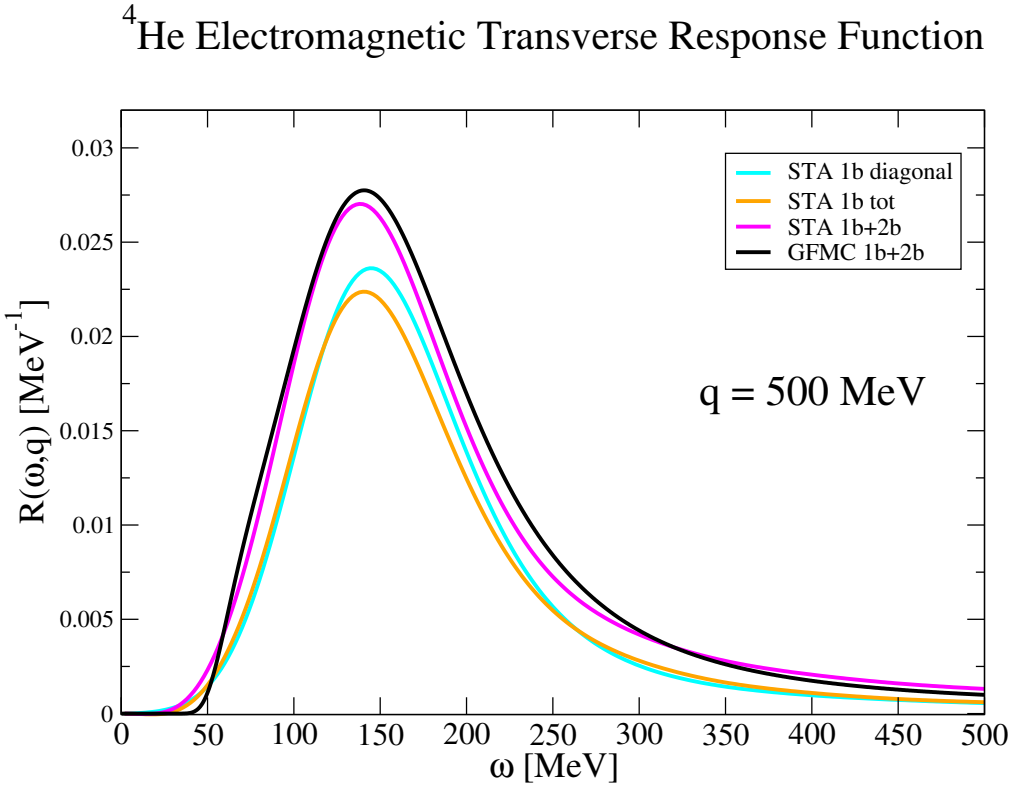




tot all pairs
tot proton-proton pairs
tot neutron-neutron pairs
(tot proton-proton pairs/tot all pairs)%
(tot neutron-neutron pairs/tot all pairs)%
(tot proton-proton pairs/tot all pairs)% from two-body momentum distributions

SP & Carlson *et al.* Phys.Rev.C 101 (2020) 4, 044612

STA: Comparison with ^{4}He GFMC exact calculations

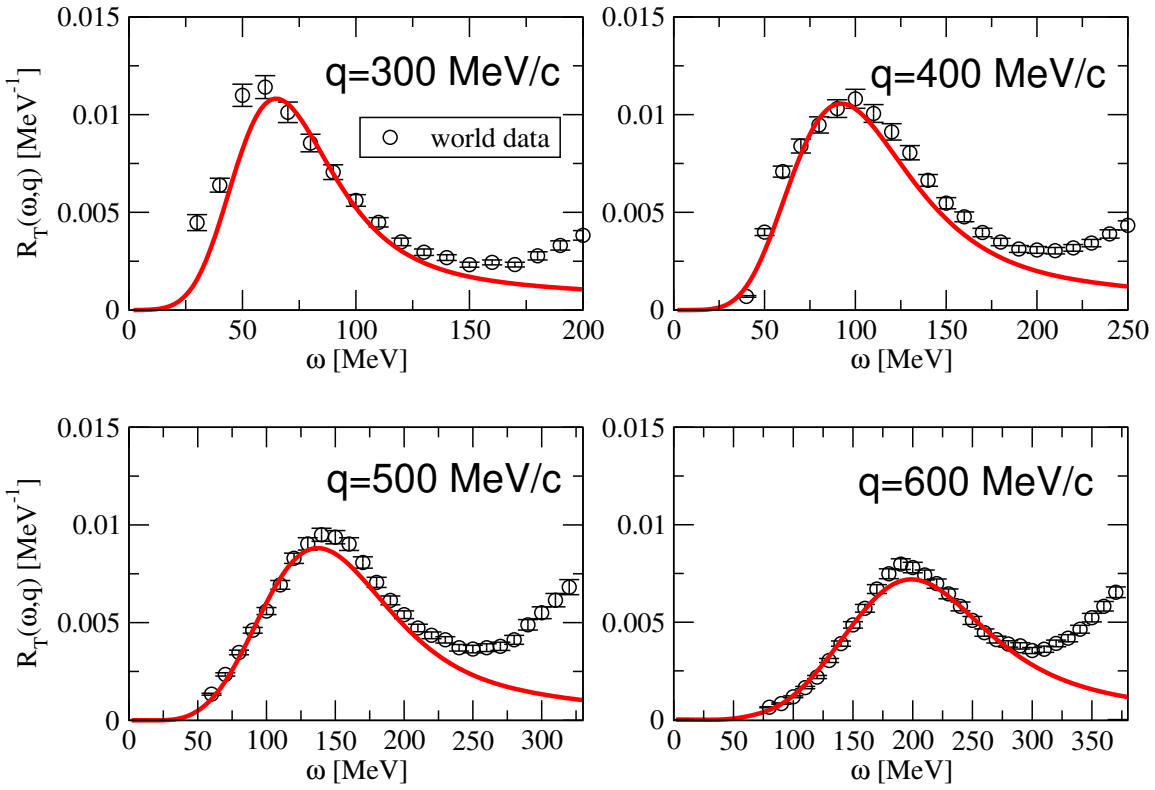


GFMC tot
STA tot
STA one-body

GFMC results for ^{4}He courtesy of A. Lovato

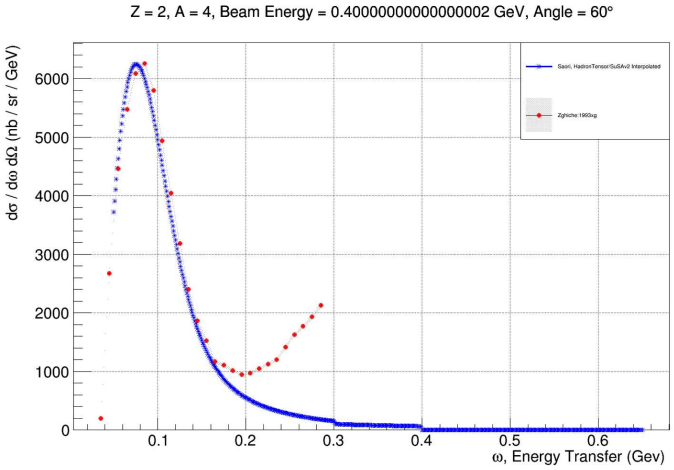
SP & Carlson *et al.* Phys.Rev.C 101 (2020) 4, 044612

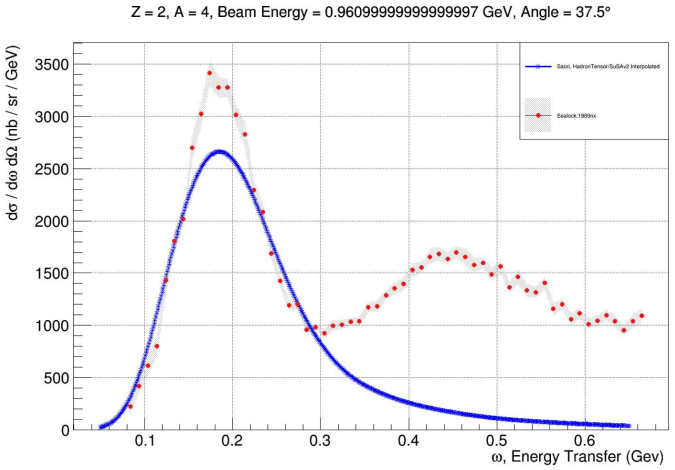
Short-Time Approximation Comparison with data: Responses



SP & Carlson *et al.* Phys.Rev.C 101 (2020) 4, 044612

STA Comparison with data: cross sections

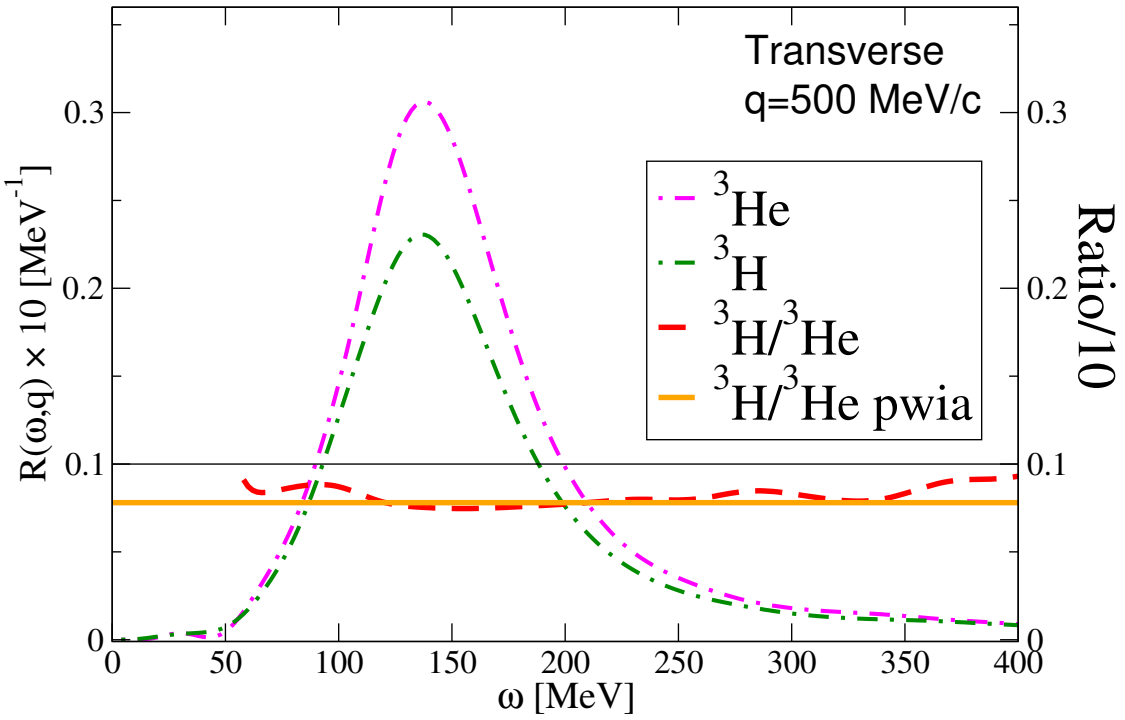




* PRELIMINARY RESULTS *

by Josh Barrow & Steven Gardiner (FNAL)

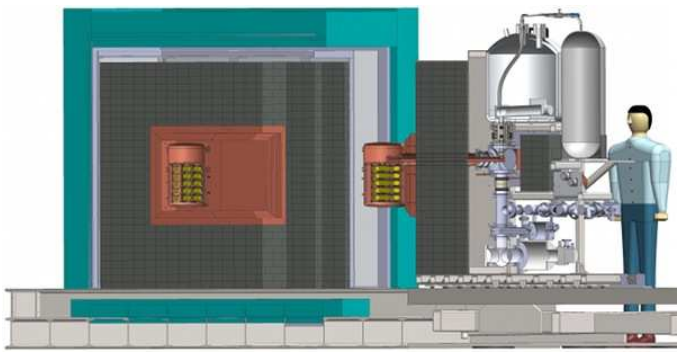
STA: Preliminary results for ^{3}H and ^{3}He

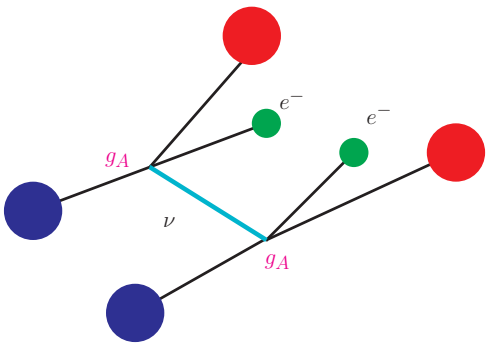


* PRELIMINARY RESULTS *

work is in progress in collaboration with N. Rocco and A. Lovato to derive $A = 3$ cross sections within the STA, SP, and GFMC frameworks

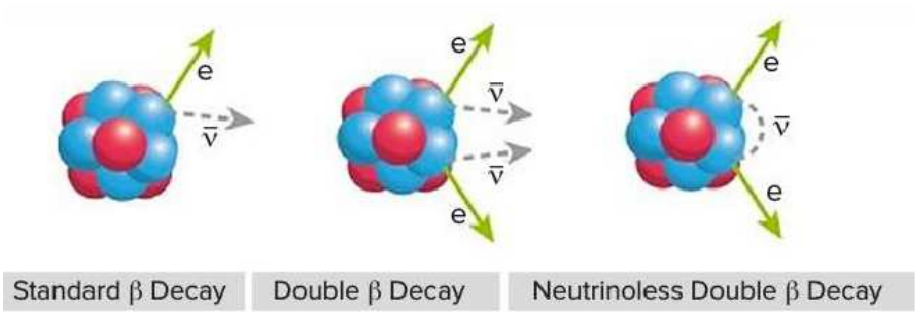
Neutrinoless Double Beta Decay



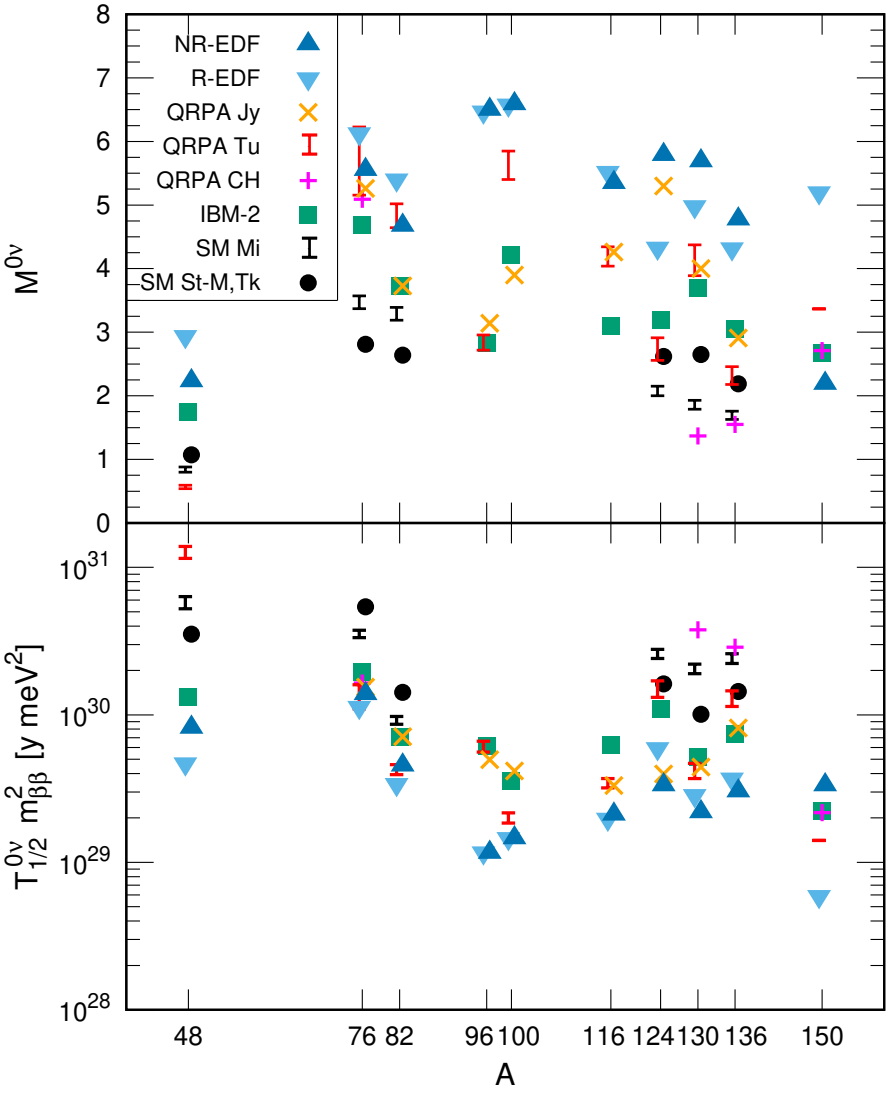


"The average momentum is about 100 MeV, a scale set by the average distance between the two decaying neutrons" cit. Engel&Menéndez

$$* \text{ Decay rate} \propto (\text{nuclear matrix elements})^{\,2} \times \langle m_{\beta\beta} \rangle^2 \; *$$

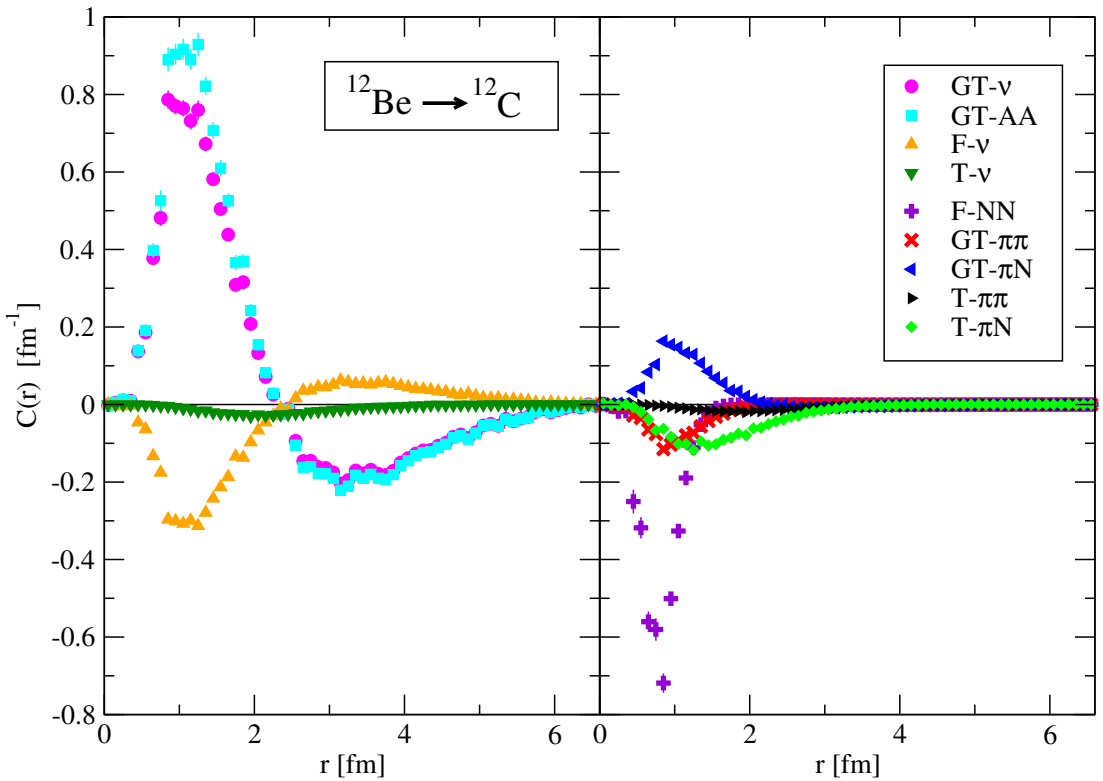


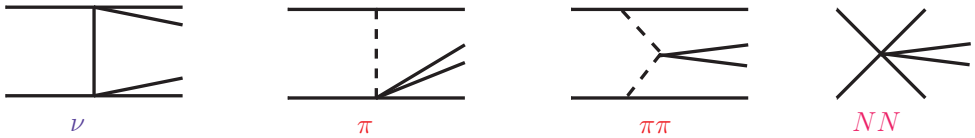
Neutrinoless Double Beta Decay: STATUS



Jon Engel and Javier Menéndez - Reports on Progress in Physics 80, 046301 (2017)

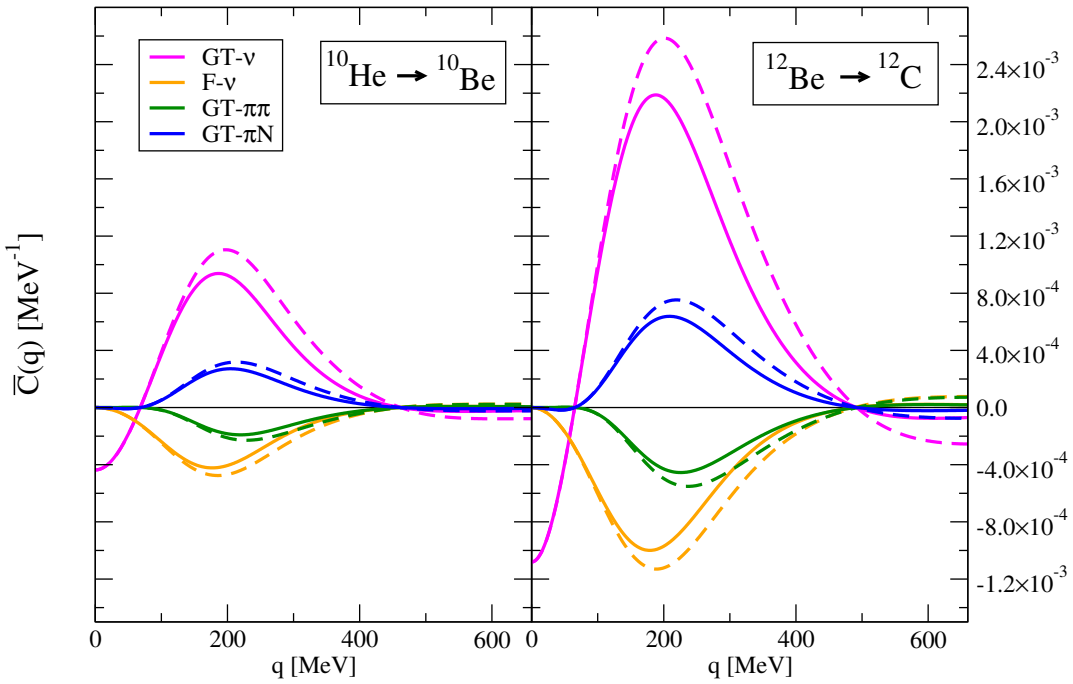
Double beta-decay Matrix Elements





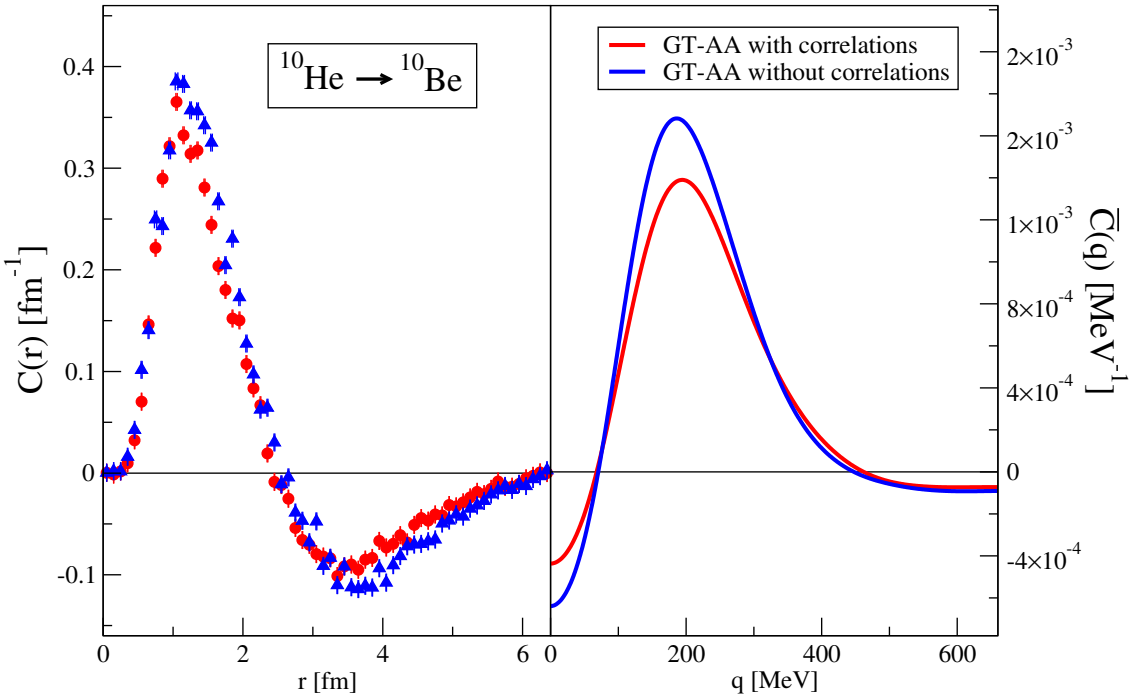
SP *et al.* PRC97(2018)014606

Momentum Dependence



* Peaks at ~ 200 MeV
* $A = 10$ highly suppressed w.r.t. $A = 12$ (clusterization matter?)
* $A = 10$ small overlap between initial diffuse w.f. ($r_n \sim 3.66$ fm) and final compact w.f. ($r_p \sim 2.32$ fm)
* $A = 12$ large overlap between initial compact w.f. ($r_n \sim 2.99$ fm) and final compact w.f. ($r_p \sim 2.48$ fm)
* $A = 12$ 'most similar' to experimental cases

Sensitivity to ‘pion-exchange-like’ correlations



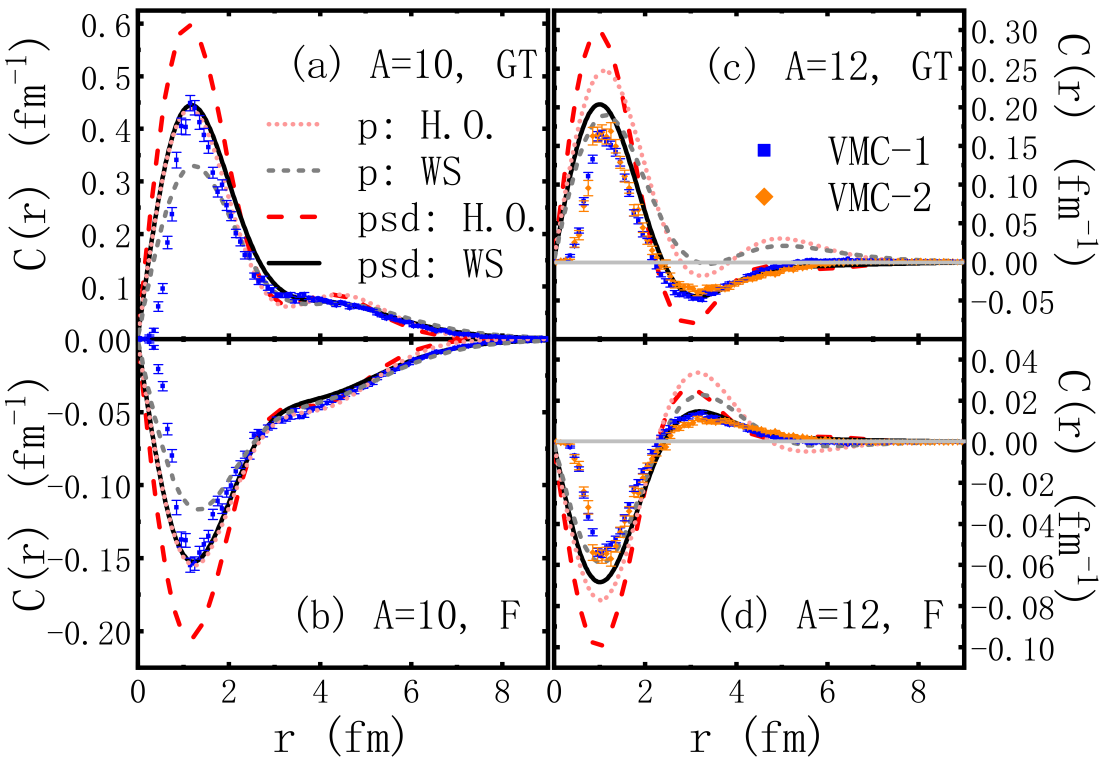
* no ‘pion-exchange-like’ correlation operators U_{ij}

* yes ‘pion-exchange-like’ correlation operators U_{ij}

* Correlations reduce the m.e.’s (also true for μ’s and GT’s) *

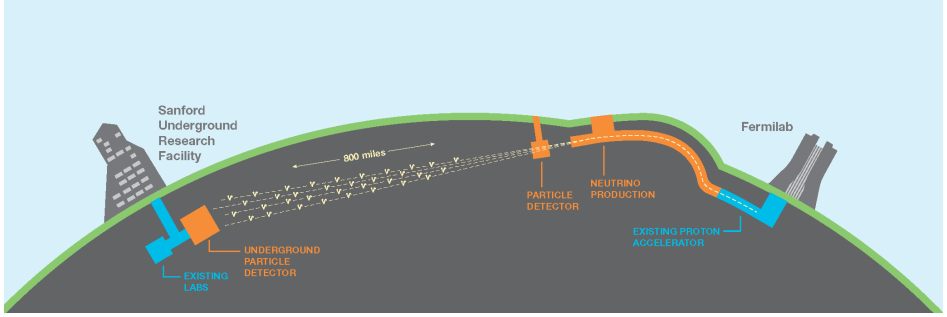
SP *et al.* PRC97(2018)014606

Benchmark with Shell Model



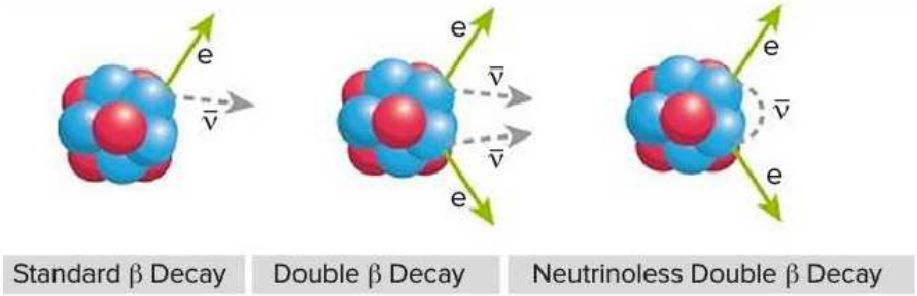
X. Wang *et al.* arXiv:1906.06662 (2019)

Summary



* Two-body currents can give $\sim 30-40\%$ contributions and improve on theory/EXPT agreement

* Calculations of $\beta-$ and $\beta\beta-$decay matrix elements in $A \leq 12$ indicate two-body physics (currents and correlations) are required

* Short-Time-Approximation developed to evaluate υ scattering off $A > 12$ nuclei is in excellent agreement with exact calculations and data

* We are developing a coherent picture for neutrino-nucleus interactions *