Nuclear interactions and quantum Monte Carlo methods

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Lecture 3: What can we calculate?

Many-body Nuclear Interactions

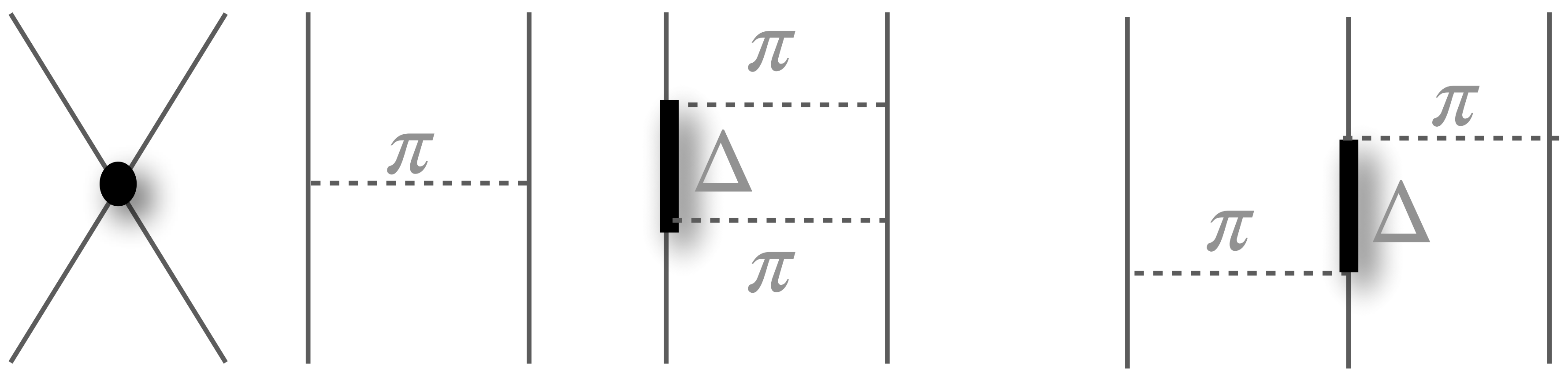
Many-body Nuclear Hamiltonian

th+exp   th+exp

$$H = \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i<j=1}^{A} v_{ij} + \sum_{i<j<k=1}^{A} V_{ijk} + \cdots$$

one-body   two-body (NN)   three-body (3N)

- Accurate understanding of the interactions/correlations between nucleons in pairs, triplets,..(v_{ij} and V_{ijk} are the two- and three-nucleon forces)
- Operators constrained by experimental data; fitted parameters encode underlying QCD dynamics



long-range $r \sim m_\pi^{-1}$: pion-exchange
intermediate range $r \sim (2m_\pi)^{-1}$: ex. two-pion exchange
short-range: ex. contact terms

In our Quantum Monte Carlo calculations we use:

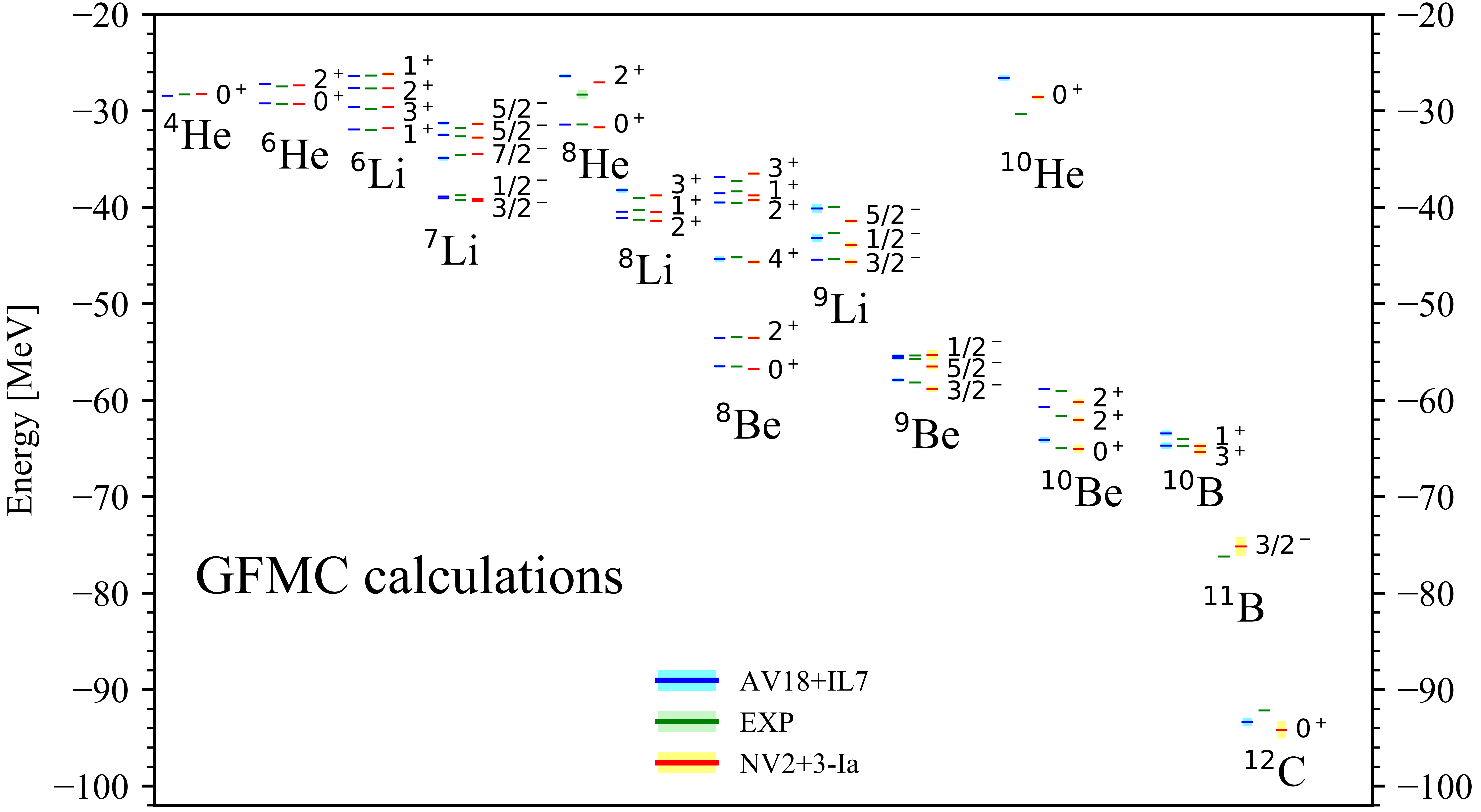
- AV18+UIX; AV18+IL7 phenomenological models

Wiringa, Stoks, Schiavilla PRC **51**, 38 (1995); J. Carlson et al. NP **A401**, 59 (1983); S. Pieper et al. PRC **64**, 014001 (2001)

- chiral $\pi N\Delta$ N3LO+N2LO Norfolk models

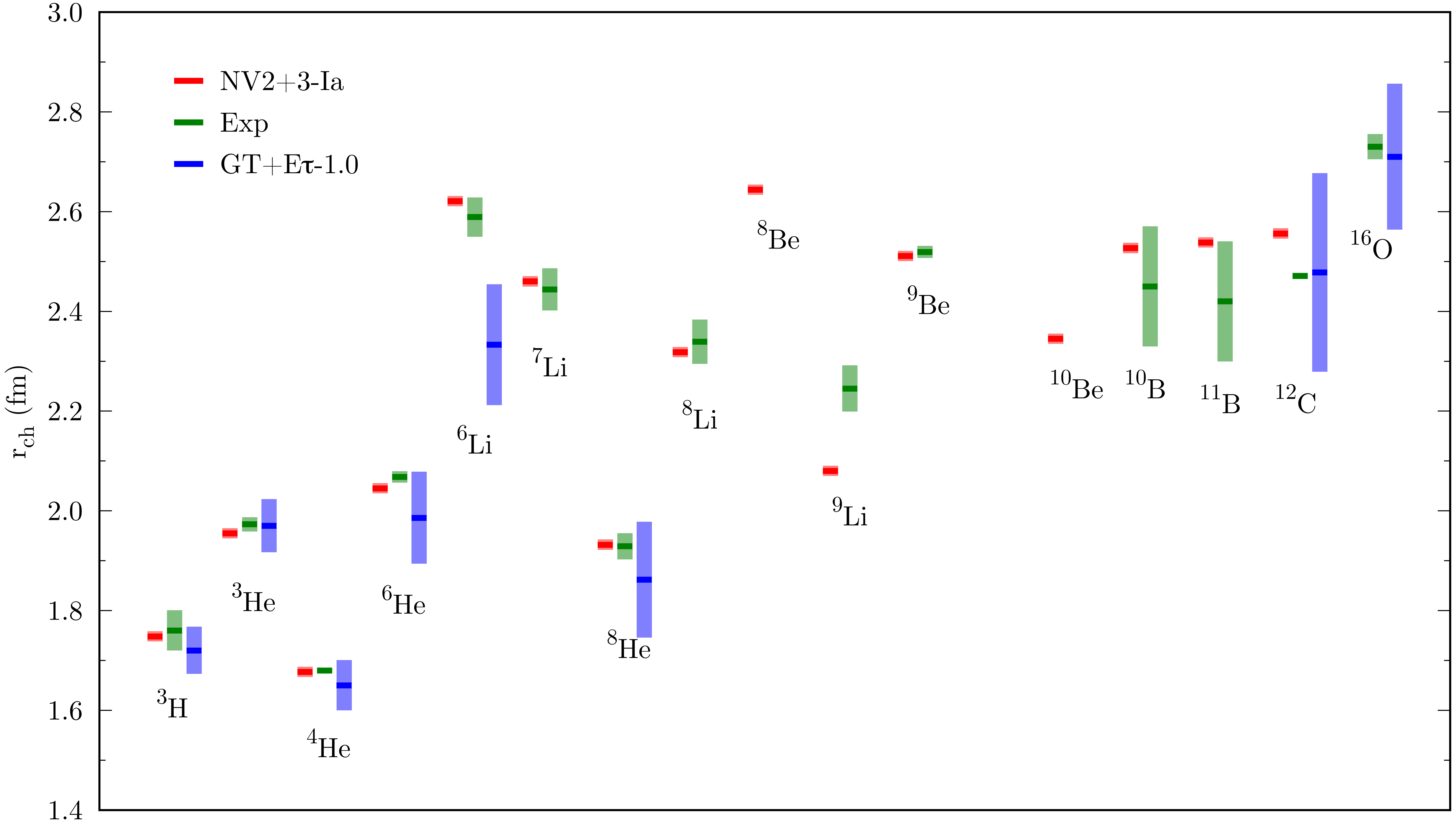
MP et al. PRC 91, 024003 2015; PRC 94, 054007 2016; MP *et al.* PRL **120**, 052503 (2018); A. Baroni, MP et al.PRC 98, 044003 (2018)

Binding energies of light nuclei



- Studied 37 different nuclear states in $A \sim 4-12$ nuclei. Comparison between the phenomenological AV18+IL7 model and experiment.
- The agreement with experiment is good for both Hamiltonians: absolute binding energies very close to experiment, and excited states reproducing the observed ordering, indicating reasonable one-body spin orbit splittings.

Charge radii of light nuclei



- Charge radii with respect to experimental data (GFMC for NV2+3-Ia and AFDMC for GT+Eτ-1.0)
- Overall agreement with the experimental data for both models
- For NV2+3-Ia, 9Li charge radius underpredicted, 12C slightly overestimated
- For GT+Eτ-1.0, 6Li charge radius underpredicted (issue with AFDMC w.f.)

$$\langle r_{ch}^2 \rangle = \langle r_{pt}^2 \rangle + \langle R_p^2 \rangle + \frac{A-Z}{Z}\langle R_n^2 \rangle + \frac{3\hbar^2}{4M_p^2c^2} + \langle r_{so}^2 \rangle$$

point-nucleon radius

proton radius $= 0.770(9)\ \mathrm{fm}^2$

neutron radius $= -0.116(2)\ \mathrm{fm}^2$

Darwin-Foldy correction $\approx 0.033\ \mathrm{fm}^2$

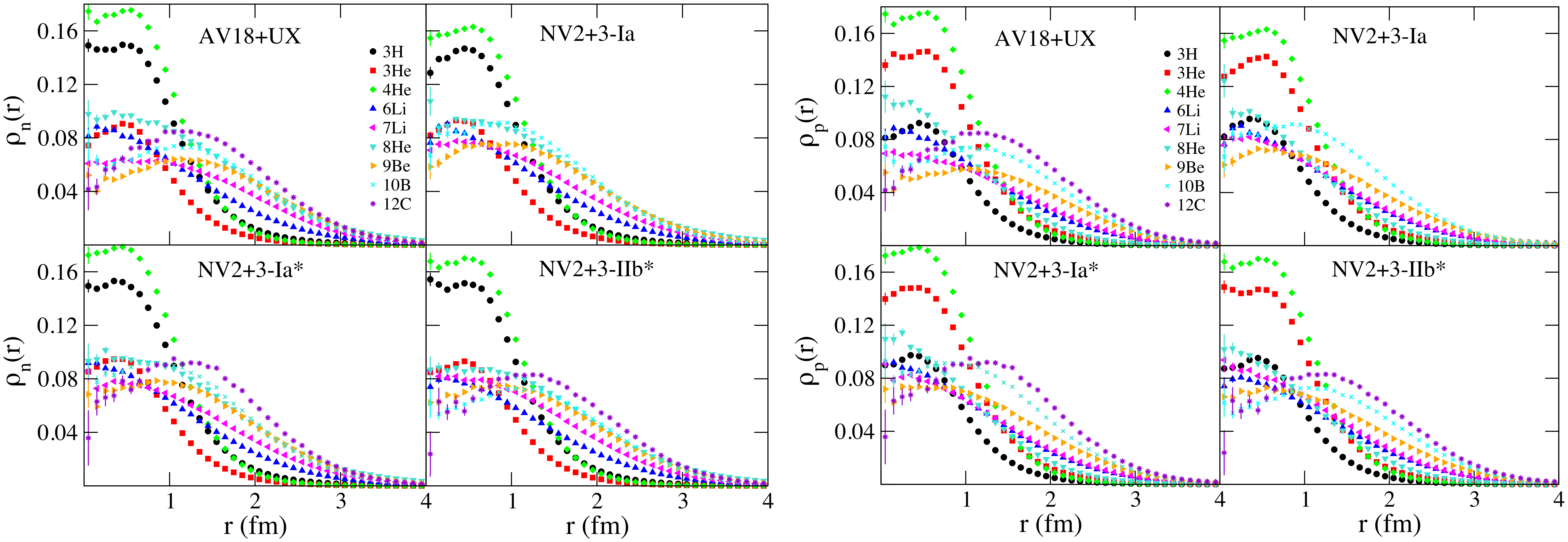
spin-orbit correction

point-nucleon radius $\langle r_N^2 \rangle = \frac{1}{\mathcal{N}}\langle \Psi | \sum_i \mathcal{P}_{N_i} |\mathbf{r}_i|^2 | \Psi \rangle$

- $\mathbf{r}_i$ is the intrinsic nucleon coordinate
- $\mathcal{N}$ is the number of protons or neutrons,
- $\mathcal{P}_{N_i} = \frac{1 \pm \tau_{z_i}}{2}$

Single-nucleon densities

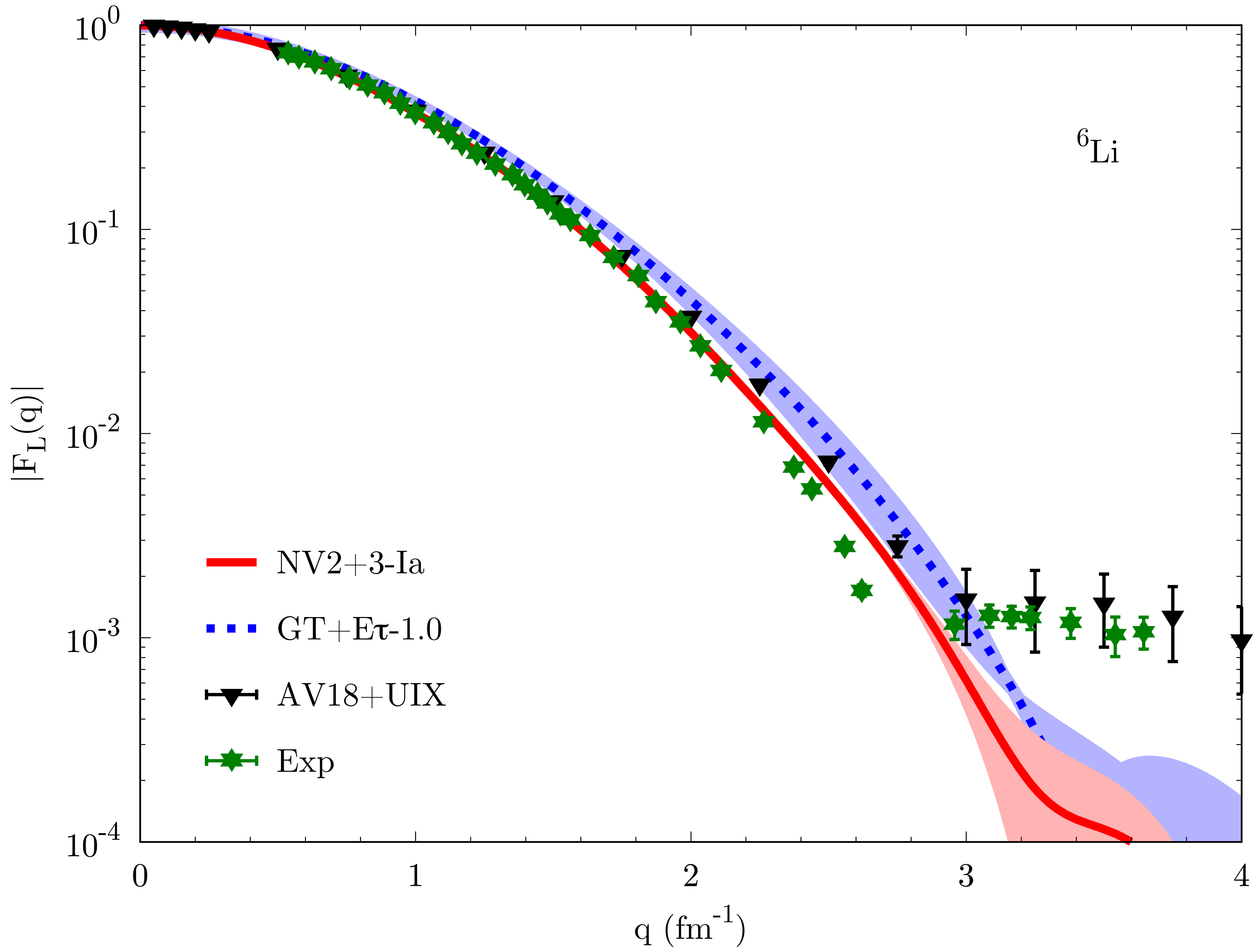
- In QMC methods, single-nucleon densities are calculated as: $\rho_N(r) = \frac{1}{4\pi r^2}\langle \Psi | \sum_i \mathcal{P}_{N_i} \delta(r - |\mathbf{r_i} - \mathbf{R}_{\rm cm}|) | \Psi \rangle$



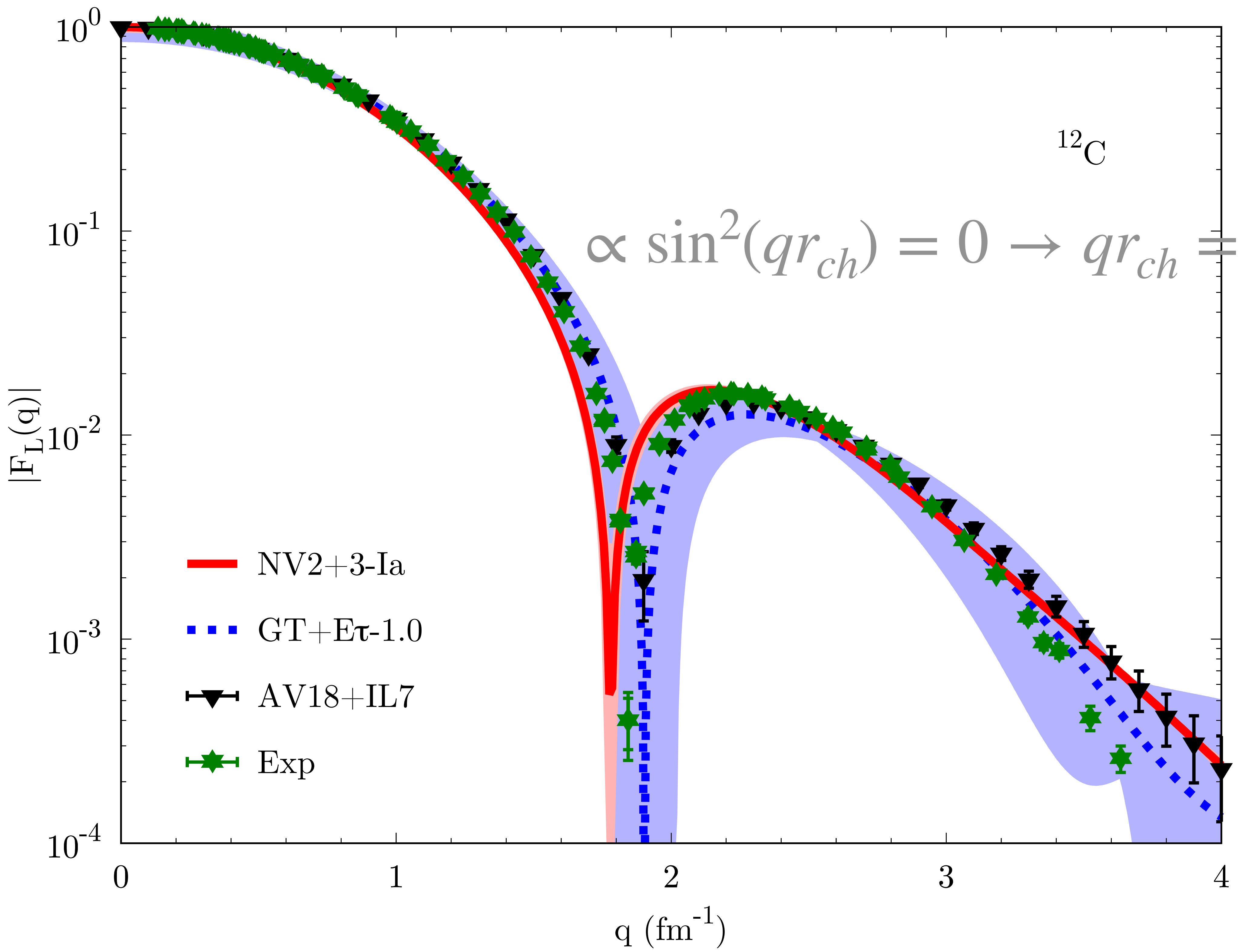
- For symmetric nuclei N = Z nuclei, proton and neutron densities are the same.
- s-shell nuclei (A ≤ 4) exhibit large peaks at small separation, while the p-shell nuclei (A ≥ 6) are much reduced at small r and more spread out: due to cluster structure of these light p-shell nuclei puts the center of mass of these nuclei in between clusters and thus reduces the central density.
- Densities are not observables but single-nucleon density can be related to longitudinal (charge) form factor physical quantity experimentally accessible via electron-nucleon scattering processes

Charge form factors in A=6 and A=12

Longitudinal form factor for 6Li



Longitudinal form factor for 12C



$\propto \sin^2(qr_{ch}) = 0 \rightarrow qr_{ch} = \pi \rightarrow r_{\rm ch} \propto 1/q$

The charge form factor can be expressed as the ground-state expectation value of the one-body charge operator, which, ignoring small spin-orbit contributions in the one-body current, results in the following expression:

$$F_L(q) = \frac{1}{Z}\frac{G_E^p(Q_{\rm el}^2)\,\tilde{\rho}_p(q) + G_E^n(Q_{\rm el}^2)\,\tilde{\rho}_n(q)}{\sqrt{1 + Q_{\rm el}^2/(4m_N^2)}}$$

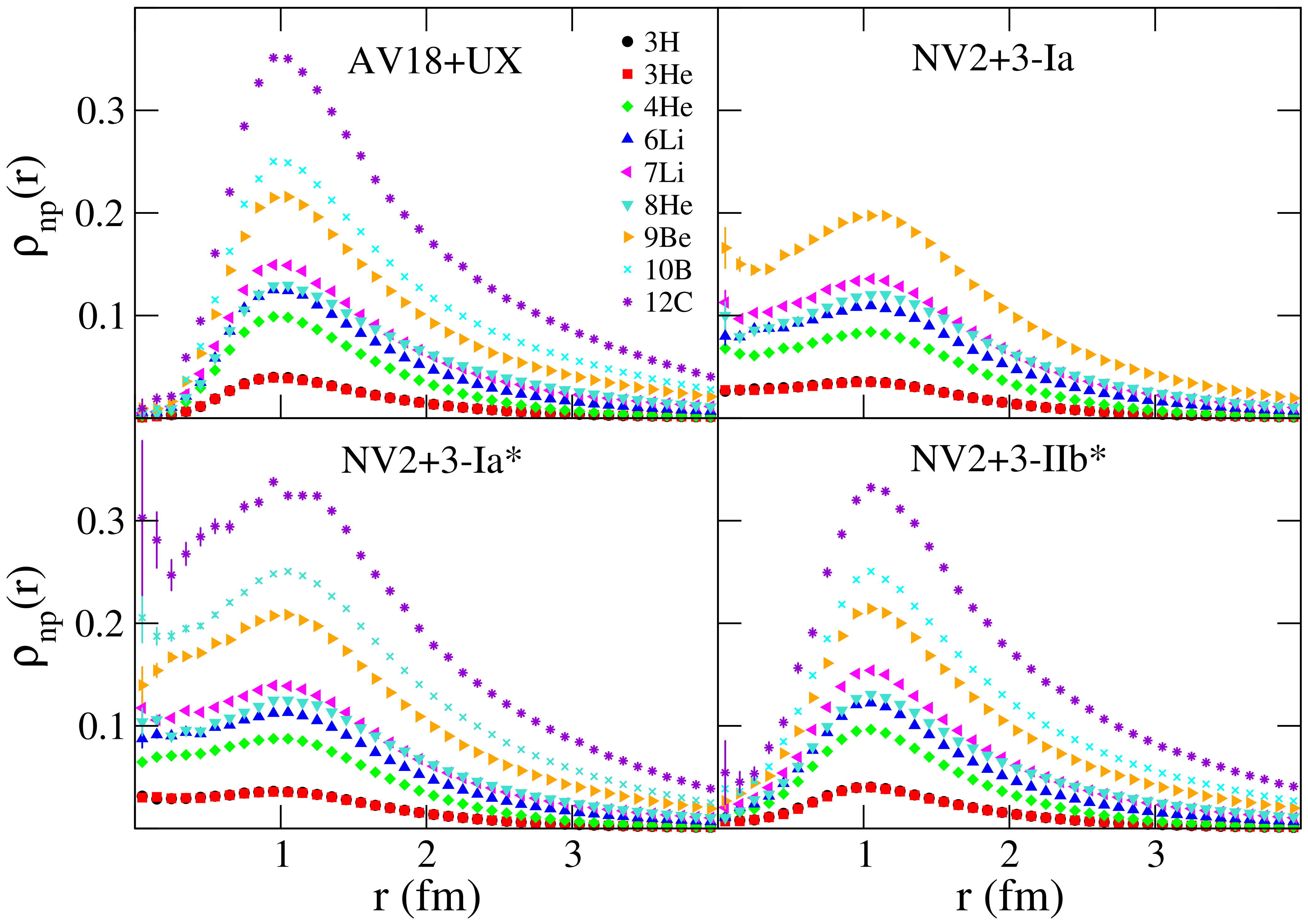
$\tilde{\rho}_N(q)$: the Fourier transform of $\rho_N(r)$

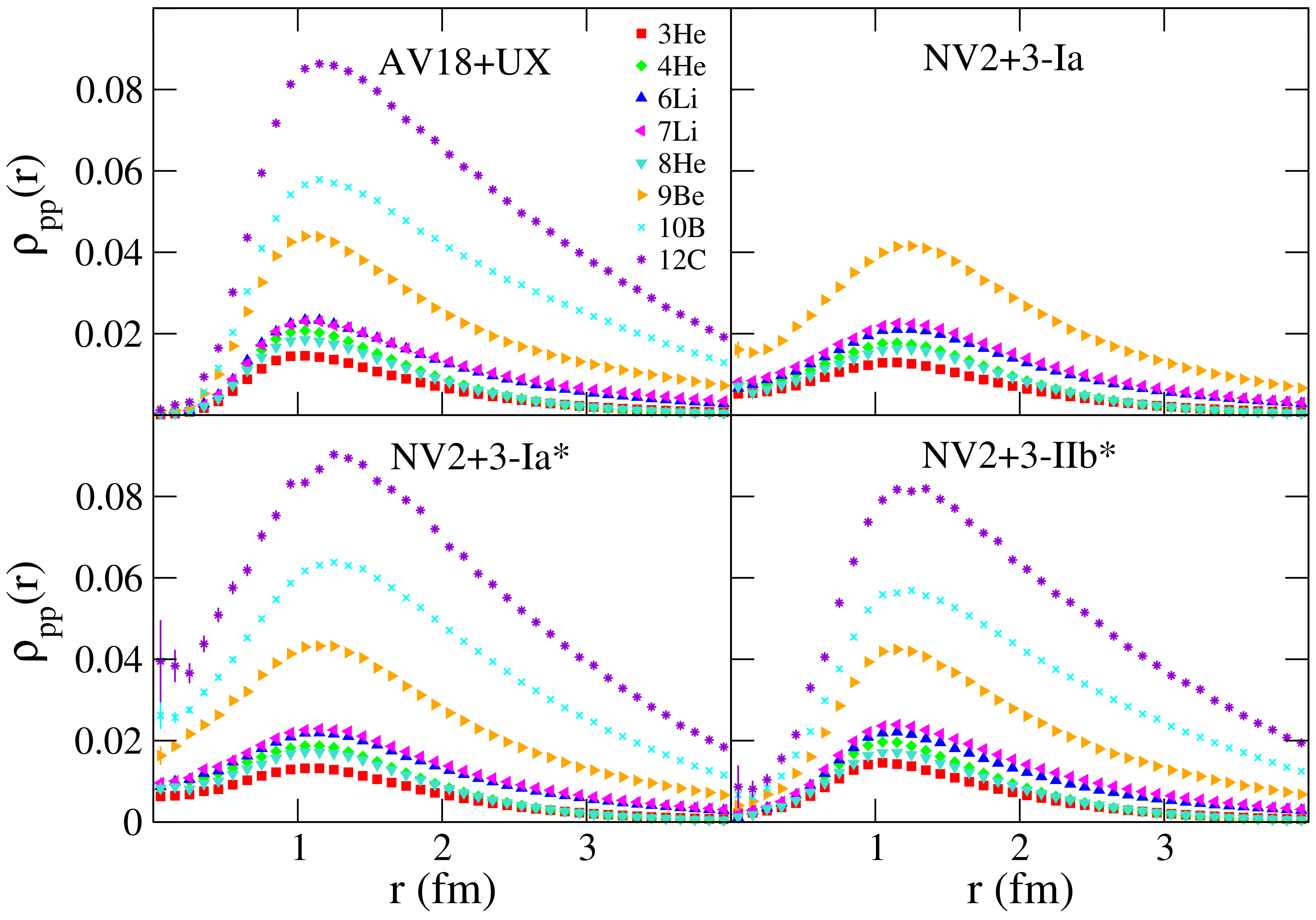
$Q_{\rm el}^2 = \mathbf{q^2} - \omega_{\rm el}^{\mathbf{2}}$ $\qquad \omega_{\rm el} = \sqrt{q^2 + m_A^2} - m_A$

$G_E^N(Q^2)$: electric nucleonic form factor

Nuclear structure: two-nucleon densities

- In QMC methods, two-nucleon densities are calculated as: $\rho_{NN}(r) = \frac{1}{4\pi r^2}\langle\Psi|\sum_{i<j}\mathcal{P}_{N_i}P_{N_j}\delta(r-|\mathbf{r_i}-\mathbf{r_j}|)|\mathbf{\Psi}\rangle$





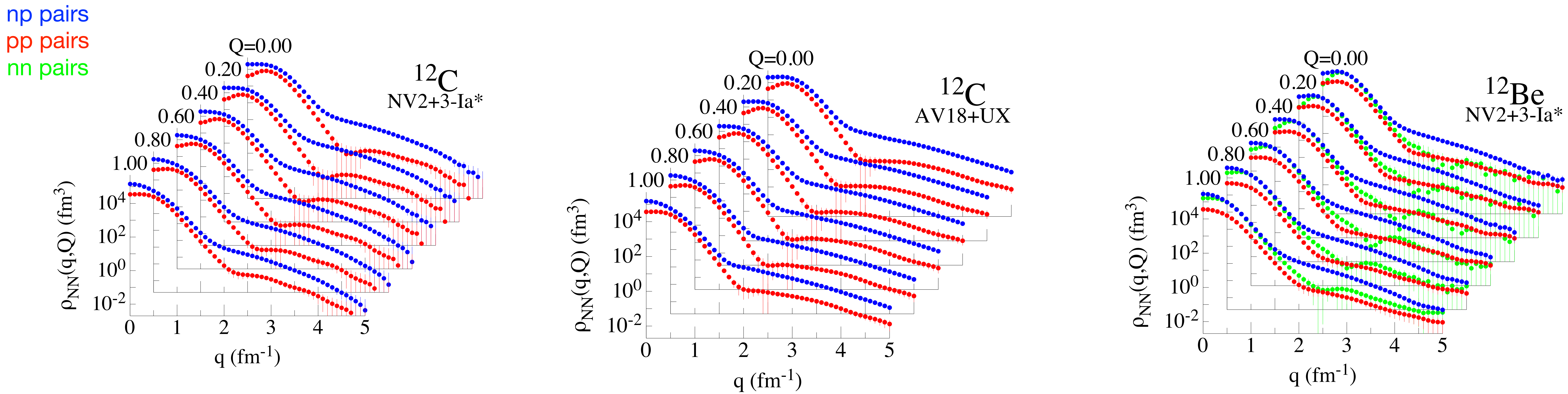
- Within a fixed interaction model, $\rho_{\mathrm{NN}}(r)$ at $r \lesssim 1.5$ fm for various nuclei exhibit a similar behavior: cooperation of the short-range repulsion and the intermediate-range tensor attraction of the NN interaction, with the tensor force being responsible of the large overshooting at $r \sim 1.0$ fm between a *np* pair compared to a *pp* pair.
- While the short-distance behavior is the same for all nuclei, it differs for each interaction. Indeed, the probability of finding two nucleons at short distances is finite for the "soft" NV2+3-Ia and NV2+3-Ia* chiral models, but approaches to zero as we progress from the "hard" local chiral interaction NV2+3-IIb* to the "hardest" phenomenological AV18+UX.

Nuclear structure: two-nucleon densities

- The probability of finding two nucleons in a nucleus with relative momentum **q** and total-center-of-mass momentum **Q** in a spin-isospin projection

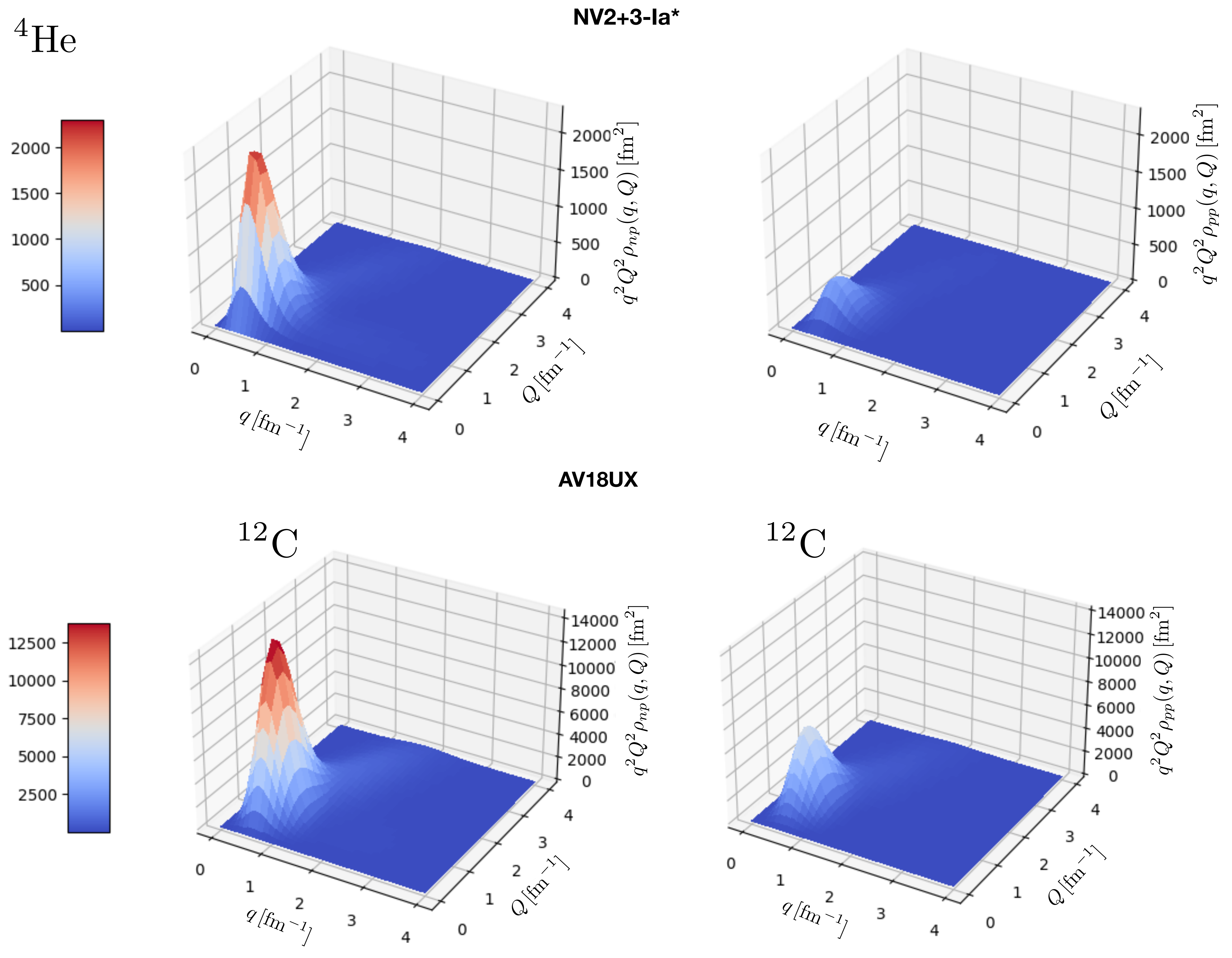
$$\rho_{ST}(\mathbf{q},\mathbf{Q}) = \int d\mathbf{r}'_1 d\mathbf{r}_1 d\mathbf{r}'_2 d\mathbf{r}_2 d\mathbf{r}_3 \cdots d\mathbf{r}_A \psi^\dagger_{JM_J}(\mathbf{r}'_1,\mathbf{r}'_2,\mathbf{r}_3,\ldots,\mathbf{r}_A)\, e^{-i\mathbf{q}\cdot(\mathbf{r}_{12}-\mathbf{r}'_{12})}$$
$$\times e^{-i\mathbf{Q}\cdot(\mathbf{R}_{12}-\mathbf{R}'_{12})}\, P_{ST}(12)\, \psi_{JM_J}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\ldots,\mathbf{r}_A)$$

The total normalization is: $N_{ST} = \int \frac{d\mathbf{q}}{(2\pi)^3}\frac{d\mathbf{Q}}{(2\pi)^3}\rho_{ST}(\mathbf{q},\mathbf{Q})$



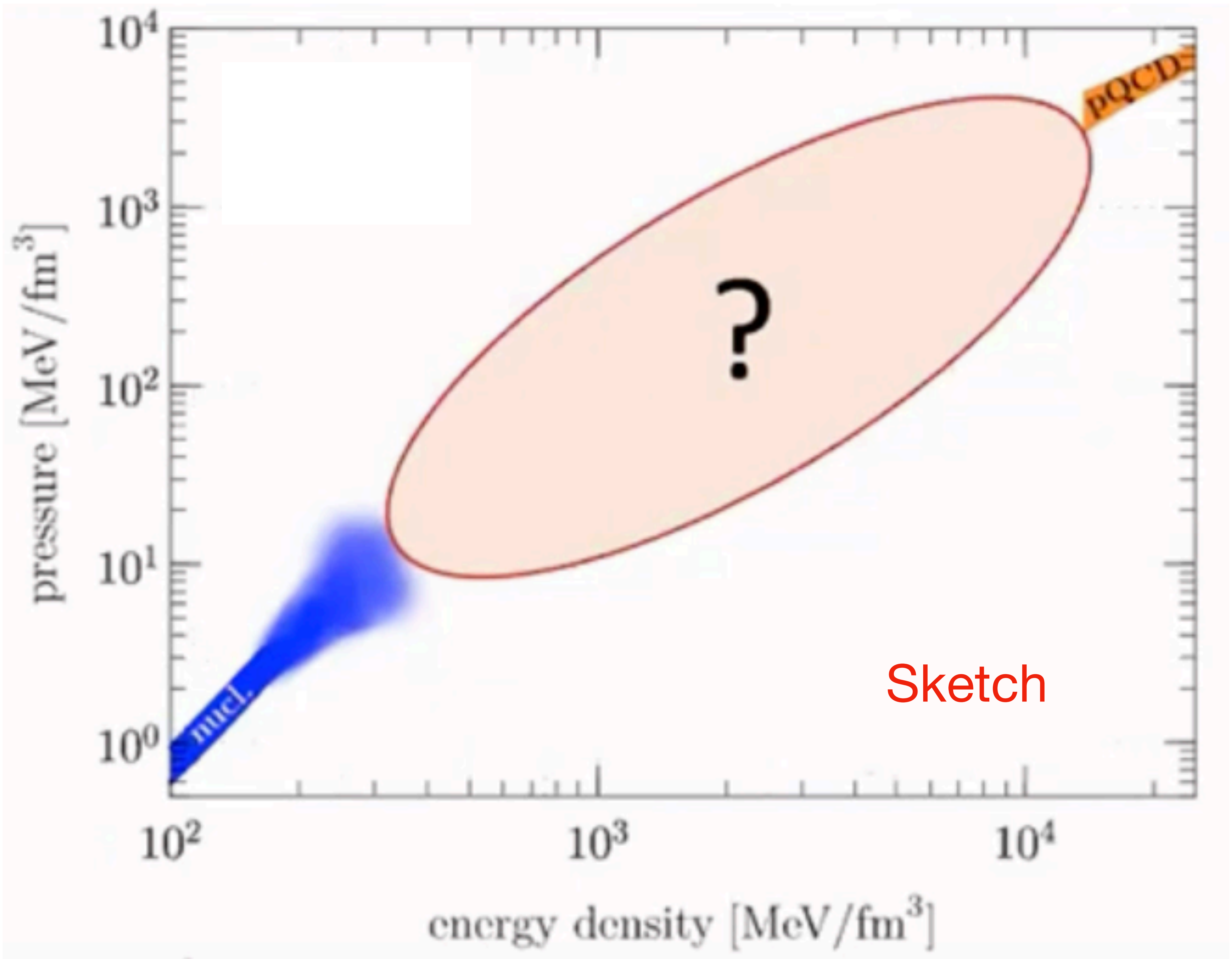
- In 12C both Hamiltonian exhibit the large pn/pp ratio around q = 2 fm^{-1} for small Q, which gradually reduces as Q increases. They also show the high-momentum tail in q, but it decays more rapidly with increasing q for the “soft” chiral force.

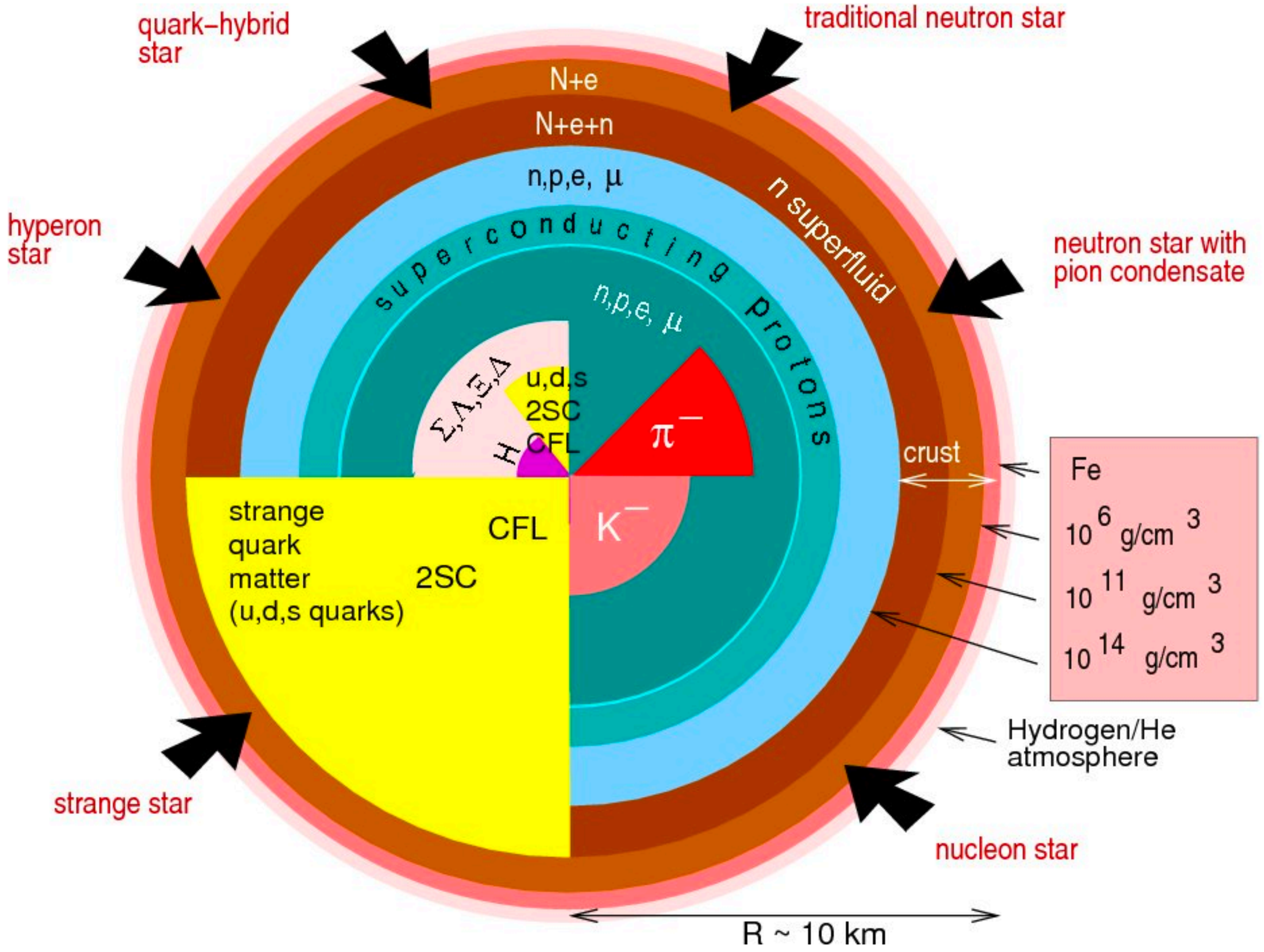
Nuclear structure: two-nucleon momentum distribution



- Tables and figures that tabulate the single-nucleon momentum distribution (including proton and neutron spin momentum distribution) and two-nucleon momentum distribution (including pair distributions in different combinations of ST) will be available online
- A new capability in the VMC code: constraint in the momentum distribution according to pair separation distance

Dense matter equation of state of neutron matter



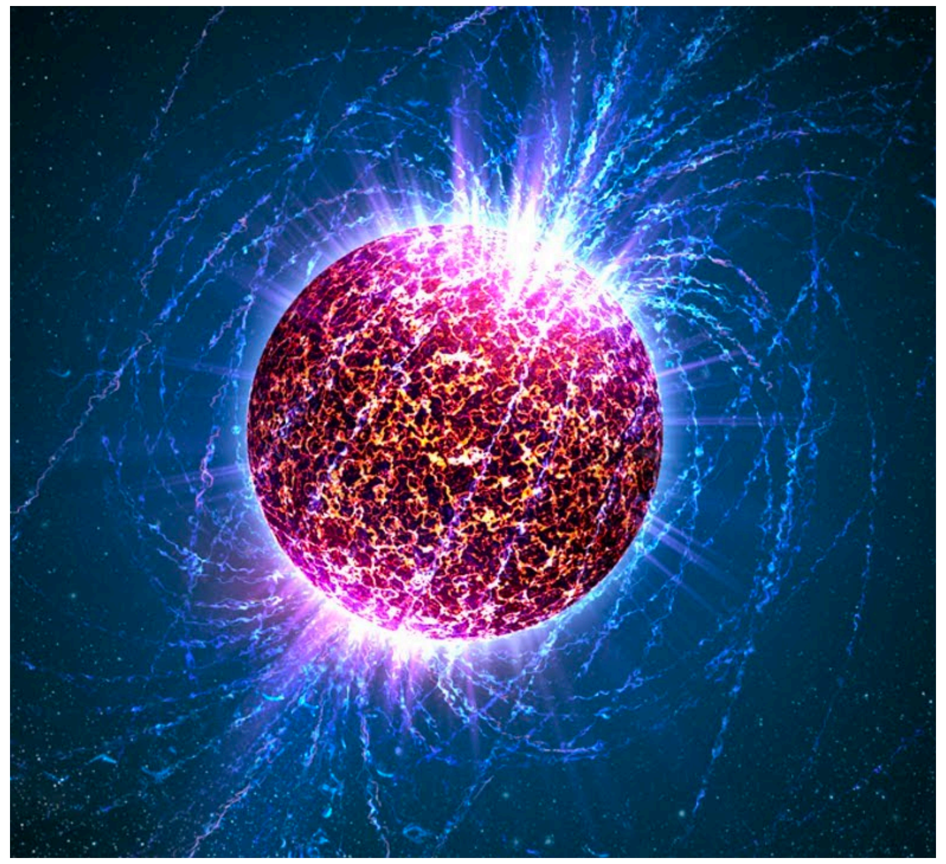


Constraints:

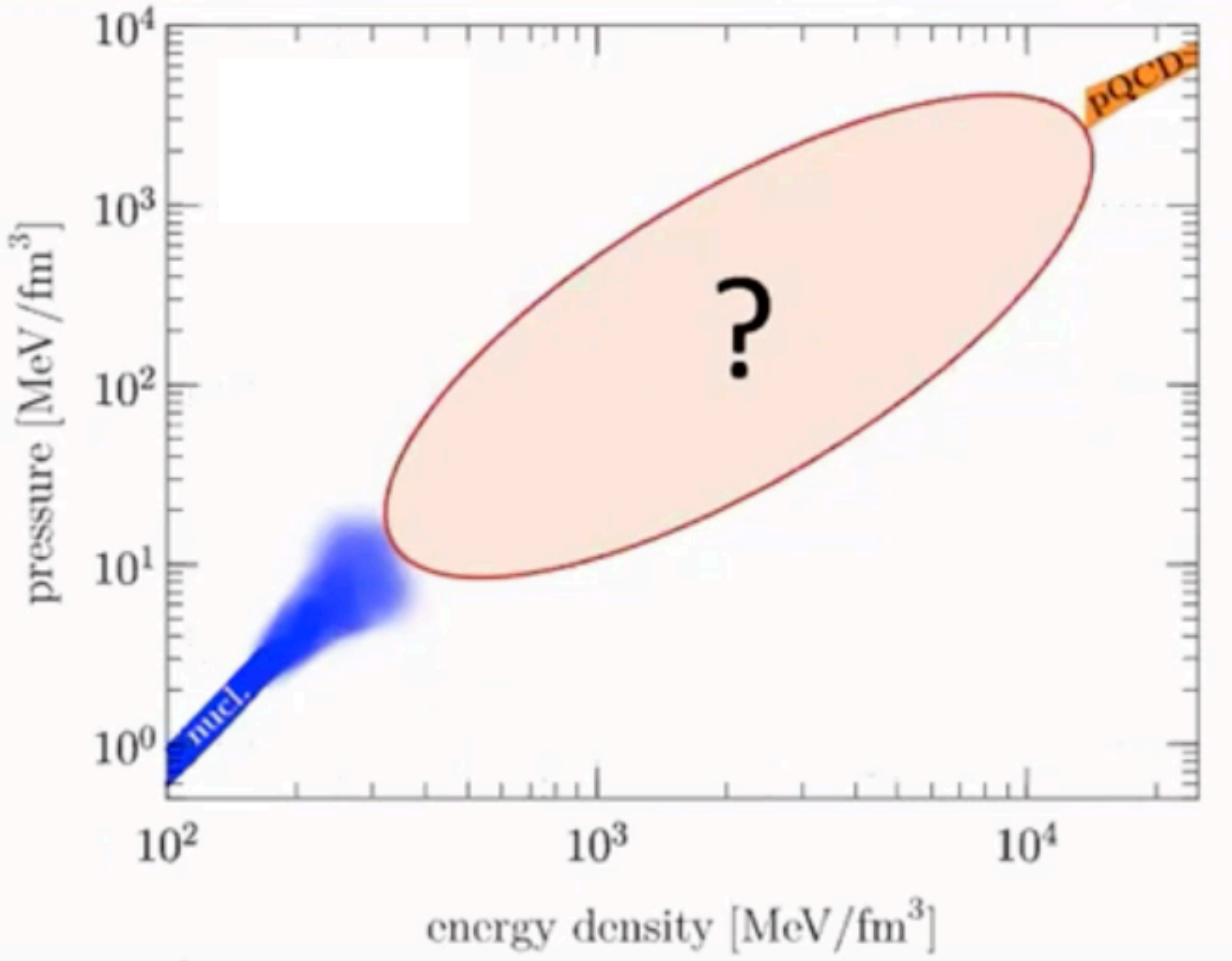
- At low density from nuclear theory and experiment
- At very high density from pQCD
- No robust constraint ay intermediate densities from nuclear physics

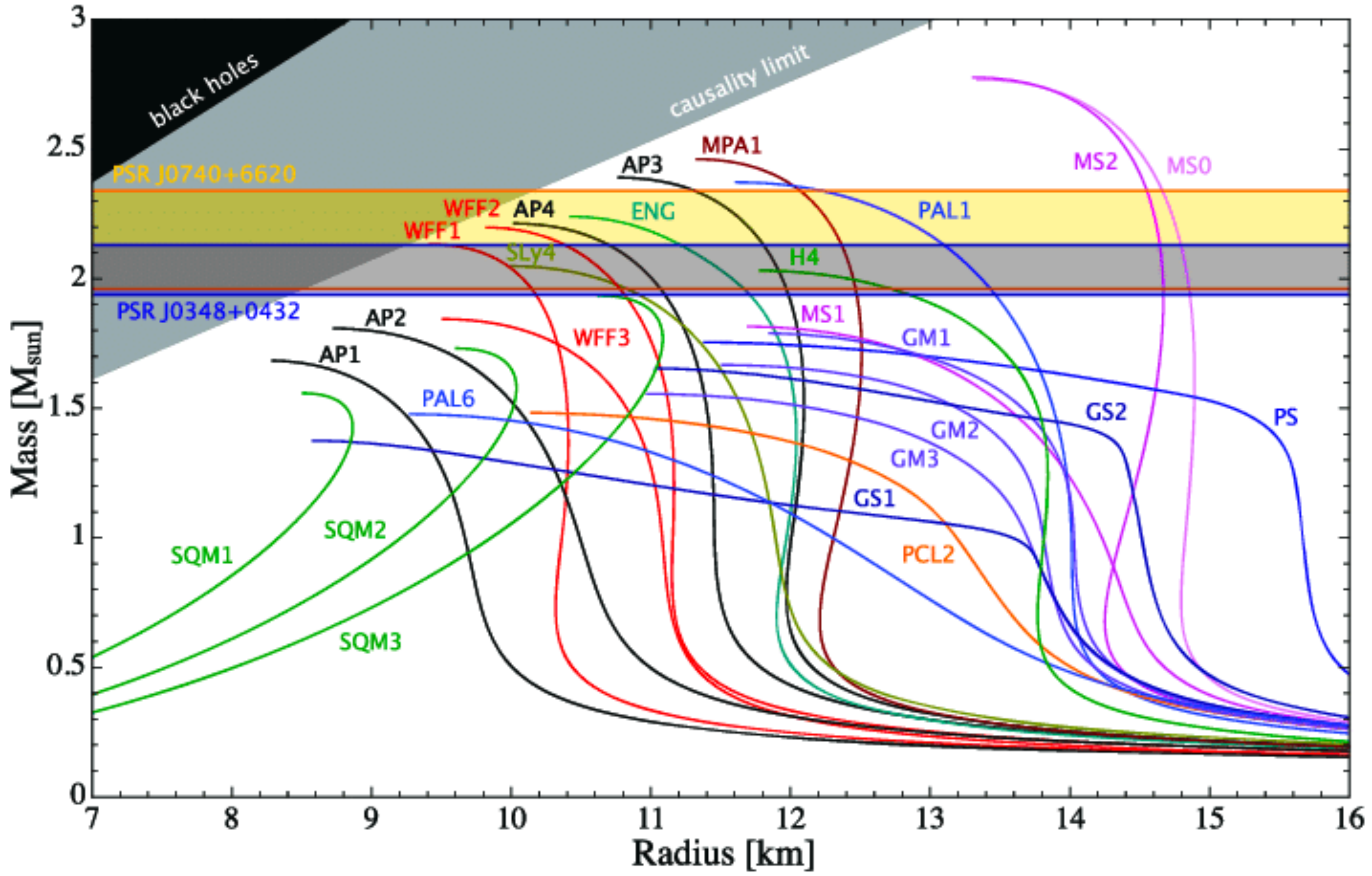
Dense matter equation of state of neutron matter

- The EoS of pure neutron matter (PNM): neutrons stars



- Compact objects: R ~ 10km,
- Composed predominantly of neutrons between the inner crust and the outer core
- NS from gravitational collapse of a massive star after a supernova explosion





Constraints:

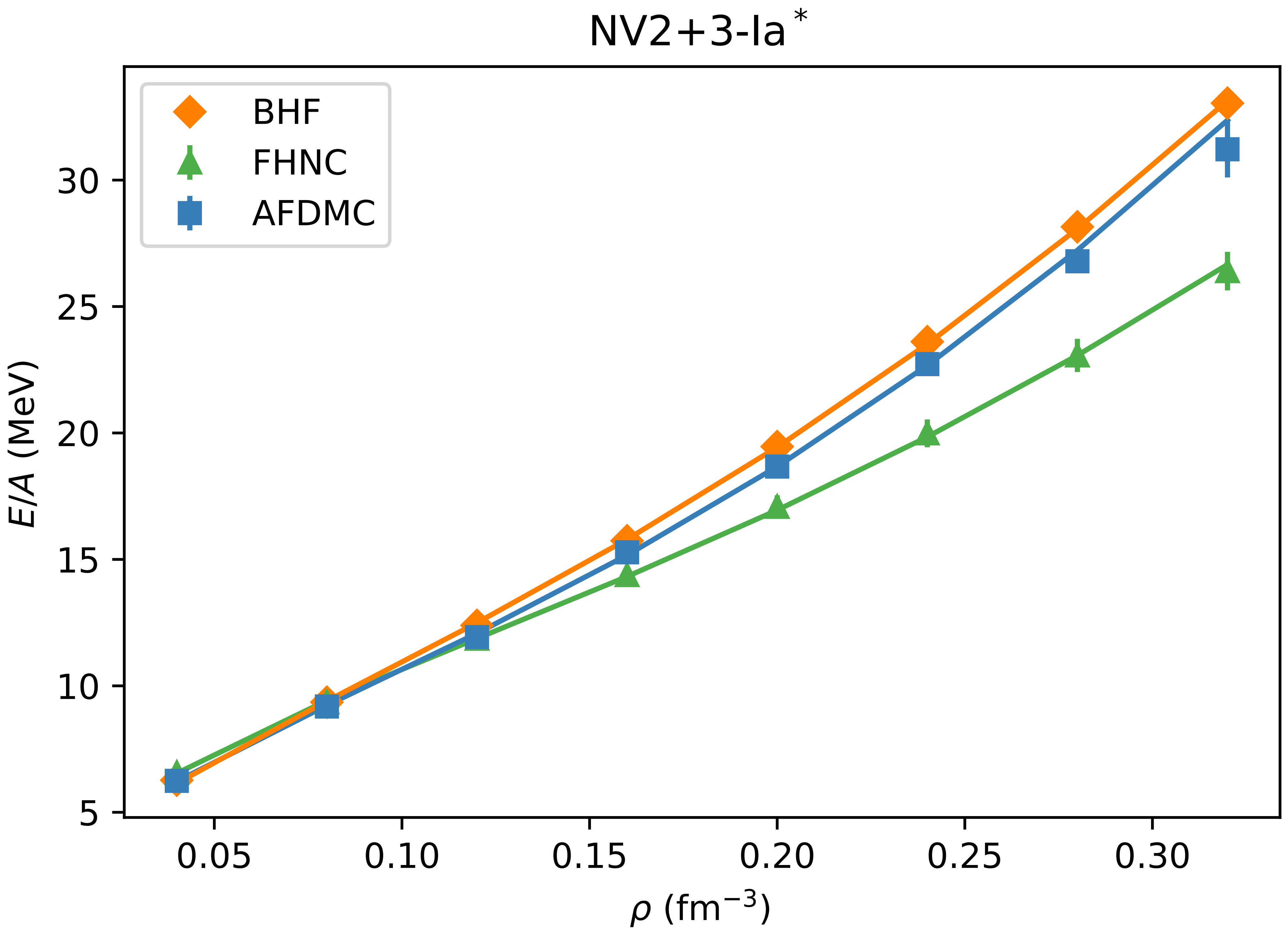
At low density from nuclear theory and experiment

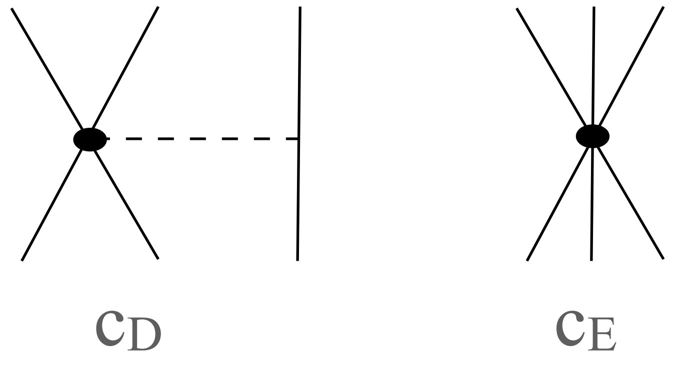
At very high density from pQCD

No robust constraint ay intermediate densities from nuclear physics

Neutron matter with realistic NN+3N potentials

- Benchmark calculations between BHF, FHNC/SOC, AFDMC-UP for both the AV18 and chiral-EFT interactions

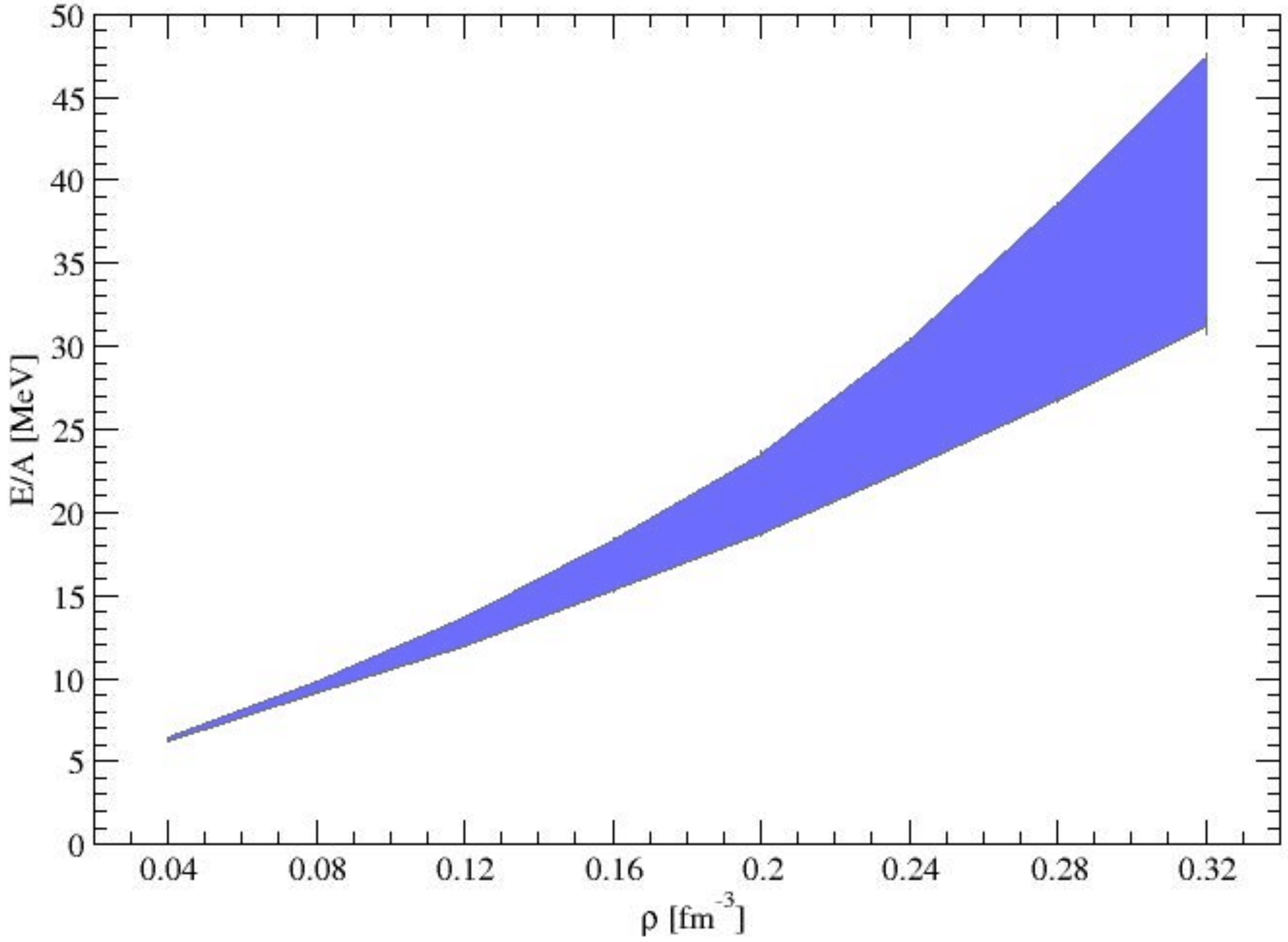




$\sim \tau_i \cdot \tau_j$

NV2+3s*

Model	c_D	c_E
Ia*	–0.635(255)	–0.09(8)
Ib*	–4.705(285)	0.550(150)
IIa*	–0.610(280)	–0.350(100)
IIb*	–5.250(310)	0.05(180)

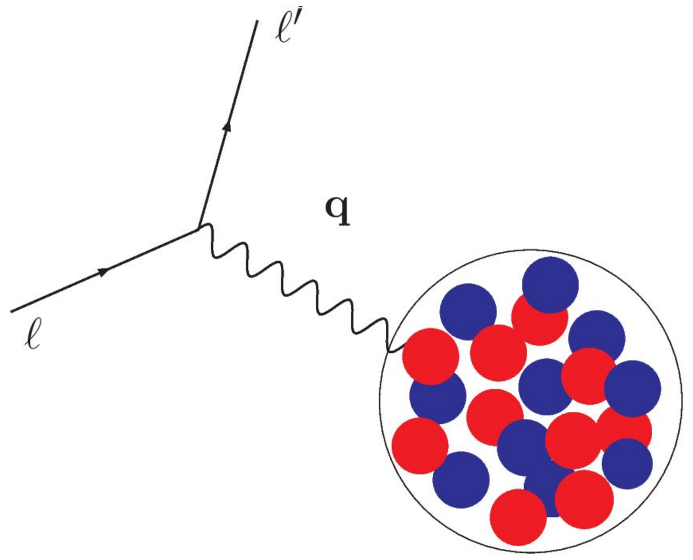


- AFDMC-UC, BHF, FHNC/SOC are very close to each other up to $\rho = \rho_0$ (~1 MeV)
- FHNC/SOC is below AFDMC and BHF at higher density; due to limited three-body terms into the cluster expansion $\rho = 2\rho_0$ (~6 MeV)
- Model dependence of the EOS at three-body level $\rho = 2\rho_0$ (~16 MeV)
- The exp error on the 3H beta decays in the NV2+3s* (numbers in parenthesis) is not propagated yet

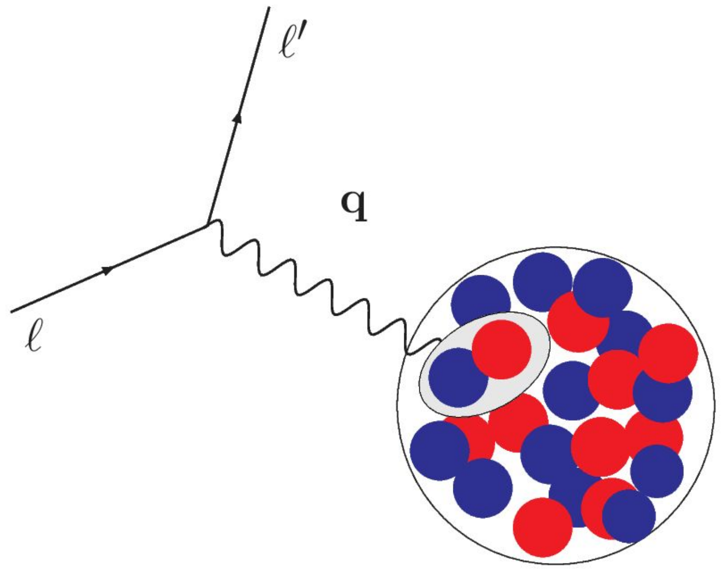
MP *et al*. Phys. Rev. C 101, 045801 (2020)
Lovato, MP *et al*. arxiv 2202.10293 (2022)

Many-body Nuclear Electroweak Currents

- Electroweak structure and reactions:



one-body



two-body

- Electroweak form factors
- Magnetic moments and radii
- Electroweak Response functions
- Radiative/weak captures
- G.T. matrix elements involved in beta decays
- ....

- Accurate understanding of the electroweak interactions of external probes with nucleons, correlated nucleon-pairs,...
- Two-body currents are a manifestation of two-body 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

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

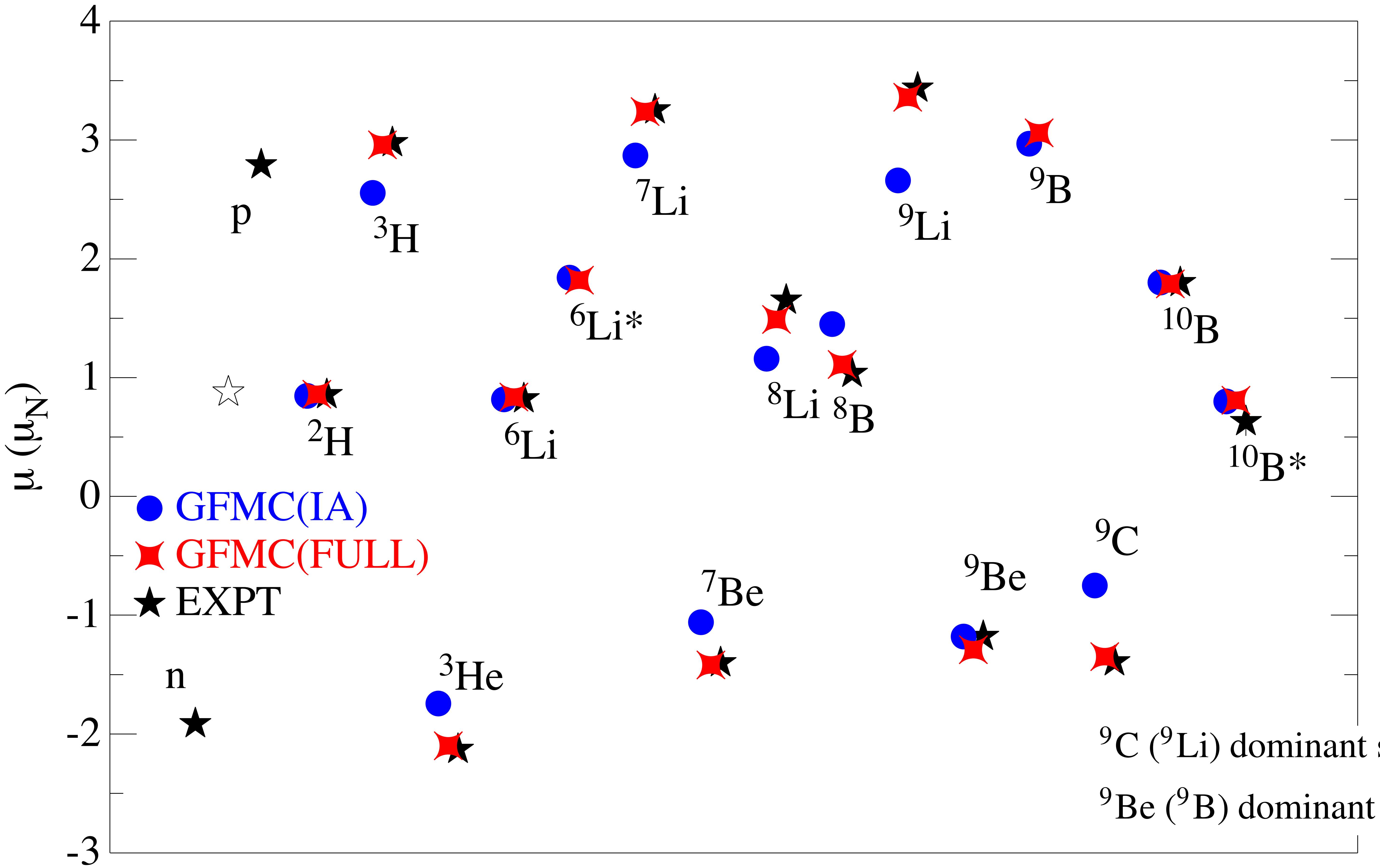
Nuclear vector operator

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

- Meson exchange currents: R. Schiavilla et al., PRC 45, 2628 (1992), Marcucci *et al.* PRC **72**, 014001 (2005), L. Marcucci et al., PRC 78, 065501 (2008)
- Chiral EFT currents: Park *et al.* NPA **596**, 515 (1996); Pastore *et al.* PRC **78**, 064002 (2008), PRC **80**, 034004 (2009); Piarulli *et al.* PRC **87**, 014006 (2013), Baroni *et al.* PRC **93**, 015501 (2016); Phillips et al. PRC **72**, 014006 (2005), Kölling *et al.* PRC **80**, 045502 (2009), PRC **84,** 054008, PRC **86**, 047001 (2012); Krebs et al., Ann. Phys. **378**, 317 (2017)

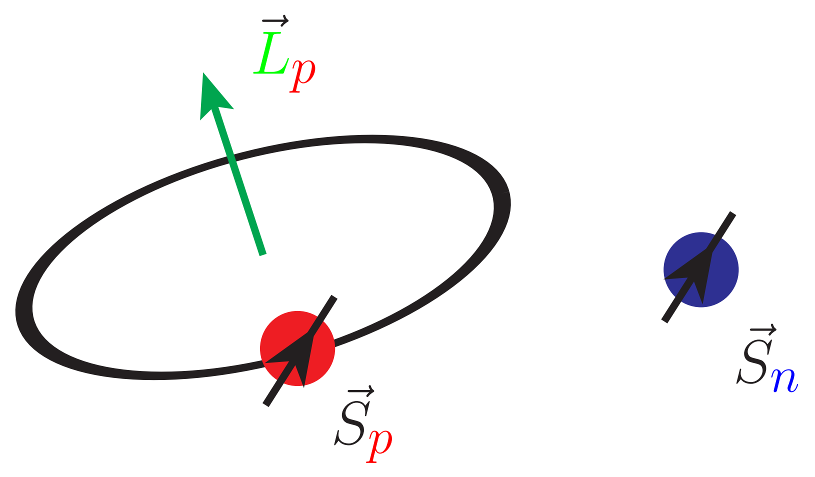
Magnetic moment and EM decay

- GFMC calculations using AV18/IL7 (rather then chiral) and EM χEFT currents— hybrid calculation



Pastore *el al.* PRC **87**, 035503 (2013)

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



$$\langle J_f^\pi, M_f \mid \mu^{\mathrm{MEC}} \mid J_i^\pi, M_i \rangle = -i \lim_{q\to 0} \frac{2\, m_N}{q} \langle J_f^\pi, M_f \mid j_y^{\mathrm{MEC}}(q\,\hat{\mathbf{x}}) \mid J_i^\pi, M_i \rangle$$

^{9}C (^{9}Li) dominant spatial symmetry [s.s.] = [432] = [α, ^{3}He(^{3}H), $pp(nn)$] $\rightarrow$ Large MEC

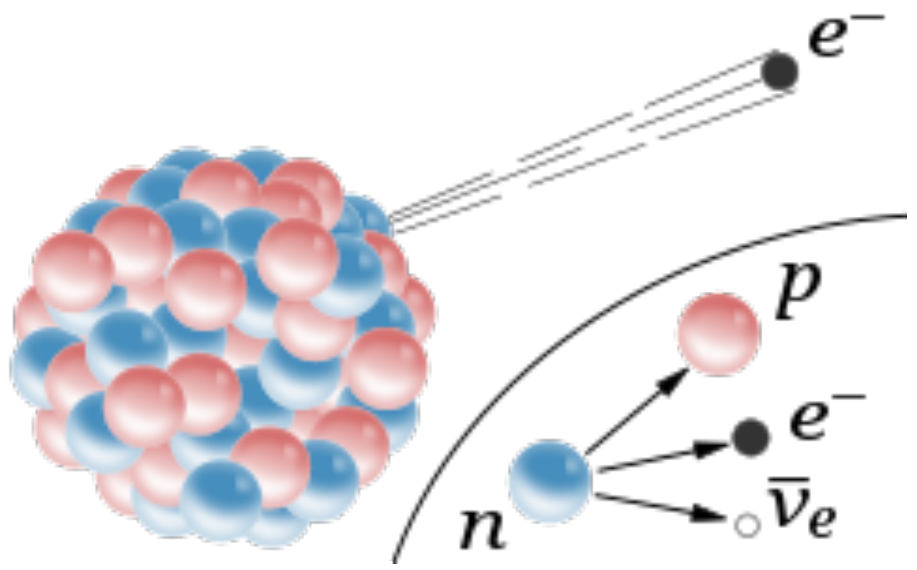
^{9}Be (^{9}B) dominant spatial symmetry [s.s.] = [441] = [$\alpha, \alpha, n(p)$]

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

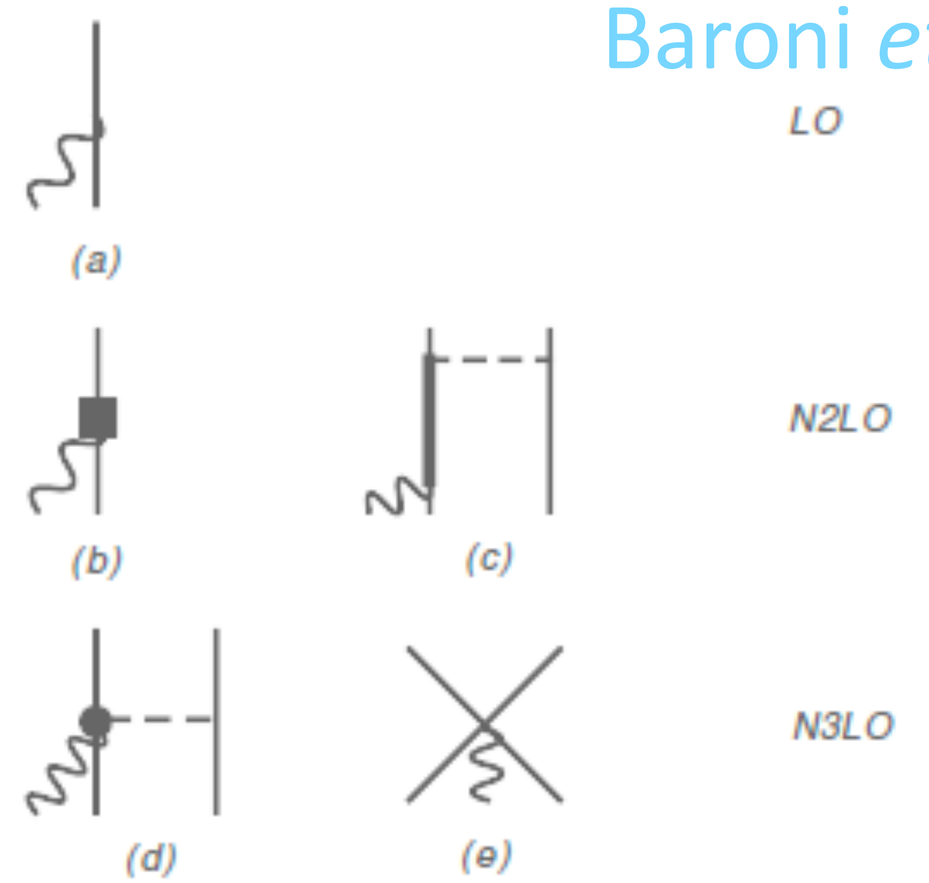
Single-Beta decay matrix elements

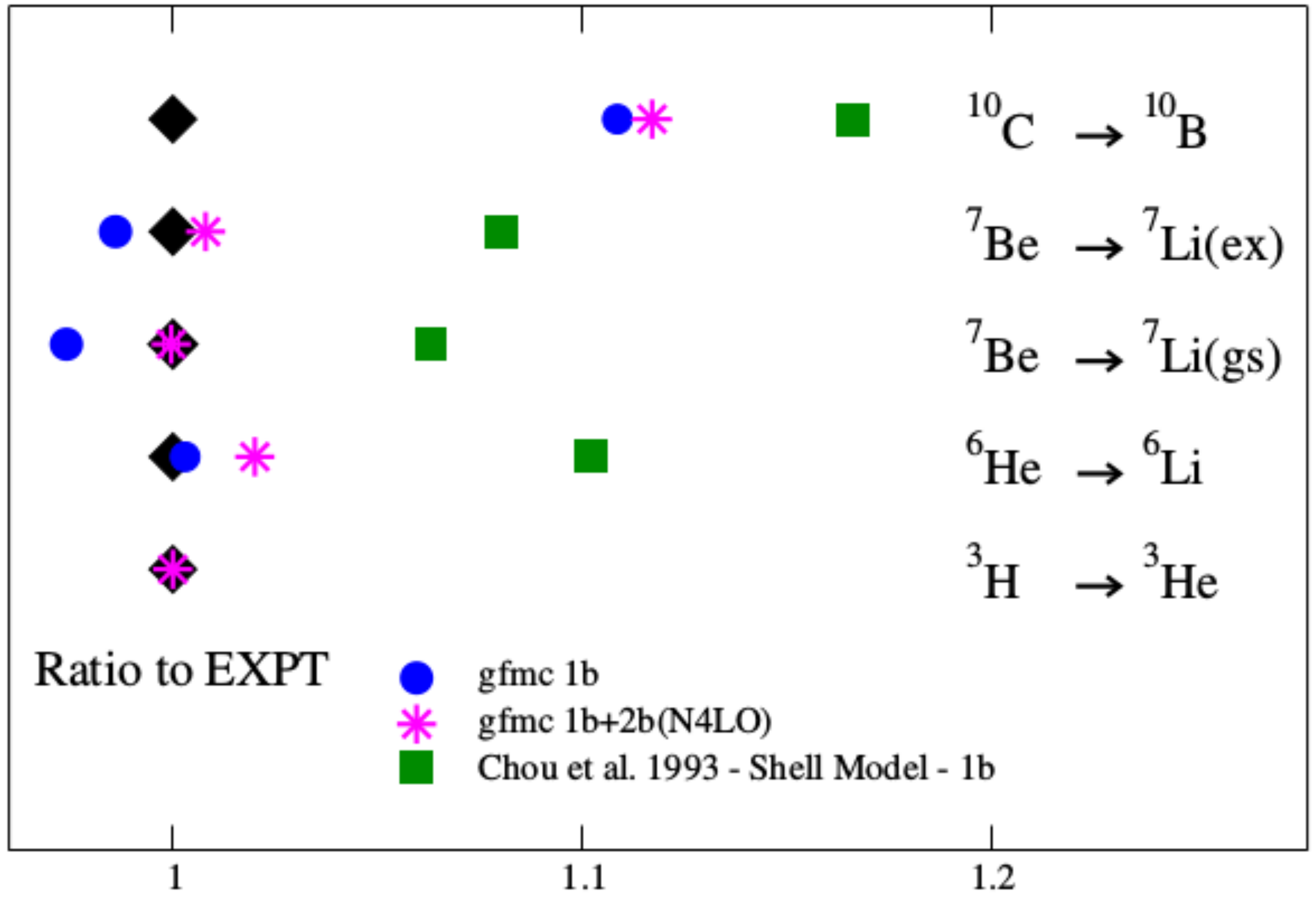
- Beta decay occurs when, in a nucleus with too many protons or too many neutrons, one of the protons or neutrons is transformed into the other.

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



Baroni *et al.* PRC **93**, 015501 (2016)



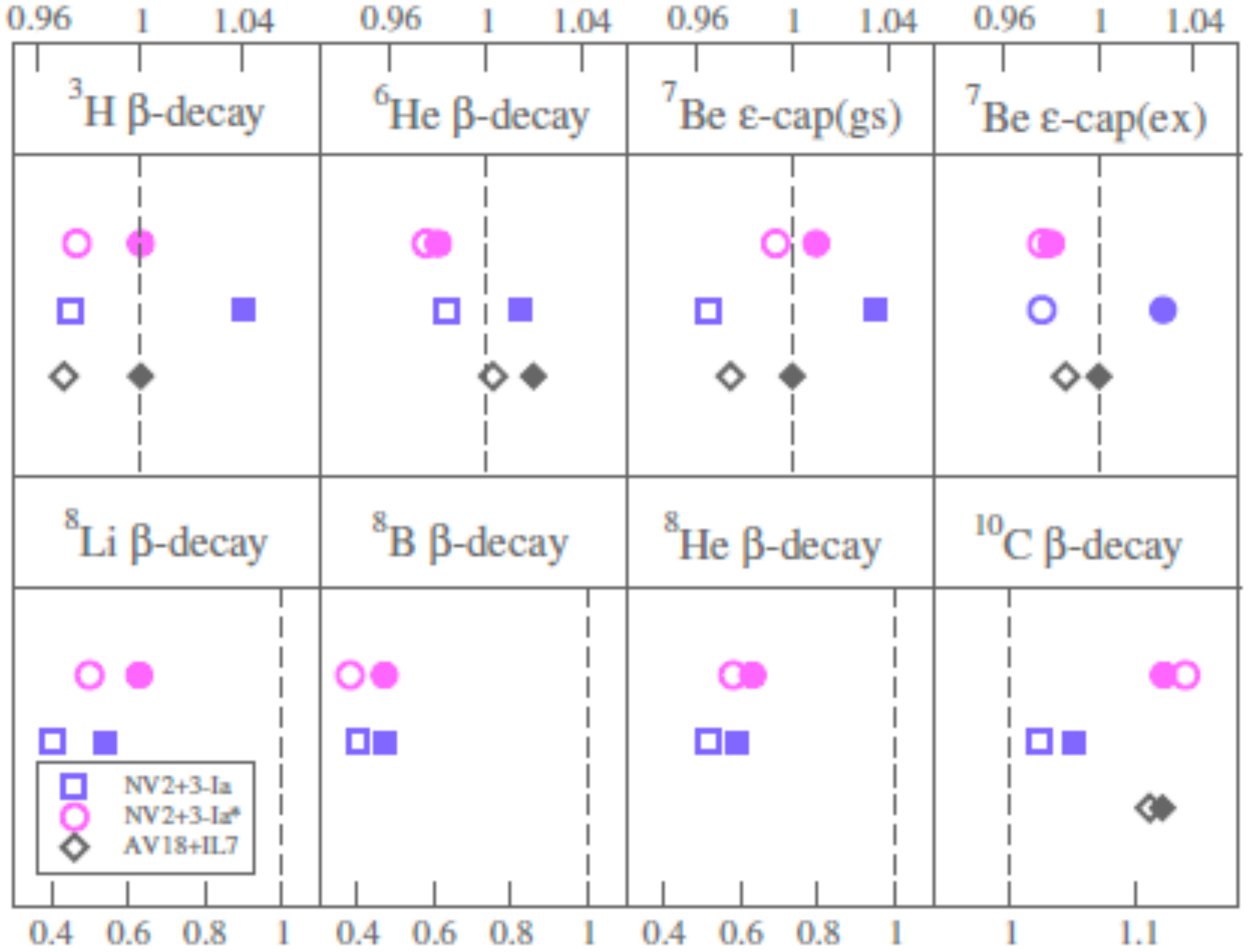


gfmc (1b) and gfmc (1b+2b); shell model (1b)

GFMC calculations using AV18/IL7 (rather then chiral) and axial χEFT currents— hybrid calculation

Pastore et al. PRC **97** 022501 (2018)

G. King *et al.* PRC 102, 025501 (2020)



GFMC calculations using chiral and axial χEFT currents— consistent calculation

Neutrinoless Double Beta Decay

In the hypothesis that the 0νDBD is mediated by the exchange of a light neutrino:

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

Javier Menendez arXiv:1703.08921 (2017)

Lepton space-phase integral

- Depends on the Q-value of the decay and the charge of the final state of the nucleus
- Can be calculated precisely: for most of the emitters of interest

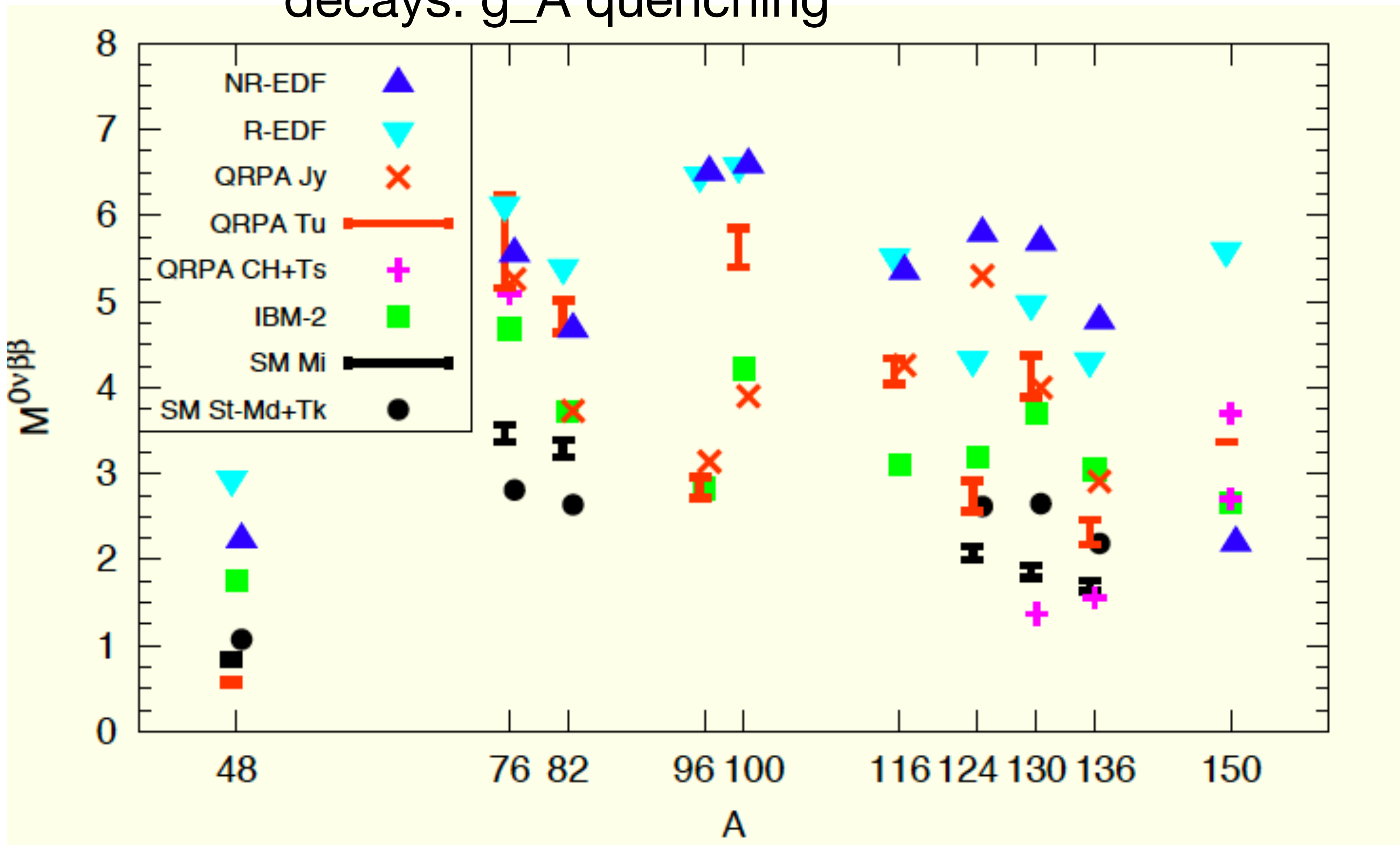
$$10^{-15} - 10^{-16}\text{yr}^{-1}$$

Nuclear matrix element (NME)

- Open issues for theorists
- Spread of about a factor 2-3 in the predicted values for NME for a given isotope
- Theoretical predictions for these models compared with single beta decays: g_A quenching

Effective Majorana mass

- Depends on combination of neutrino masses and oscillation parameters
- Uncertainties in the parameters extracted by oscillation experiments and cosmology



Neutrinoless double-beta decay

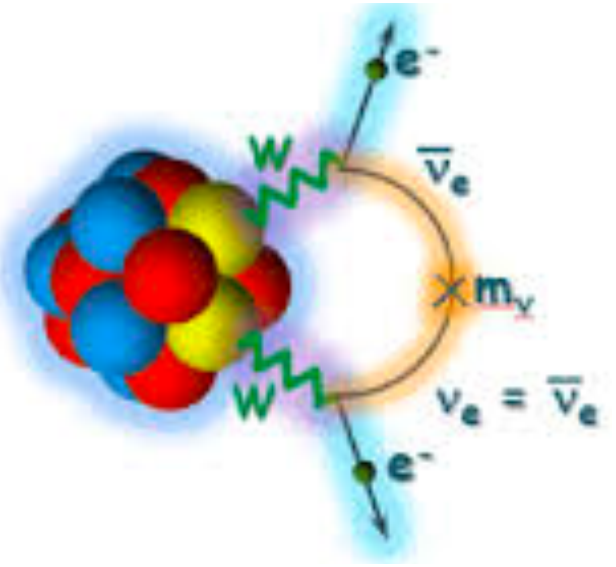
- OvDBD: decay mode with the emission of two electrons but without the associated neutrinos:

  Light-neutrino exchange

  Supersymmetric particle exchange

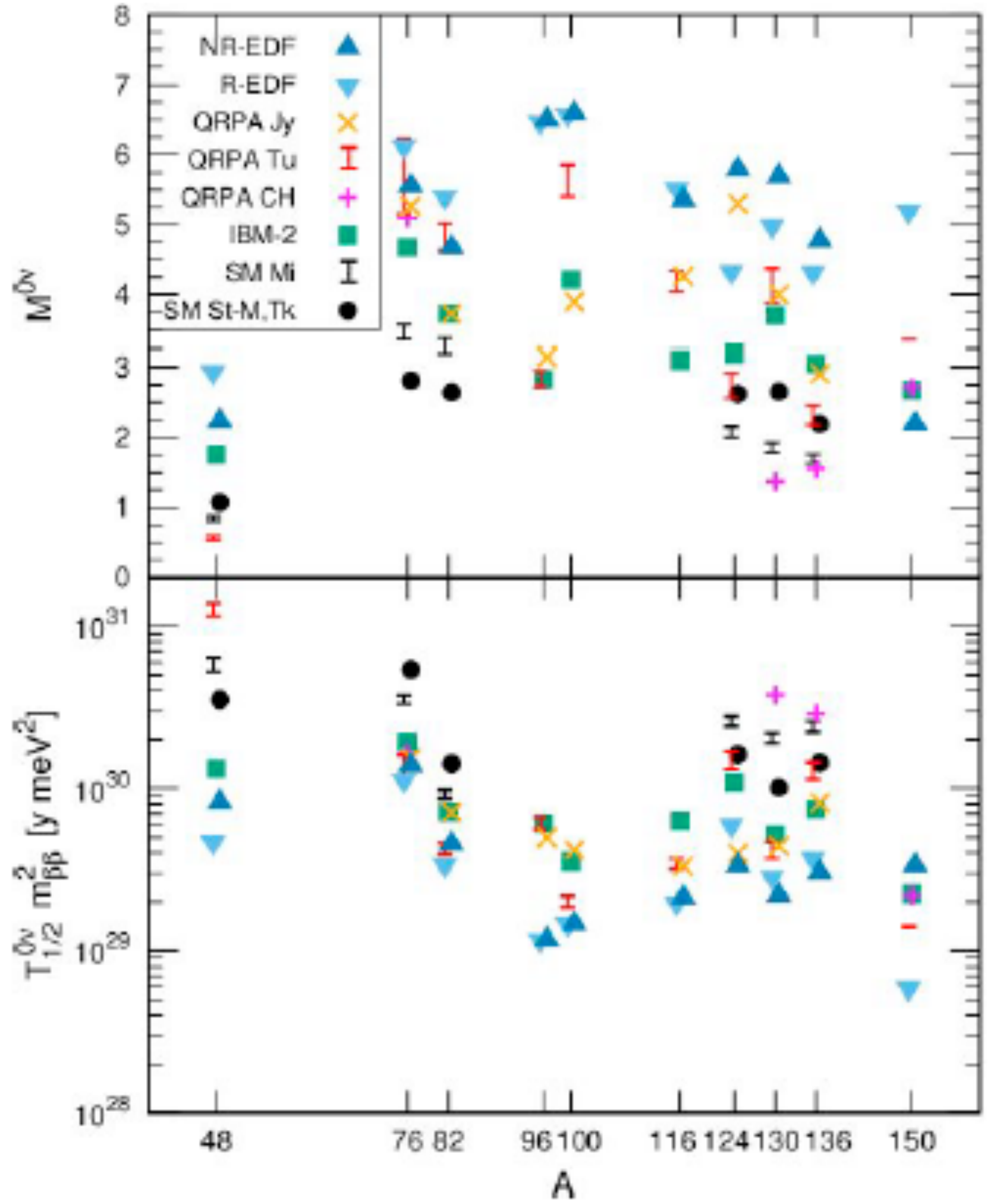
  Emission of Majorons (heavy bosons)

  ……..



W. Furry, Phys. Rev. 56 1134 (1939).

- Neutrino physics: Majorana particles
- Lepton number violation
- B-L number violation: relevant to explain asymmetry matter-antimatter



- Matrix elements for nuclei of experimental interest are currently affected by large uncertainties due to truncation in the model space and partial (or missing) inclusion of many-body effects

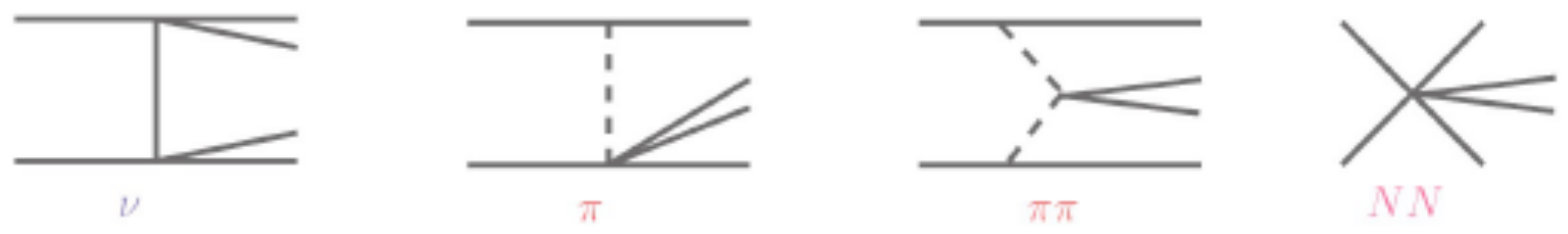
- We study neutrinoless double beta decay in light nuclei that have been successfully described by ab initio models where correlations and currents can be fully accounted for

- These studies serve as benchmark and to establish the relevance of the various two-body (or more) dynamics inducing the decay

Engel and Menéndez, Rep. Prog. Phys. 80 046301 (2017)

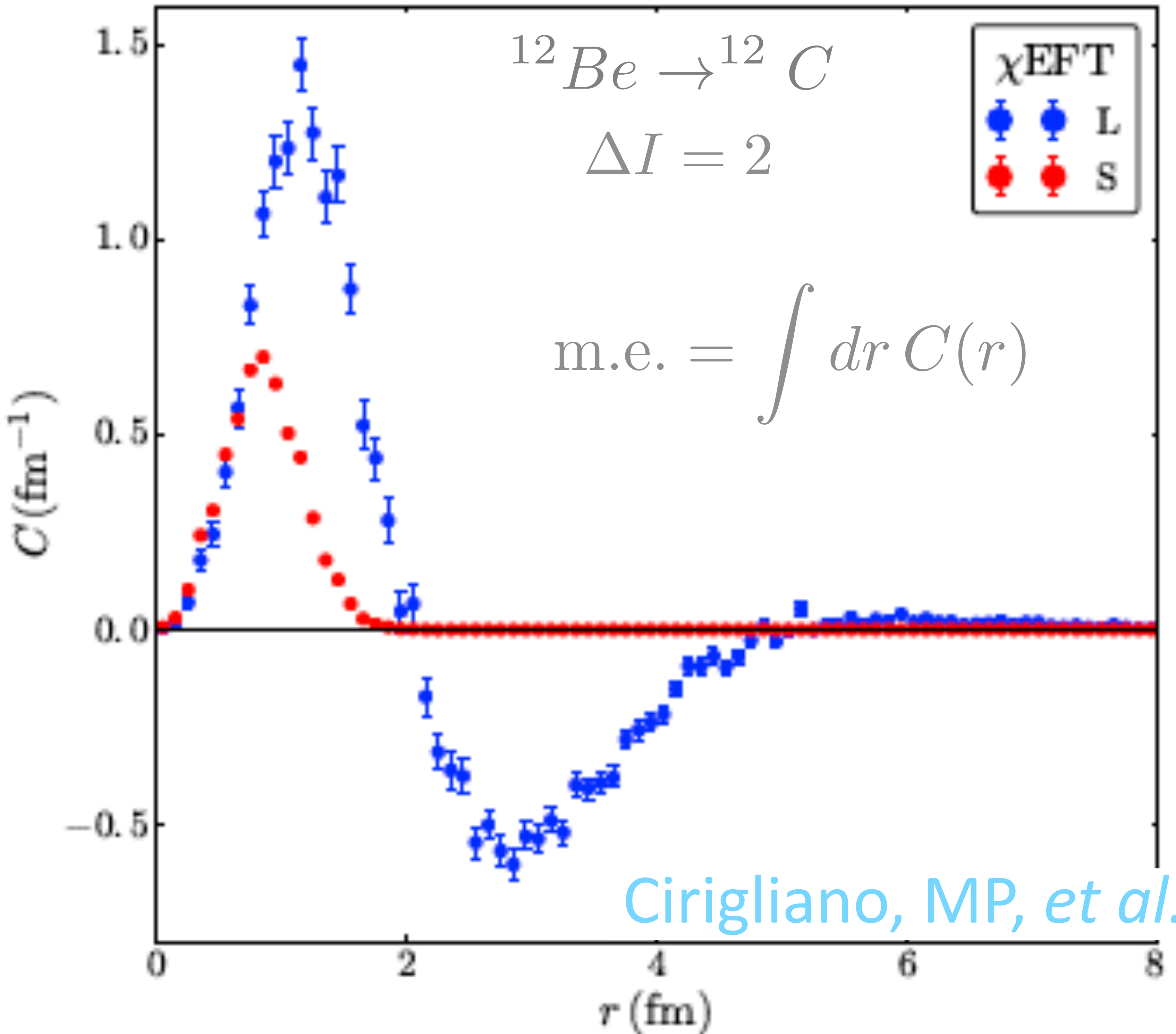
Neutrinoless double beta matrix elements

- 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 $\sim$ 200 MeV



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

- Study impact of short-range versus long-range neutrino potential: $C(r) = C_L(r) + C_S(r)$l
- The CIB counter term extracted from potential: $g^{\nu}_{NN} = C_{\mathrm{CIB}}$



- ΔI=2 transitions: orthogonal initial and final-state wave functions
- Feature of all isotopes of experimental interest: 48Ca, 76Ge, 136Xe
- Presence of nodes in the long-range transition densities
- 100% corrections to ΔI=2 transitions from: g^{ν}_{NN}
- If similar in heavier nuclei: large impact on neutrino mass extractions

Cirigliano, MP, *et al.* Phys. Rev. C 100, 055504 (2019)

A	Model	M_F	M_{GT}	M_T	M_L	M_S
6	AV18	1.56	−3.66	0.03	7.45	0.48
	χEFT	1.62	−3.85	0.03	7.82	1.15
12	AV18	0.198	−0.349	0.068	0.653	0.518
	χEFT	0.223	−0.394	0.083	0.725	0.533

Partial Muon Capture in Light Nuclei

Weak-interaction Hamiltonian

$$H_W = \frac{G_V}{\sqrt{2}} \int d\mathbf{x} e^{-i\mathbf{k}_\nu \cdot \mathbf{x}} \tilde{l}_\sigma(\mathbf{x}) j^\sigma(\mathbf{x})$$

- Momentum transfer q~100MeV
- Validation of vector and axial charges and currents
- For light nuclei, you can approximate the muon as at rest in a Hydrogen-like 1s orbital

$$\Gamma = \frac{G_V^2}{2\pi} \frac{|\psi_{1s}^{\text{av}}|^2}{(2J_i+1)} \frac{E_\nu^{*2}}{\text{recoil}} \sum_{M_f, M_i} |\langle J_f, M_f | \rho(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2 + |\langle J_f, M_f | \mathbf{j}_z(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2$$

$$+ 2\,\text{Re}\left[\langle J_f, M_f | \rho(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle \langle J_f, M_f | \mathbf{j}_z(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle^* \right] + |\langle J_f, M_f | \mathbf{j}_x(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2$$

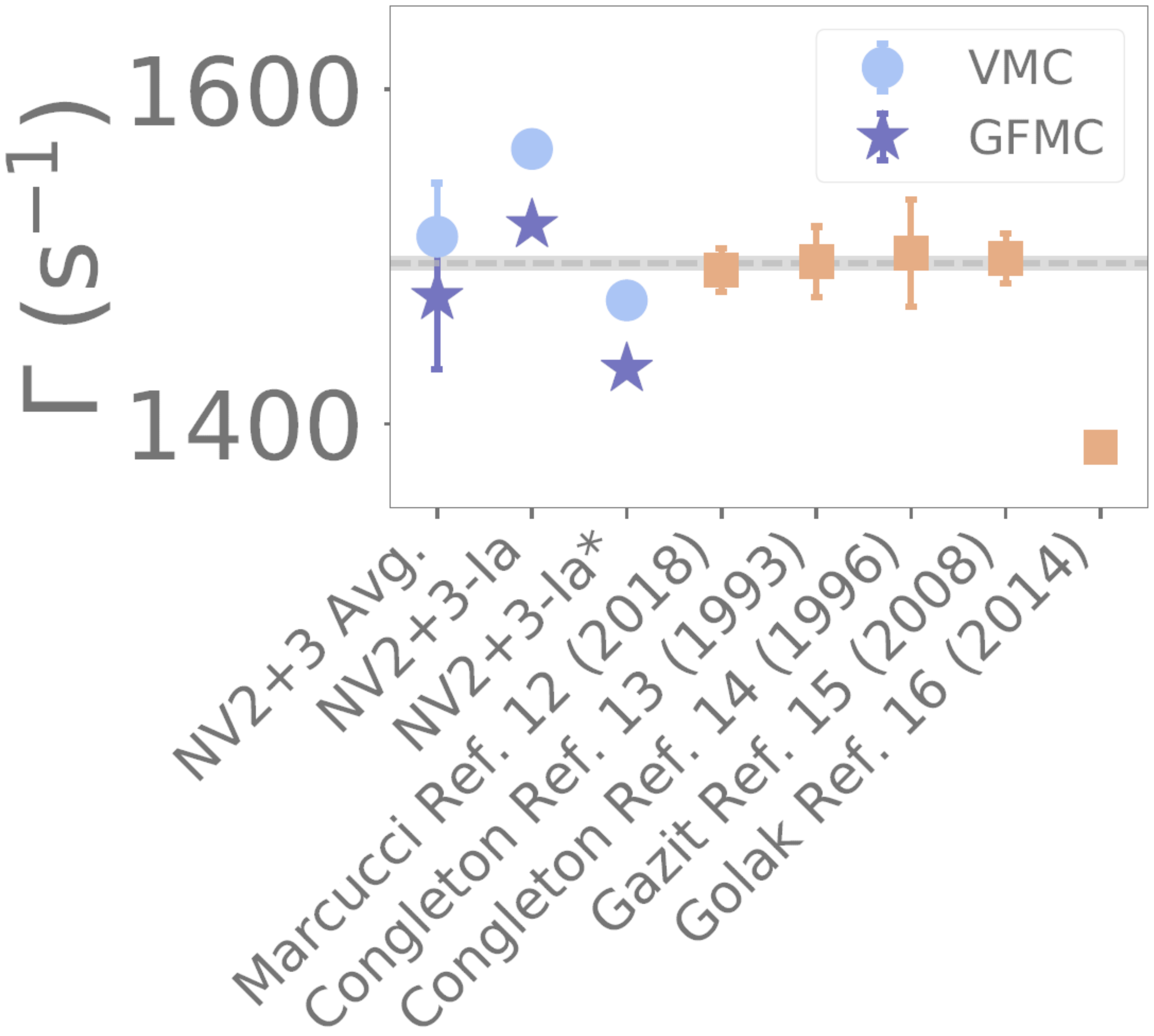
$$+ |\langle J_f, M_f | \mathbf{j}_y(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle|^2 - 2\,\text{Im}\left[\langle J_f, M_f | \mathbf{j}_x(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle \langle J_f, M_f | \mathbf{j}_y(E_\nu^* \hat{\mathbf{z}}) | J_i, M_i \rangle^* \right.$$

Partial Muon Capture Rates with QMC: $^3\mathrm{He}(\mu^-, \nu_\mu)^3\mathrm{H}$

Momentum transfer q~100 MeV

- QMC rate for ^{3}He(1/2$^+$;1/2) → ^{3}H(1/2$^+$;1/2)
  - Γ_{VMC} = 1512 s^{-1} ± 32 s^{-1}
  - Γ_{GFMC} = 1476 s^{-1} ± 43 s^{-1}
  - Γ_{expt} = 1496.0 s^{-1} ± 4.0 s^{-1}

  [Ackerbauer et al. Phys. Lett. B417 (1998)]



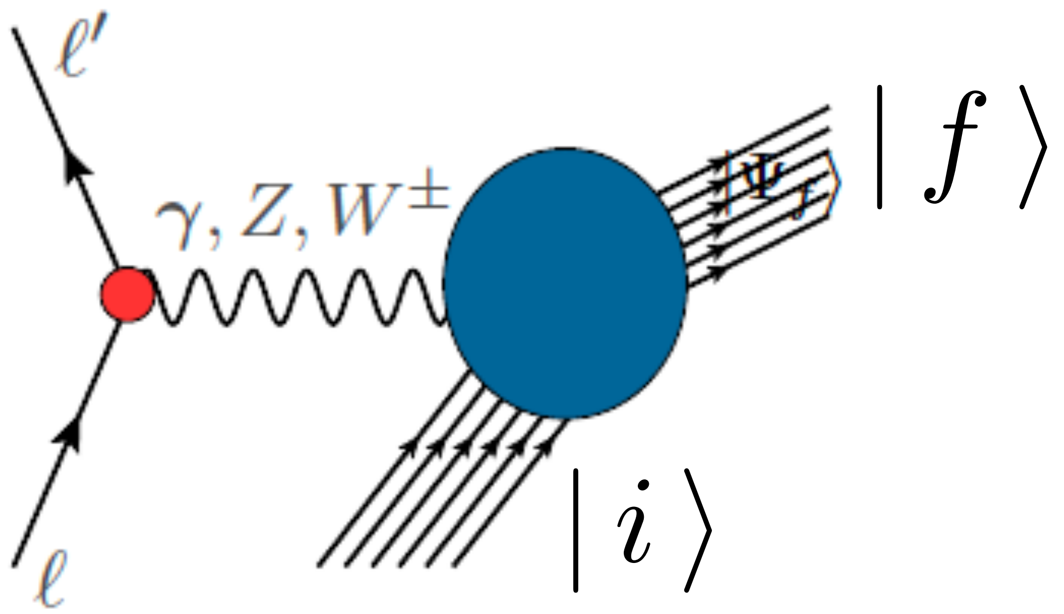
- The inclusion of 2b electroweak currents increase the rate by about 9% to 16%.

- uncertainty estimates:

  - Cutoff: 8 s^{-1} (0.5%)
  - Energy range of fit: 11 s^{-1} (0.7%)
  - Three-body fit: 27 s^{-1} (1.8%)
  - Systematic: 9 s^{-1} (0.6%)

King et al. PRC 105 (2022) 4, L042501

Lepton-Nucleus Scattering: Inclusive Processes



- Inclusive lepton scattering off a the nucleus: five response functions

$$\frac{d\sigma}{d\epsilon_l' d\Omega_l} \propto \left[v_{00}\, R_{00} + v_{zz}\, R_{zz} - v_{0z}\, R_{0z} + v_{xx}\, R_{xx} \mp v_{xy}\, R_{xy} \right]$$

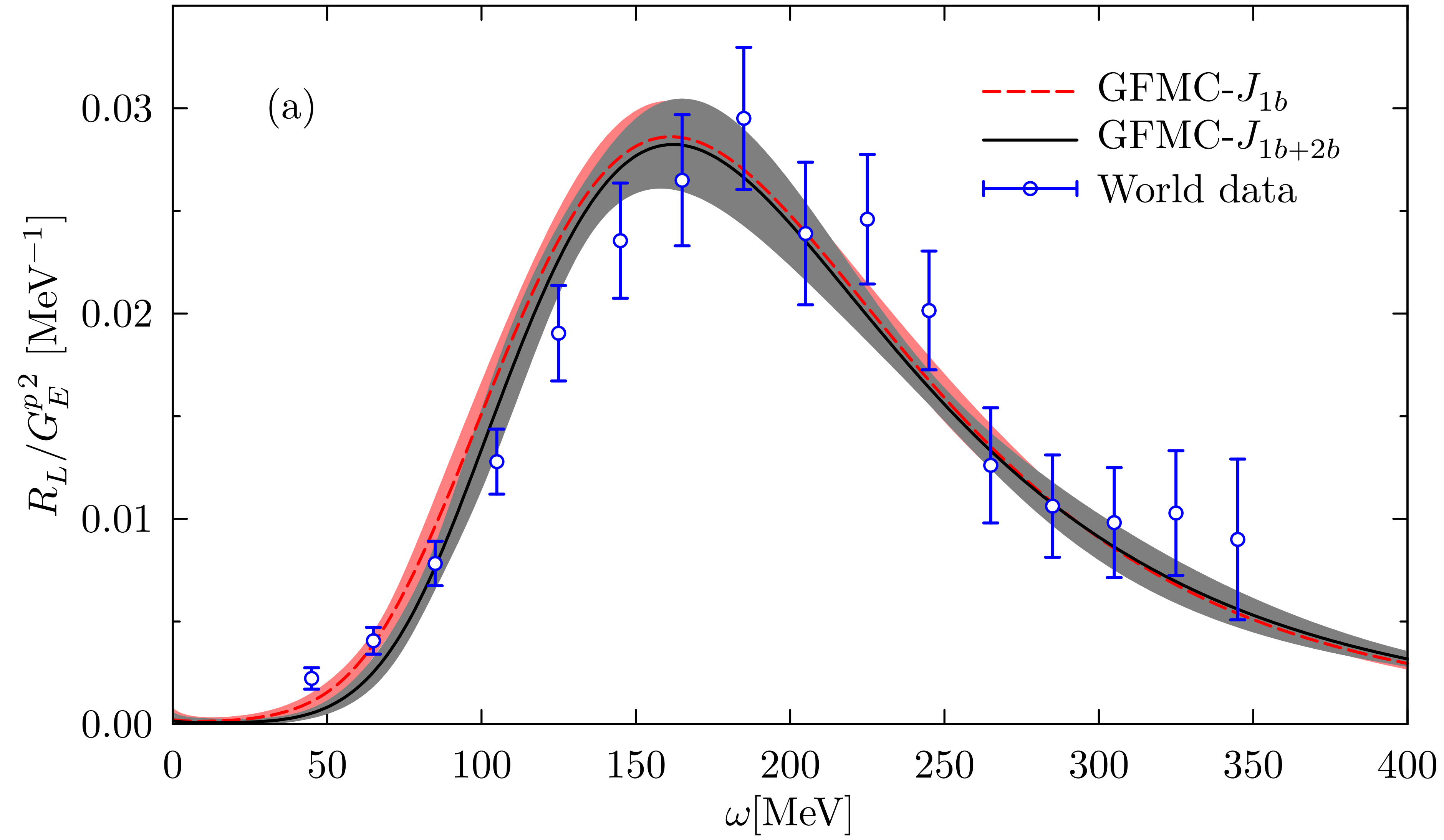
- For the EM case only two response functions survive: longitudinal R_{00} and transverse R_{xx} which are obtained from the charge and transverse current operators $R_\alpha(q,\omega) = \sum_f \delta\left(\omega + E_0 - E_f\right) |\langle\, f | O_\alpha(\mathbf{q}) | 0 \rangle|^2$ $\quad O_L = \rho$, $O_T = \boldsymbol{j}$

Euclidean response: GFMC calculations

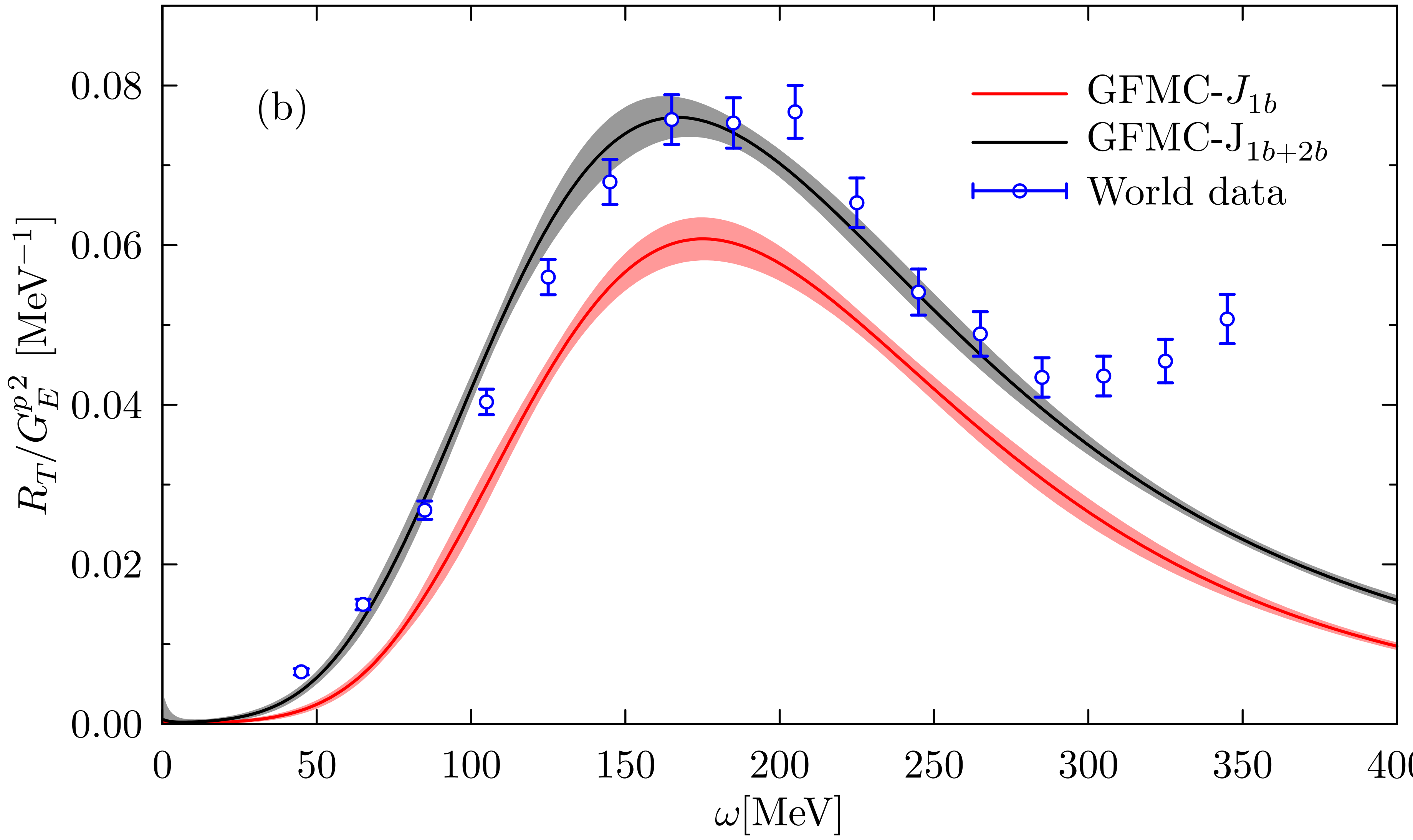
$$\int_0^\infty d\omega\, e^{-\tau\omega}\, R_{\alpha\beta}(q,\omega) = \langle i |\, j_\alpha^\dagger(\mathbf{q})\, e^{-\tau(H-E_i)}\, j_\beta(\mathbf{q})\, | i \rangle$$

Inversion back to obtain the response by maximum entropy methods

Longitudinal



Transverse

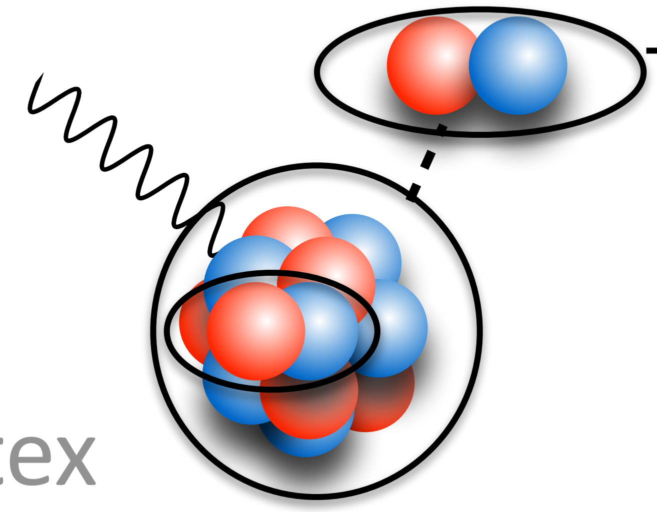


Lovato *et al.* PRL **112**, 182592 (2014) Lovato *et al.* PRC **91**, 062501 (2015) Lovato *et al.* PRL **117**, 082501 (2016)

Lepton-Nucleus Scattering: Exclusive Processes

Short-Time-Approximation:

- Based on factorization
- 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
- Describe electroweak scattering for A>12 without losing two-body physics
- Incorporate relativistic effects
- Provides “more” exclusive information in terms of nucleon-pair kinematics via the Response Densities



Response ***Functions:*** integral over real time

$$R_{\alpha\beta}(\omega,\mathbf{q}) = \int \frac{dt}{2\pi}\, e^{i(\omega+E_0)t}\langle 0|J_\alpha^\dagger(\mathbf{q})e^{-iHt}J_\beta(\mathbf{q})|0\rangle$$

The two main assumption underlying the STA are:

1. Only the one- and two-body terms are kept in the current-current correlator

$$j^\dagger(i)e^{-iHt}j(i) + j^\dagger(i)e^{-iHt}j(j) + j^\dagger(i)e^{-iHt}j(ij) + j^\dagger(ij)e^{-iHt}j(ij)$$

2. In the particle propagator the Hamiltonian is rewritten as

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{ij} v_{ij}$$

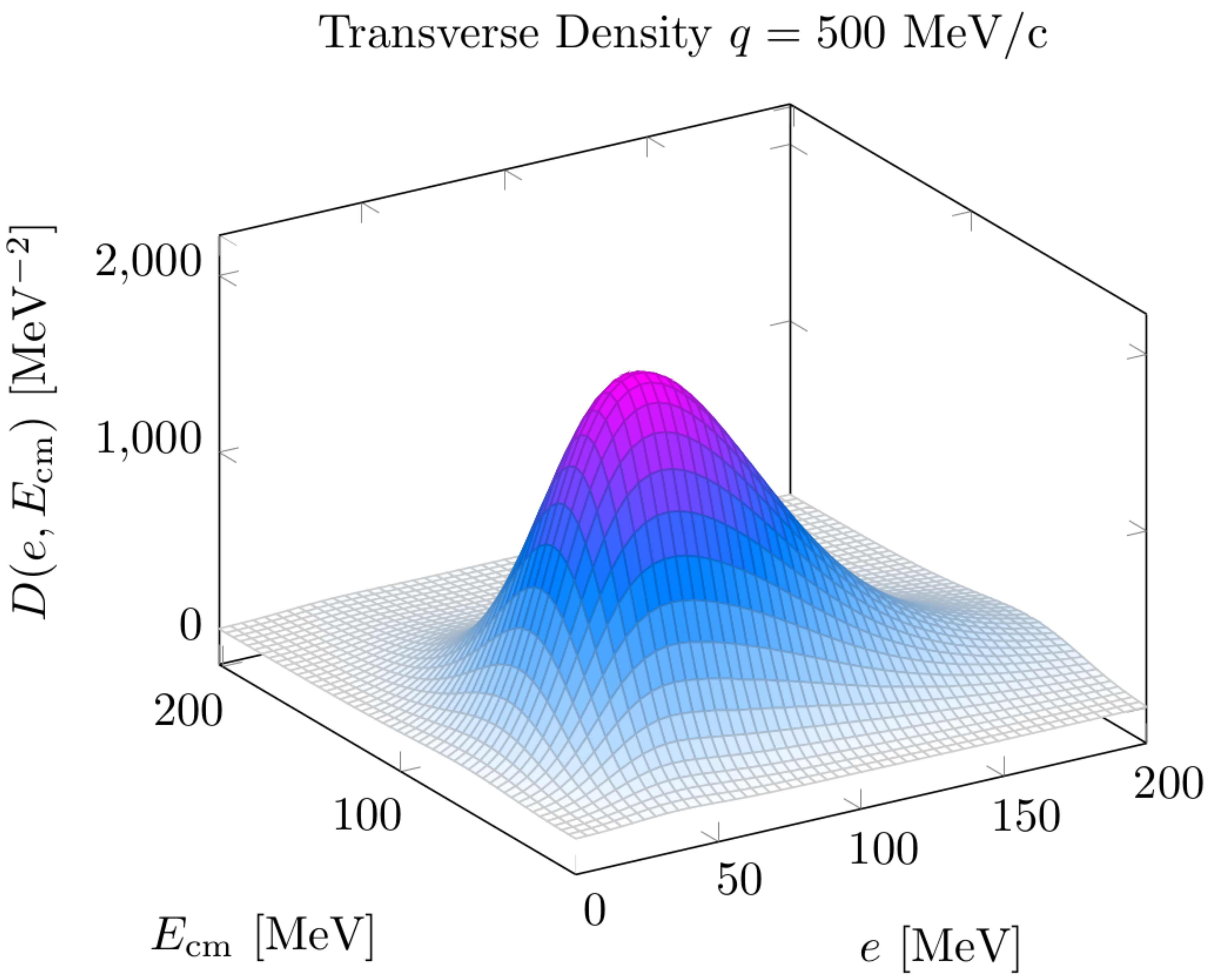
Response ***Densities:***

$$R(q,\omega) = \int_0^\infty de\, dE_{\rm cm}\delta(\omega + E_0 - e - E_{\rm cm})D(e,E_{\rm cm})$$

$E_{\rm cm}$ and *e* are the CM and relative energy of the struck nucleon pair

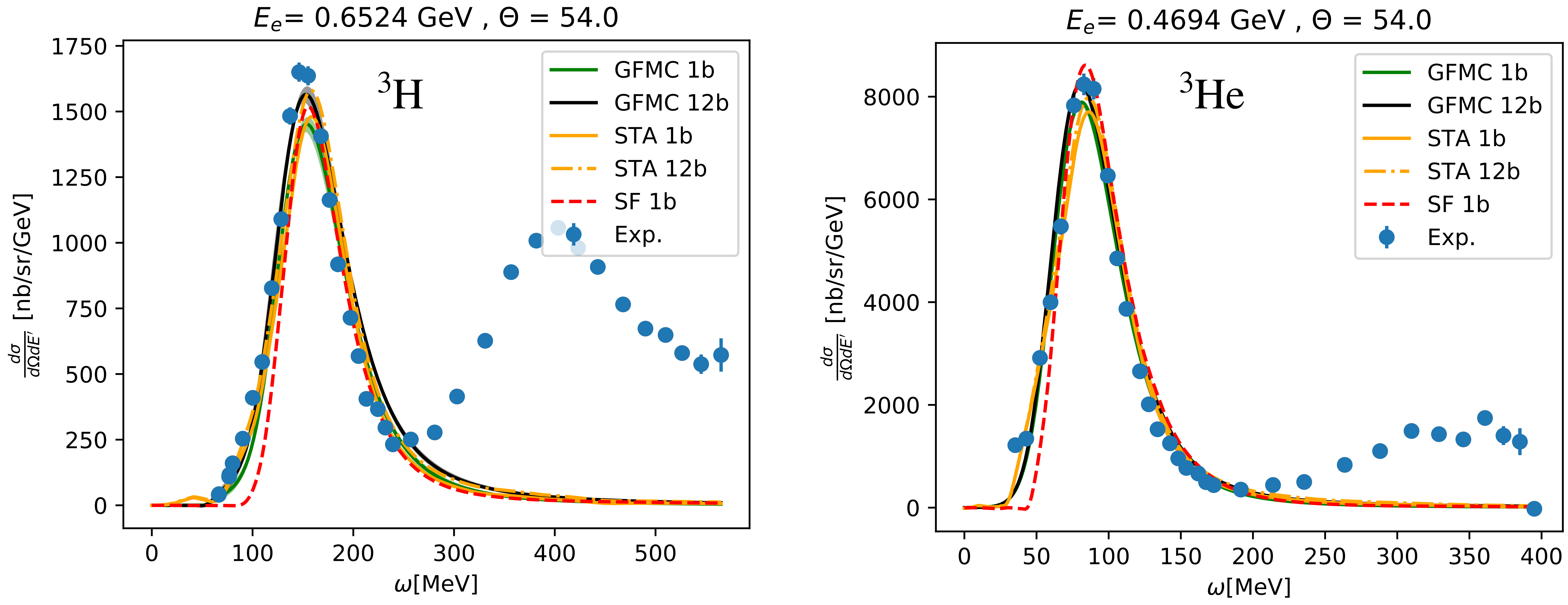
S. Pastore et al. PRC 101 (2020) 4, 044612

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



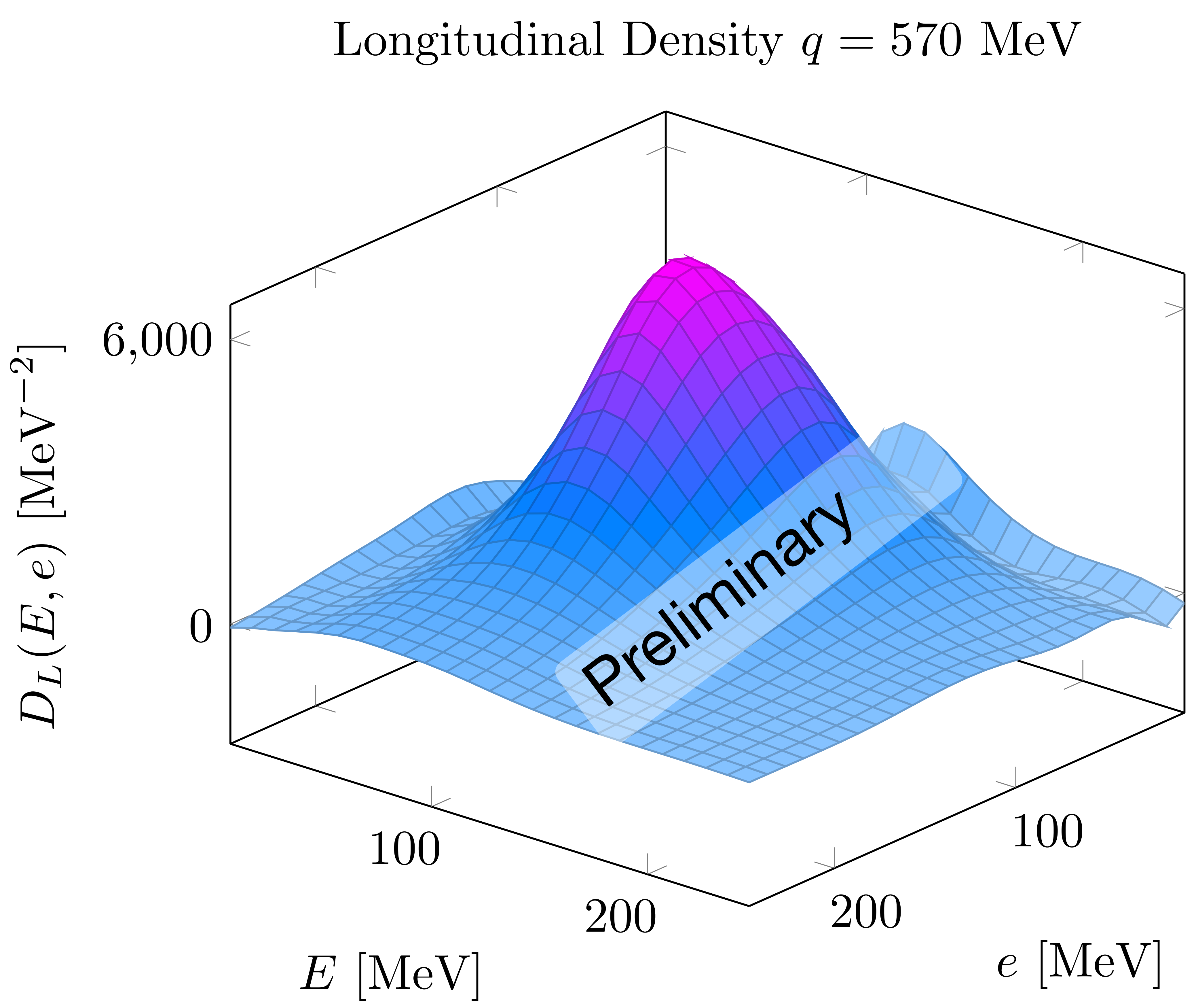
Pastore *et al.* PRC101(2020)044612

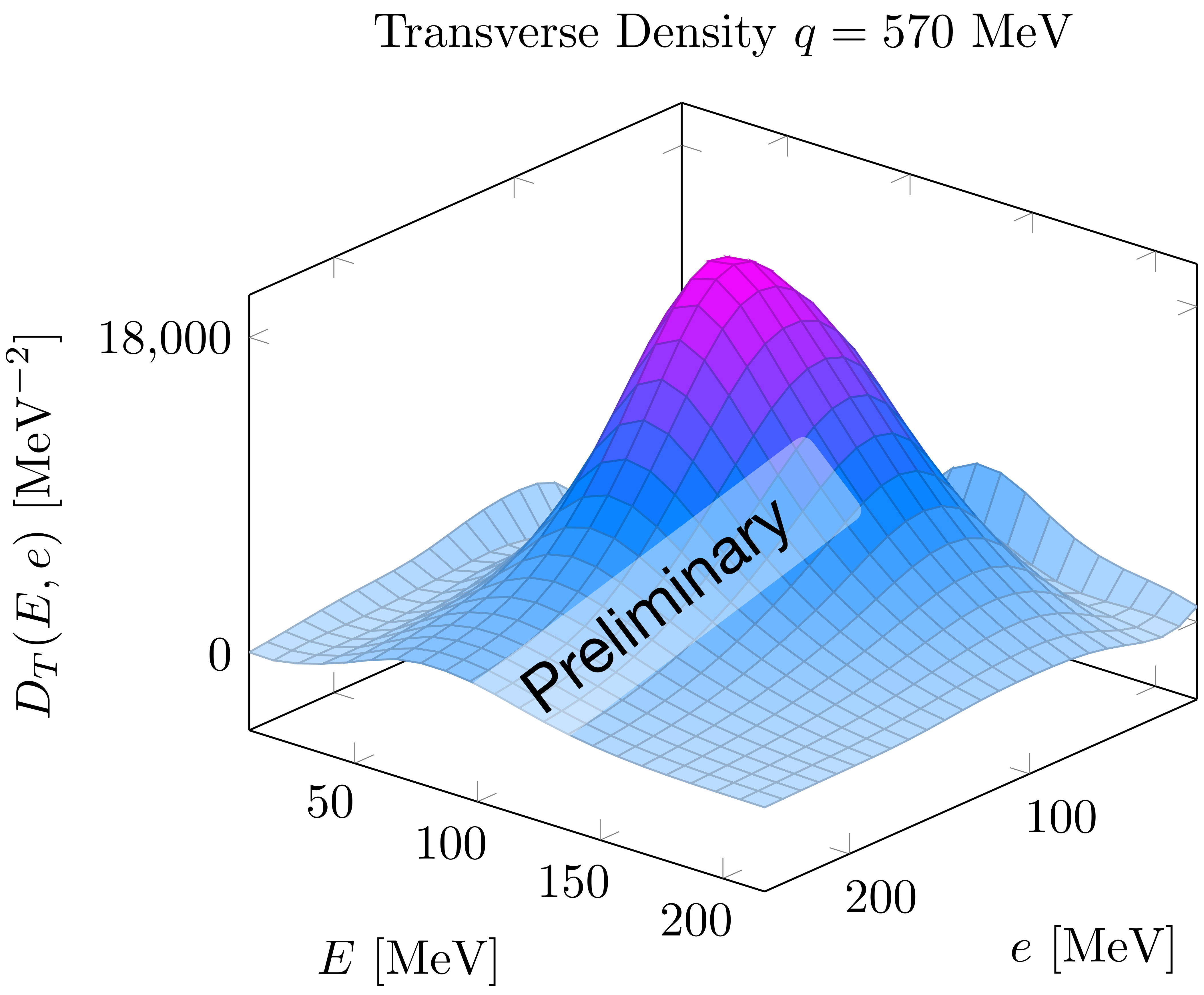
Cross sections ^3H and ^3He: benchmark between GFMC and STA



Andreoli et al. Phys. Rev. C **105**, 014002

Response densities for ^{12}C

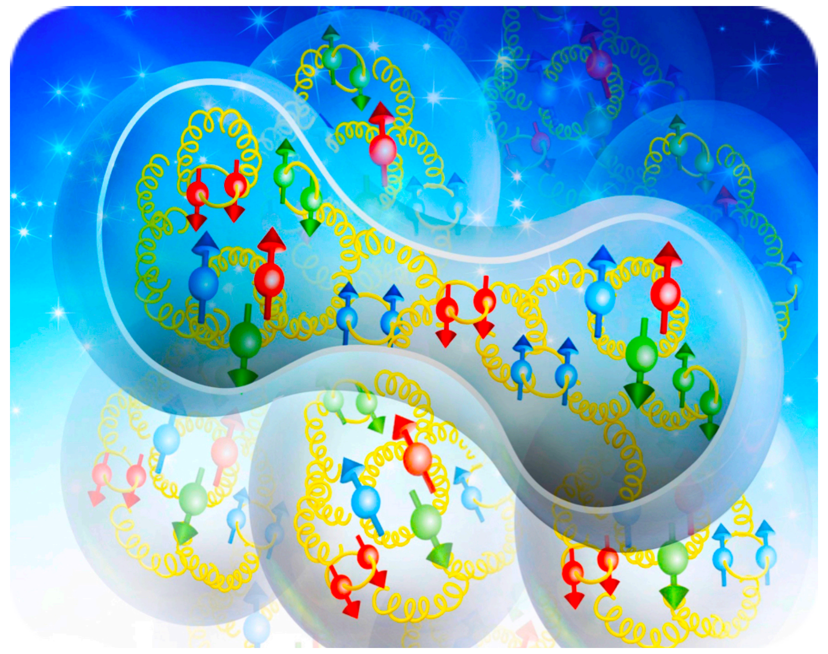


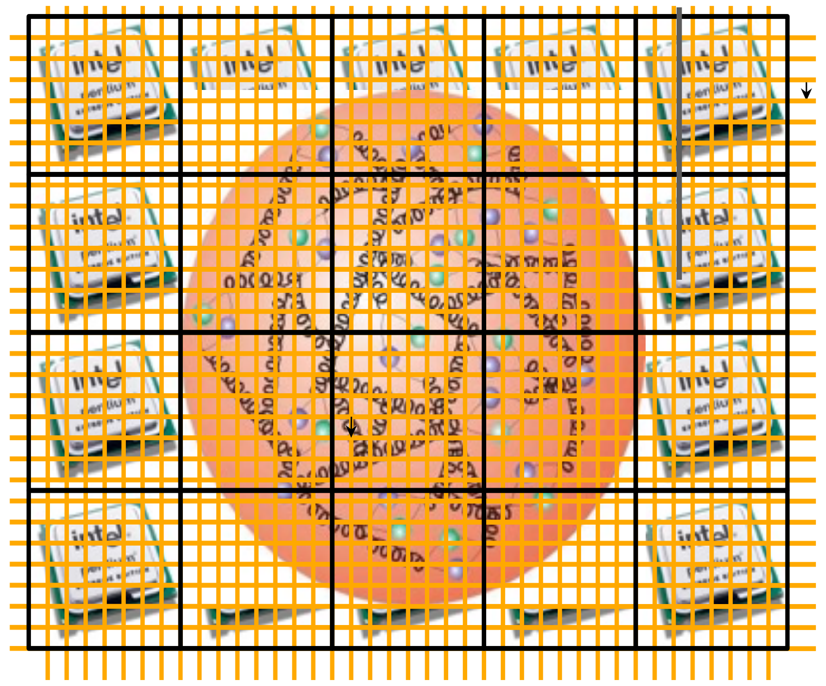


Preliminary results for longitudinal and transverse response densities in ^{12}C

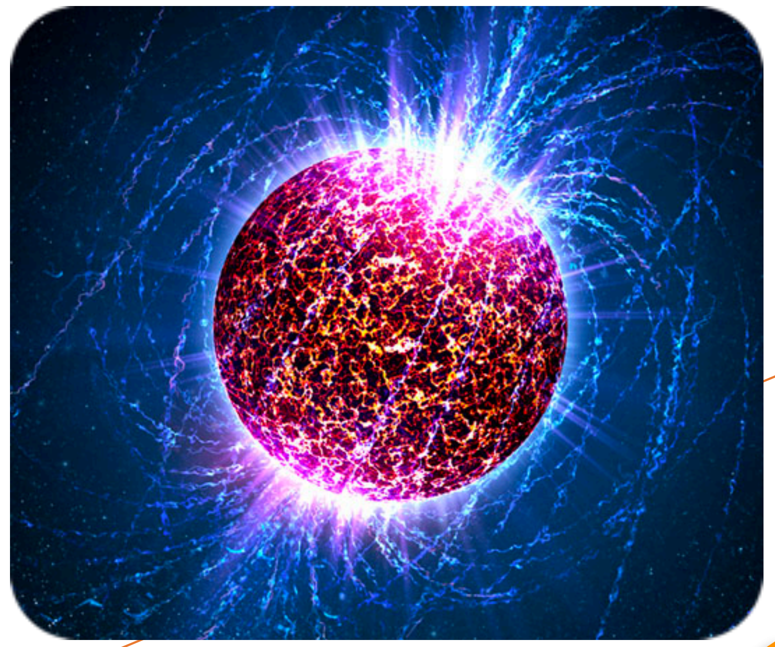
Summary: Workflow for the microscopic model nuclear theory

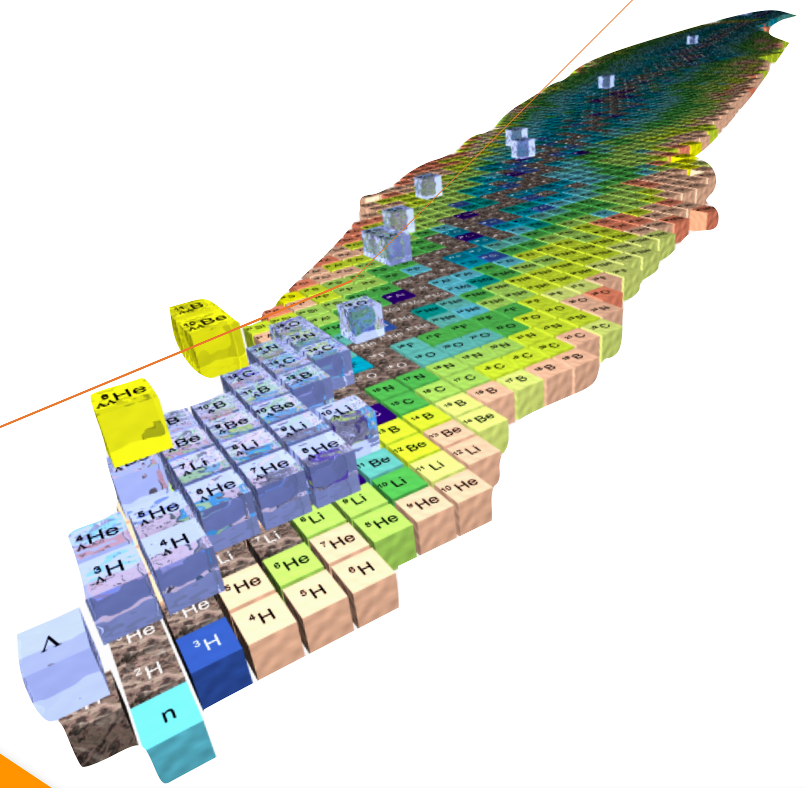
Quantum Chromodynamcs



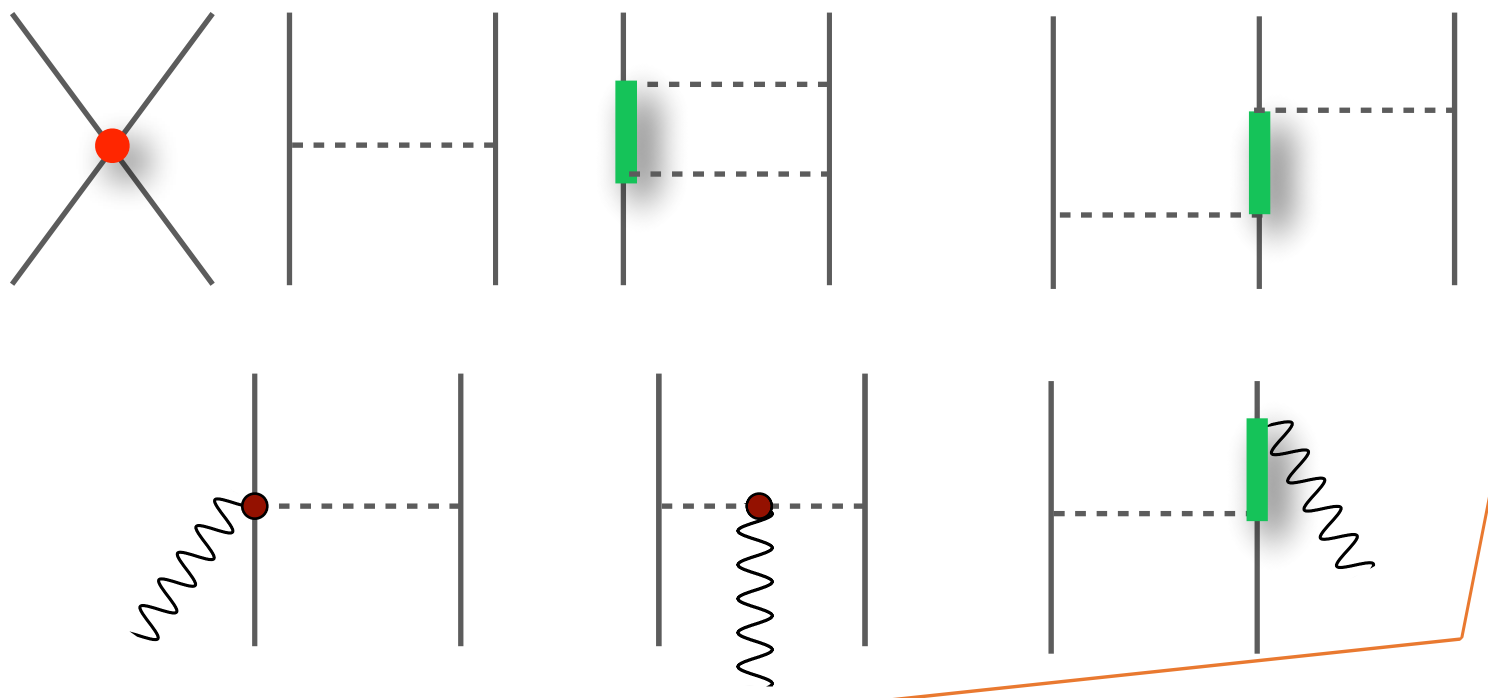


Atomic nuclei and nucleonic matter





Hamiltonian and electroweak currents



Accurate nuclear many-body methods

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

$$J_{mn} = \langle\Psi_m|J|\Psi_n\rangle$$

THANK YOU!!!