Chiral Nuclear Interactions for QMC Methods

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Quantum Monte Carlo Group for Nuclear Physics

OUR RESEARCH   GROUP MEMBERS

The QMC Group for Nuclear Physics is focused on understanding how nuclear properties emerge from the underlying nucleonic dynamics, with the broader goal of contributing to ongoing experimental efforts in nuclear physics, fundamental symmetries, neutrino physics, and astrophysics.

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Computational resources awarded by the DOE ALCC and INCITE programs

FRIB Theory Alliance

Argonne NATIONAL LABORATORY

SciDAC Scientific Discovery through Advanced Computing

NUCLEI Nuclear Computational Low-Energy Initiative

Microscopic calculations of nuclear systems

- OUR GOAL

Understand nuclear systems from a microscopic point of view, in terms of the interactions between individual nucleons and external probes

Nucleon-nucleon (NN) and 3N scattering data: "thousands" of experimental data available

Spectra, properties, and transition of nuclei: BE, radii, magnetic moments, beta decays rates, weak/radiative captures, electroweak form factors, etc,…

Nucleonic matter equation of state: for ex. EOS neutron matter

- WHAT WE NEED!

Two and many-body interactions:

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

Electroweak current operators:

$$j^{\rm EW} = \sum_{i=1}^{A} j_i + \sum_{i<j=1}^{A} j_{ij} + \sum_{i<j<k=1}^{A} j_{ijk} + \ldots.$$

Accurate many-body method:

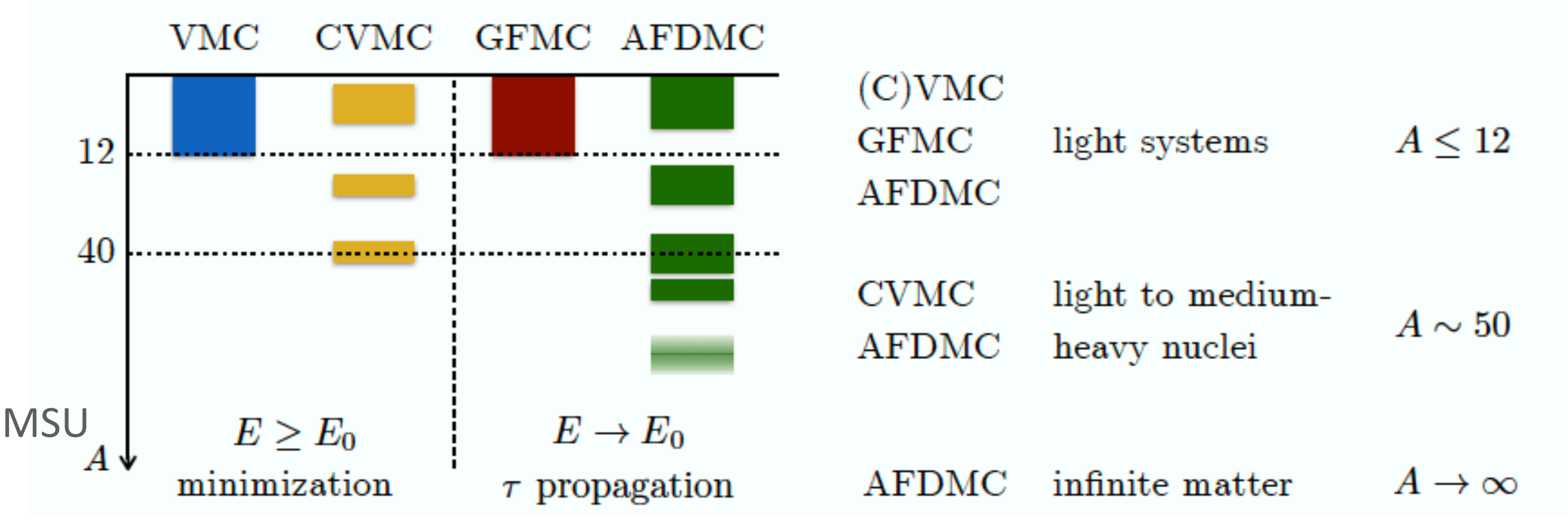
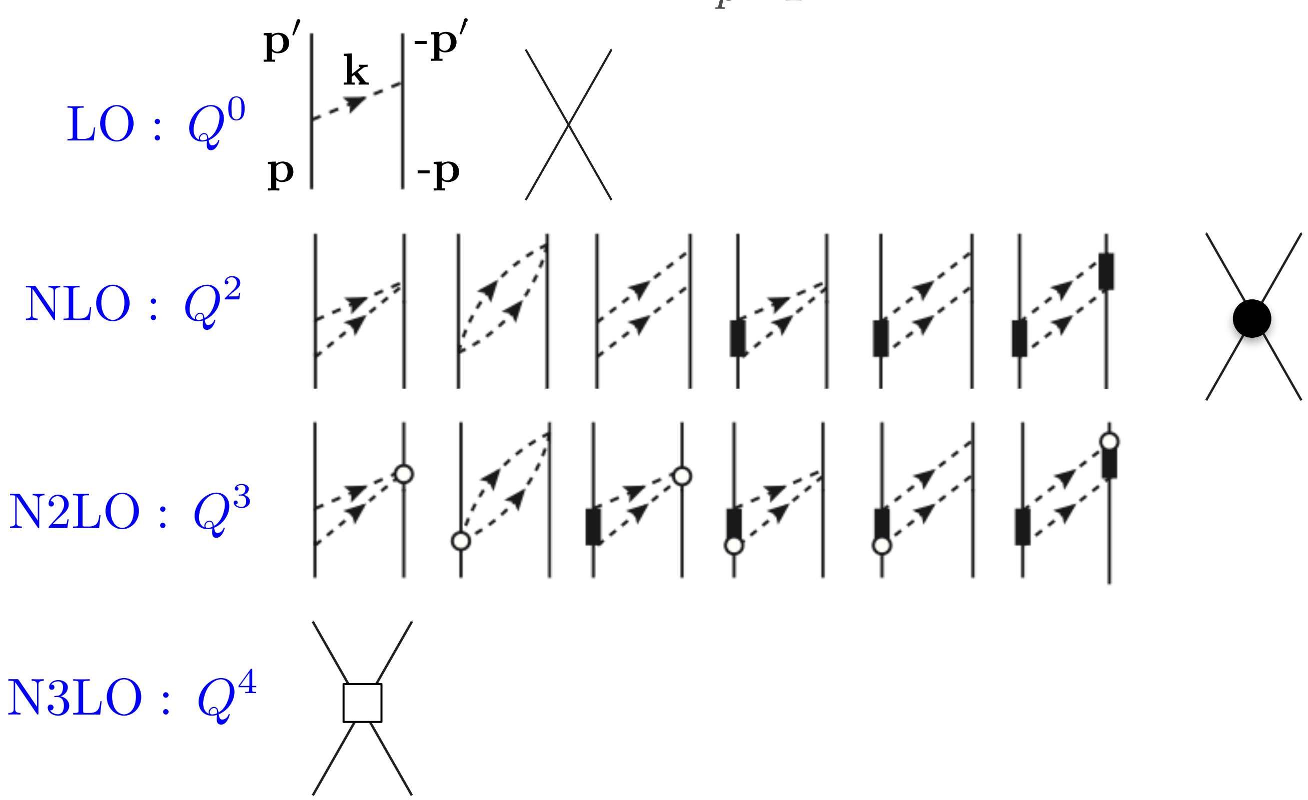


Figure by Diego Lonardoni, LANL & MSU

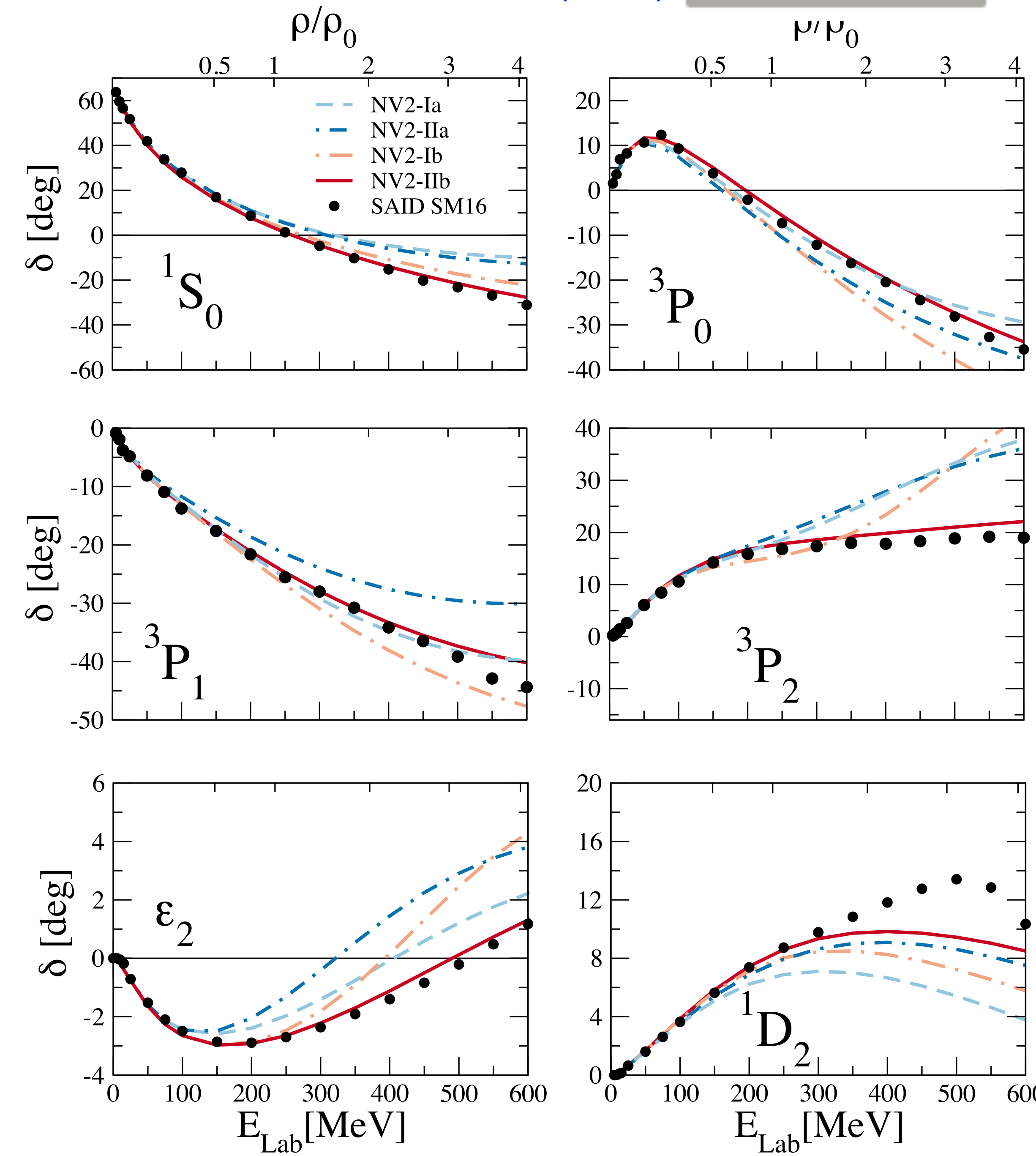
Local chiral NN Hamiltonian with Δ's

- Local NN potentials including N2LO Δ-contributions and N3LO contacts have ben also devised and expressed as a sum of 16 spin-isospin operators

$$v_{ij} = v_{ij}^{\mathrm{EM}} + v_{ij}^{\mathrm{L}} + v_{ij}^{\mathrm{S}} = \sum_{p=1}^{16} v^p(r_{ij}) O_{ij}^p$$



MP et al. PRC **101**, 045801 (2020) Editors' Suggestion



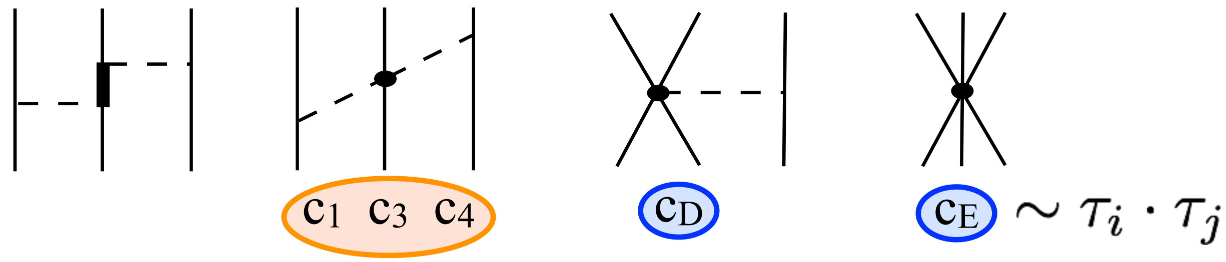
- Contact component parametrized by 26 LECs:
  - the functional form taken as $C_{R_S}(r) \propto e^{-(r/R_S)^2}$ with $R_S = 0.8\ (0.7)$ fm a (b) models
  - models a (b) cutoff~500 MeV (600 MeV) in p-space

model	order	E_{Lab} (MeV)	N_{pp+np}	χ^2/datum
Ia	N3LO	0–125	2668	1.05
Ib	N3LO	0–125	2665	1.07
IIa	N3LO	0–200	3698	1.37
IIb	N3LO	0–200	3695	1.37

MP et al. PRC **91**, 024003 (2015); PRC **94**, 054007 (2016)

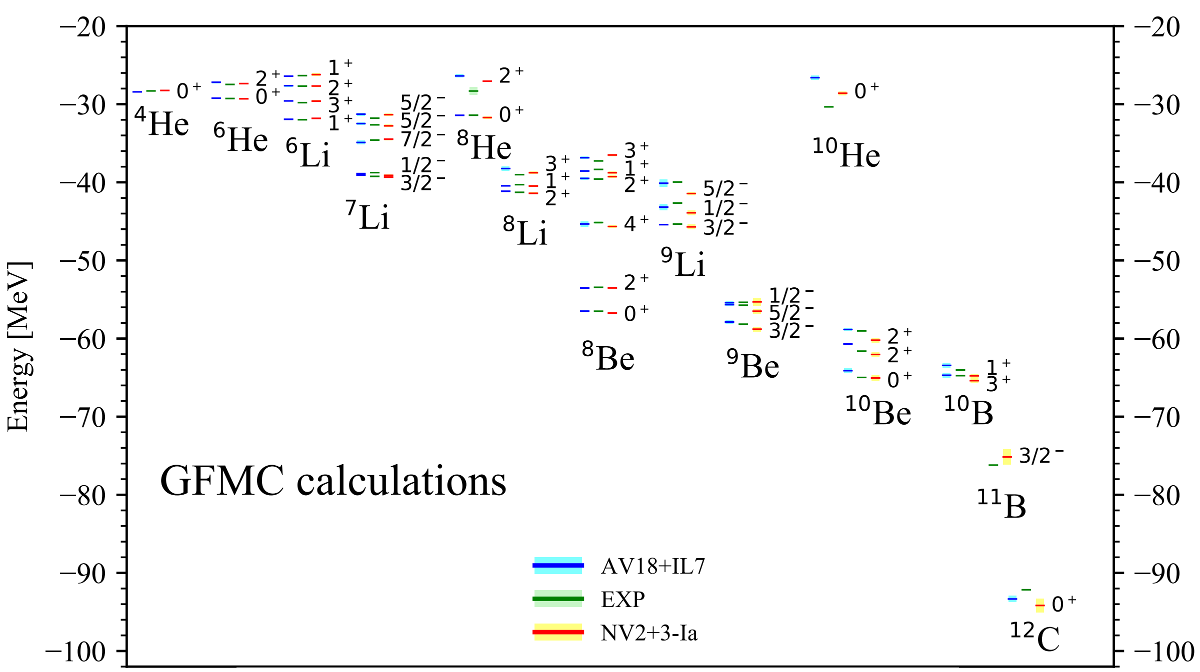
Local chiral NNN Hamiltonian with Δ's

- Inclusion of 3N forces at N2LO: $V_{ijk} = V^{2\pi}_{ijk} + V^{CT}_{ijk}$



1) Fit to:
- $E_0(^3\text{H}) = -8.482$ MeV
- $^2a_{nd} = (0.645 \pm 0.010)$ fm

Model	c_D	c_E
Ia	3.666	–1.638
Ib	–2.061	–0.982
IIa	1.278	–1.029
IIb	–4.480	–0.412

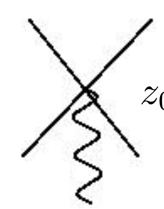


MP *et al.* PRL **120**, 052503 (2018)

GT m.e. in ^{3}H β-decay are ~3-4% away from exp data

2) Fit to:
- $E_0(^3\text{H}) = -8.482$ MeV
- GT m.e. in ^{3}H β-decay

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)



$$z_0 = \frac{g_A}{2}\frac{m_\pi^2}{f_\pi^2}\frac{1}{(m_\pi R_S)^3}\left[-\frac{m_\pi}{4\,g_A\,\Lambda_\chi}c_D + \frac{m_\pi}{3}(c_3 + 2\,c_4) + \frac{m_\pi}{6\,m}\right]$$

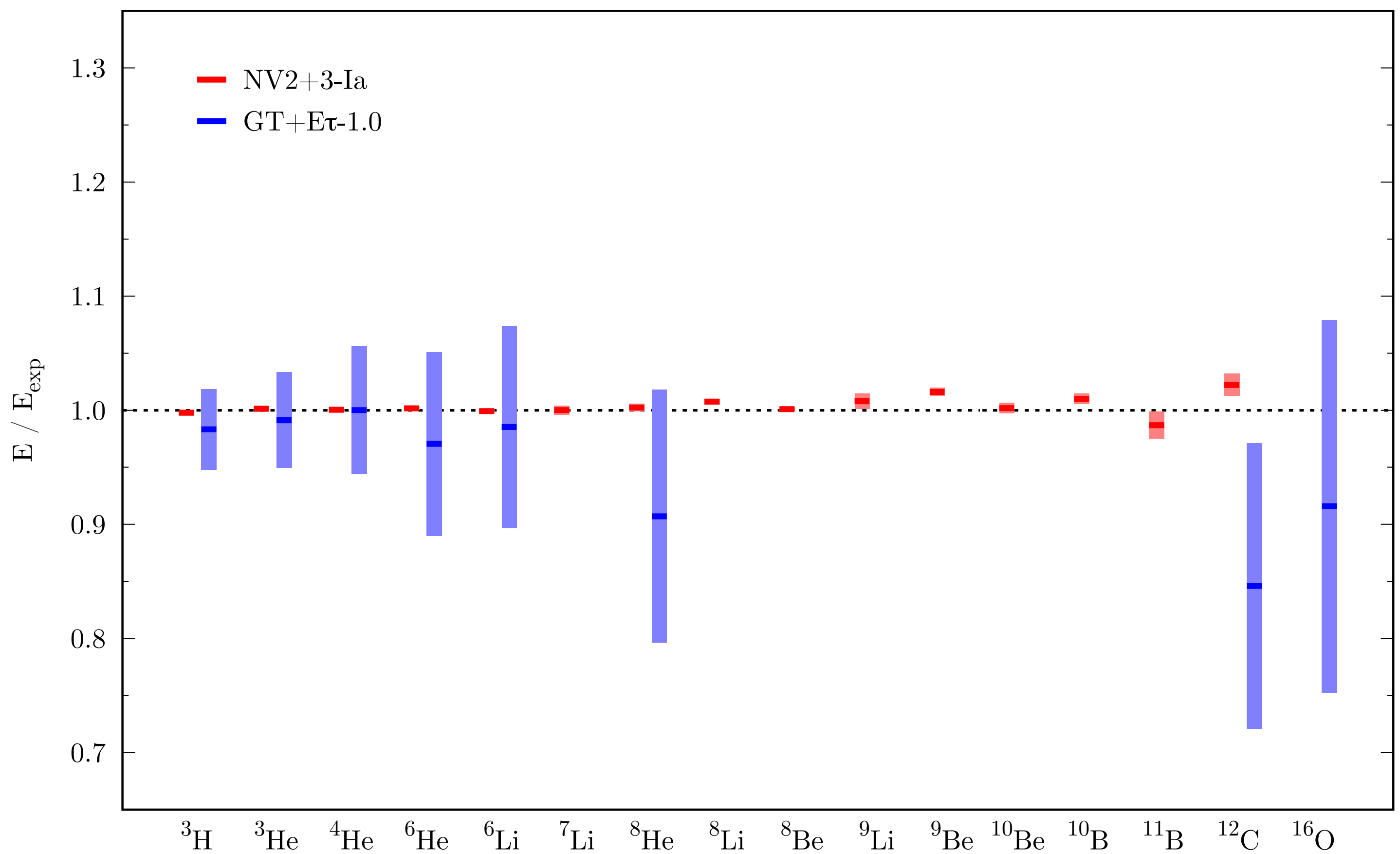
	Ia*	Ib*	IIa*	IIb*
c_D^*	−0.635	−4.71	−0.61	−5.25
c_E^*	−0.09	0.55	−0.35	0.05
LO	0.9272	0.9247	0.9261	0.9263
N2LO	0.0345	0.0517	0.0345	0.0515
N3LO(OPE)	0.0327	0.0454	0.0330	0.0465
N3LO(CT)	−0.0435	−0.0715	−0.0432	−0.0737

A.Baroni *et al.* PRC **98**, 044003 (2018)

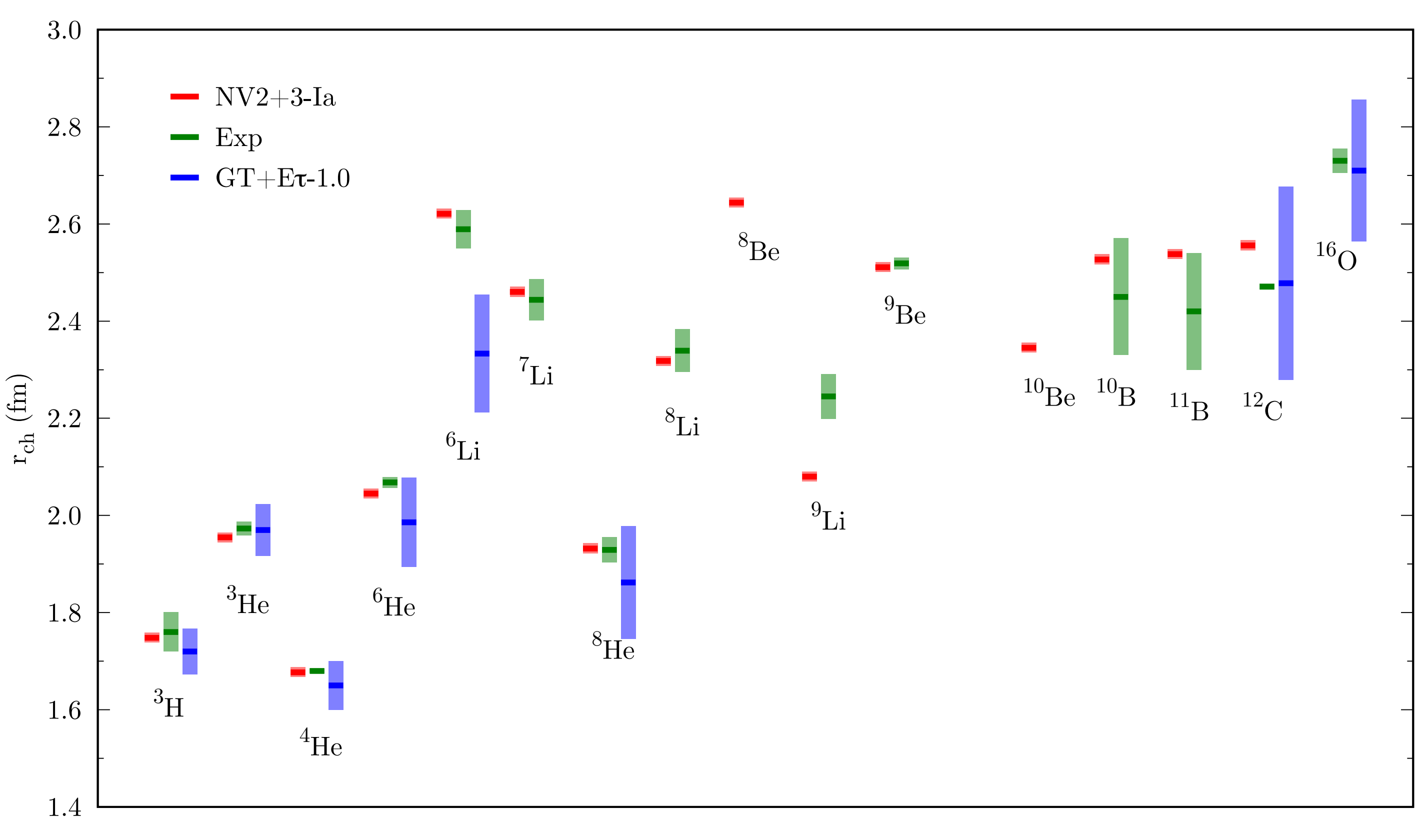
Ground state energies are ~5-6% away from exp data

Nuclear structure: spectra and radii of light-nuclei

S.Gandolfi, D.Lonardoni, A.Lovato, MP Front. Phys. 8, 117 (2020)



- Energy ratio between QMC results and experimental data (GFMC for NV2+3-Ia and AFDMC for GT+Eτ-1.0)
- For NV2+3-Ia difference with experimental data less than 0.2 MeV/A, expected to be covered by truncation error estimate
- For GT+Eτ-1.0 good agreement with experimental data within the theoretical uncertainty estimation.

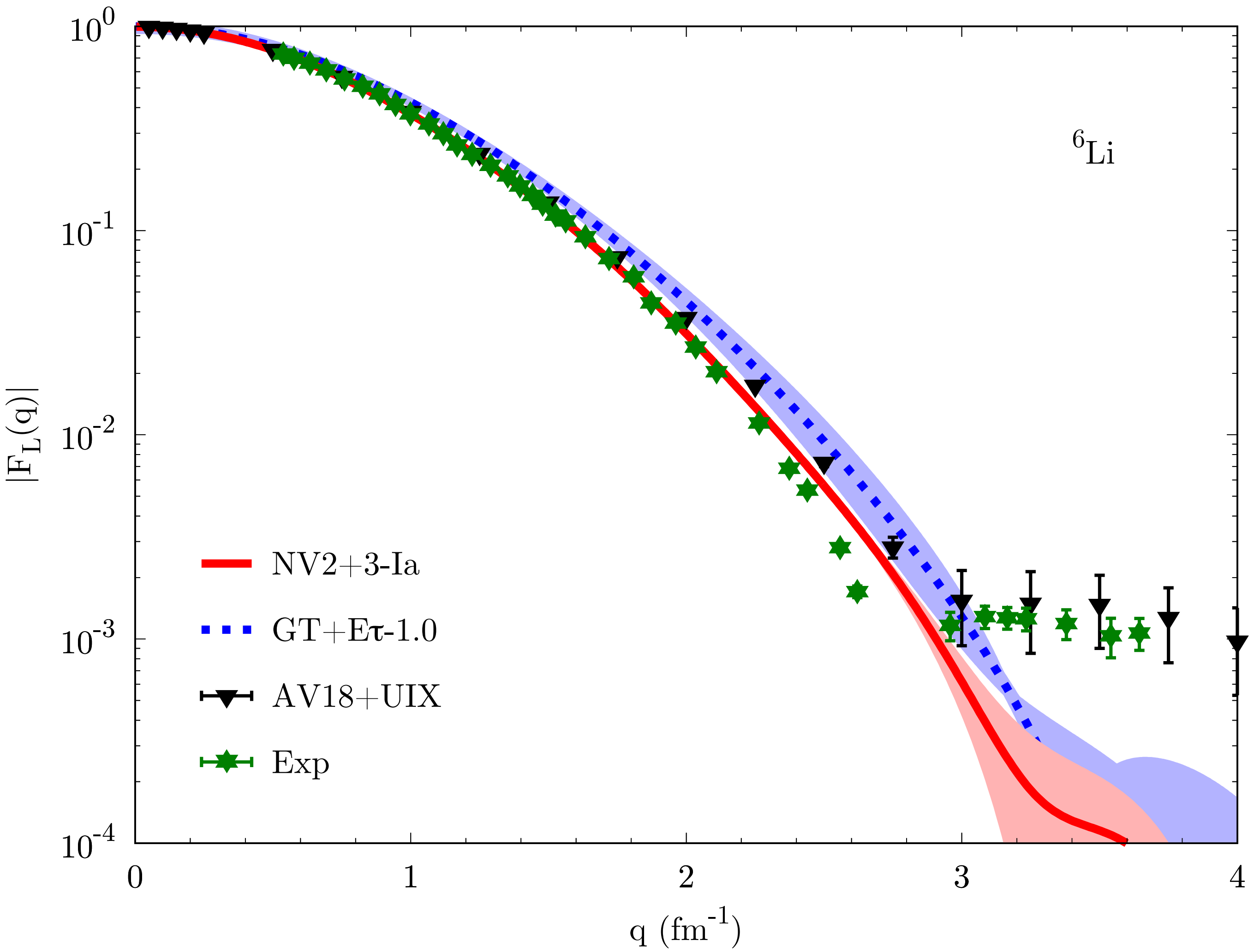


- Charge radii with respect to experimental data (GFMC for NV2+3-Ia and AFDMC for GT+Eτ-1.0)
- Overall agreement with the experimental data for both models
- For NV2+3-Ia, 9Li charge radius underpredicted, 12C slightly overestimated
- For GT+Eτ-1.0, 6Li charge radius underpredicted (issue with AFDMC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

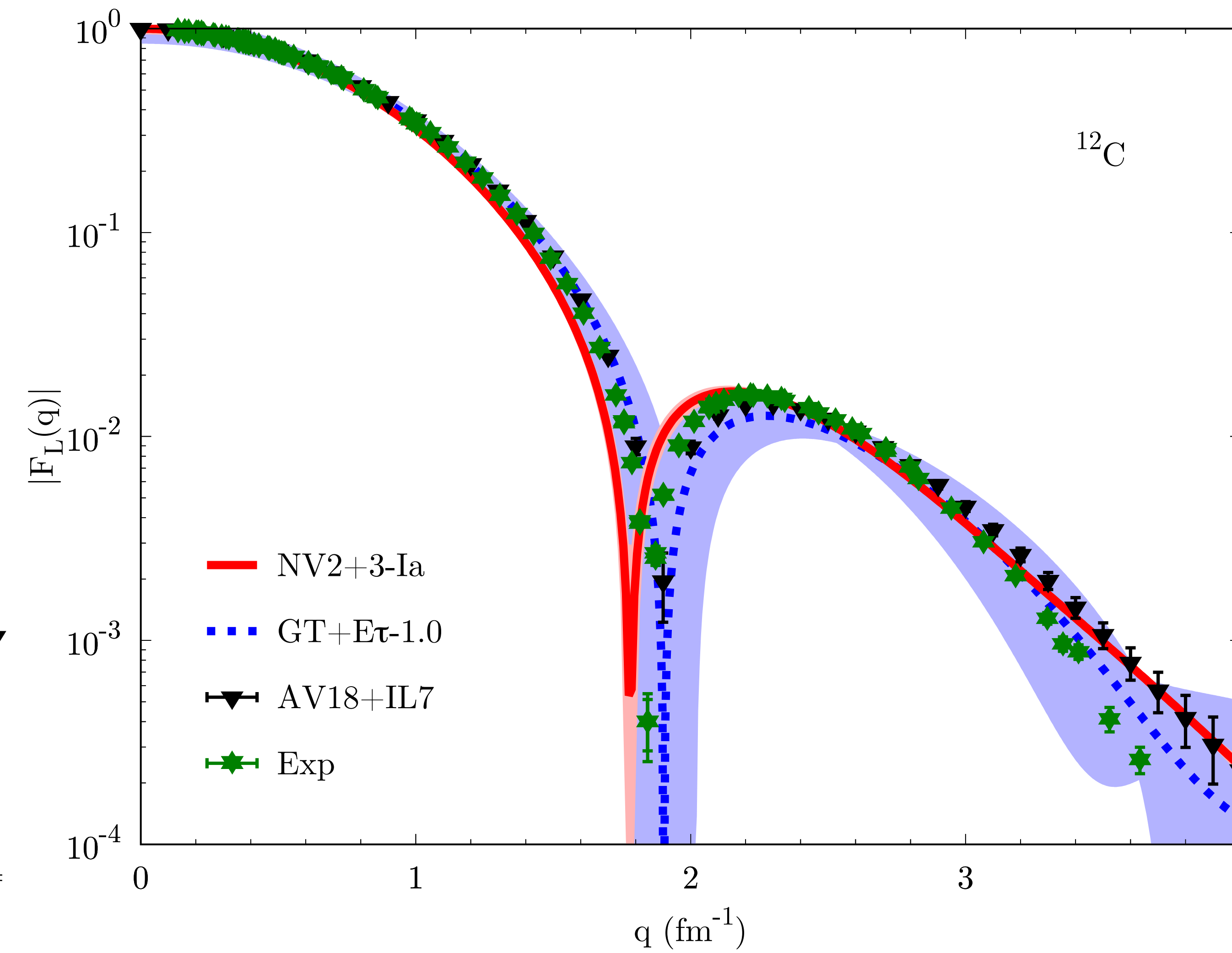
Nuclear structure: charge form factors

S.Gandolfi, D.Lonardoni, A.Lovato, MP Front. Phys. 8, 117 (2020)

Longitudinal form factor for 6Li at LO



Longitudinal form factor for 12C at LO



Calculations using NV2+3-Ia are obtained with GFMC

Calculations using GT+Eτ-1.0 are obtained with AFDMC

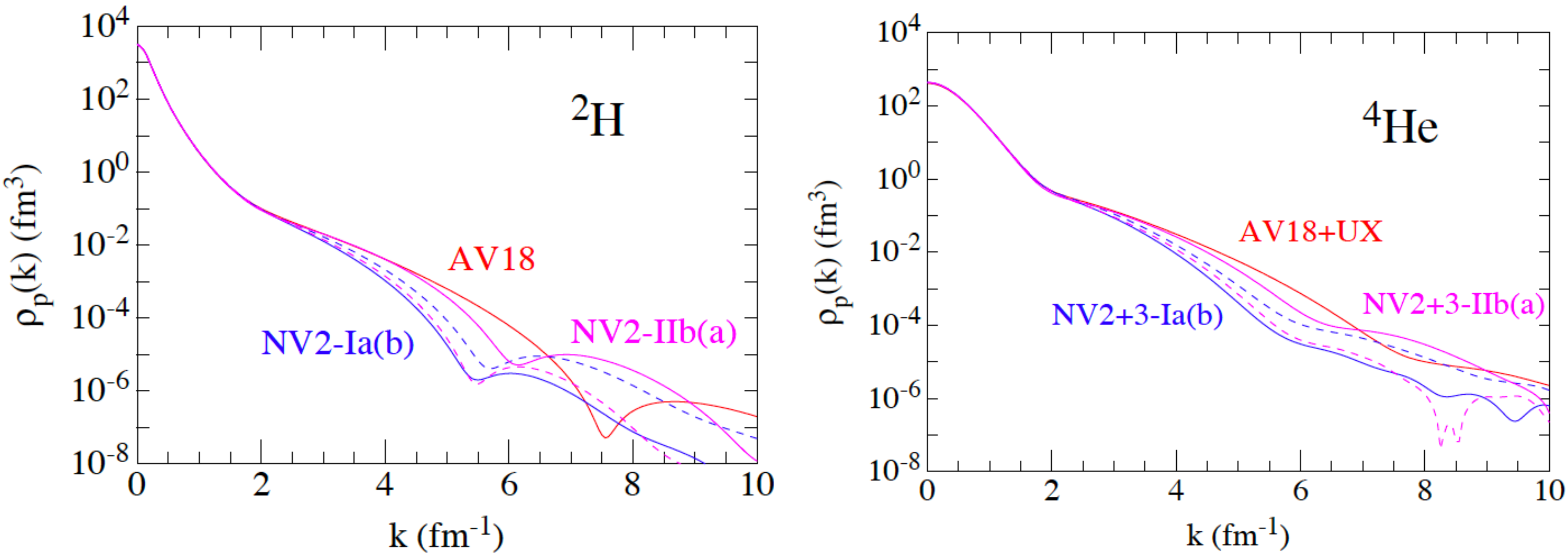
Single-nucleon momentum distribution

- The probability of finding a nucleon with momentum **k** and spin-isospin projection in a given nuclear state

$$\rho_{\sigma\tau}(\mathbf{k}) \;=\; \int d\mathbf{r}_1'\, d\mathbf{r}_1\, d\mathbf{r}_2 \cdots d\mathbf{r}_A\, \psi^\dagger_{JM_J}(\mathbf{r}_1', \mathbf{r}_2, \ldots, \mathbf{r}_A)\, e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_1')}\, P_{\sigma\tau}(1)\, \psi_{JM_J}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A)$$

The total normalization is: $N_{\sigma\tau} = \int \frac{d\mathbf{k}}{(2\pi)^3}\, \rho_{\sigma\tau}(\mathbf{k})$

MP, S.Pastore, R.Wiringa in preparation



Nucleon-pair momentum distribution

- 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

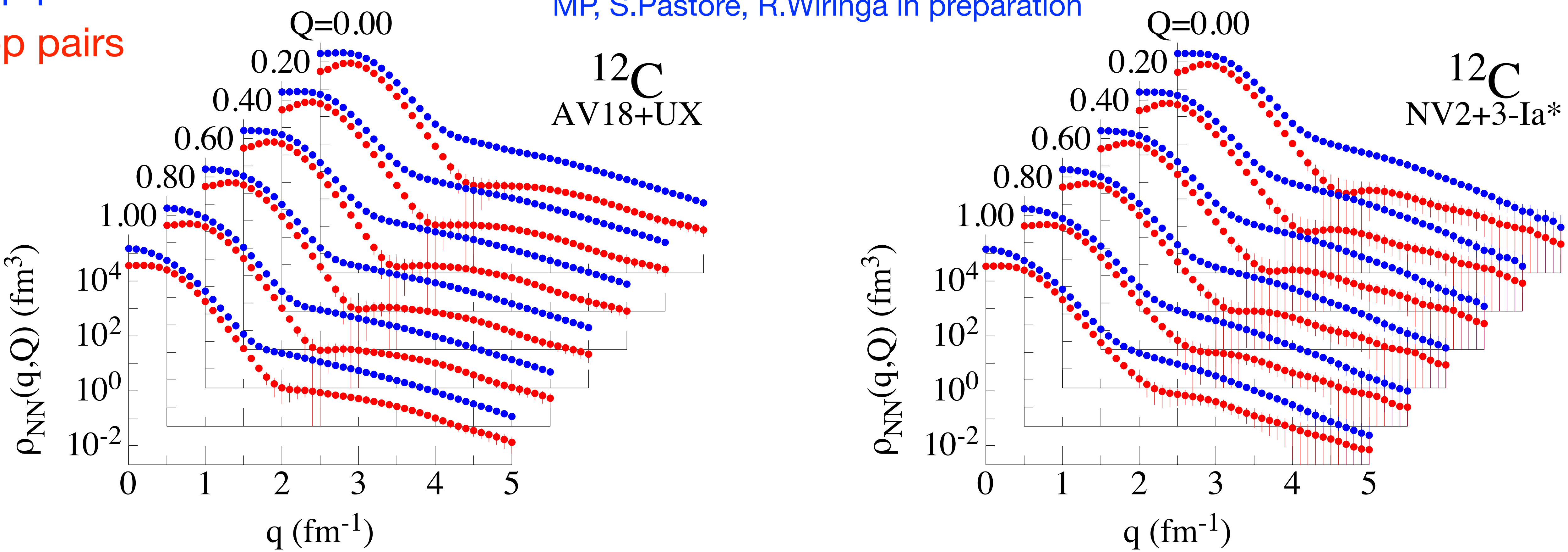
$$\rho_{ST}(\mathbf{q},\mathbf{Q}) = \int d\mathbf{r}'_1 d\mathbf{r}_1 d\mathbf{r}'_2 d\mathbf{r}_2 d\mathbf{r}_3 \cdots d\mathbf{r}_A \psi^\dagger_{JM_J}(\mathbf{r}'_1,\mathbf{r}'_2,\mathbf{r}_3,\ldots,\mathbf{r}_A)\, e^{-i\mathbf{q}\cdot(\mathbf{r}_{12}-\mathbf{r}'_{12})} \times e^{-i\mathbf{Q}\cdot(\mathbf{R}_{12}-\mathbf{R}'_{12})}\,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

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

np pairs

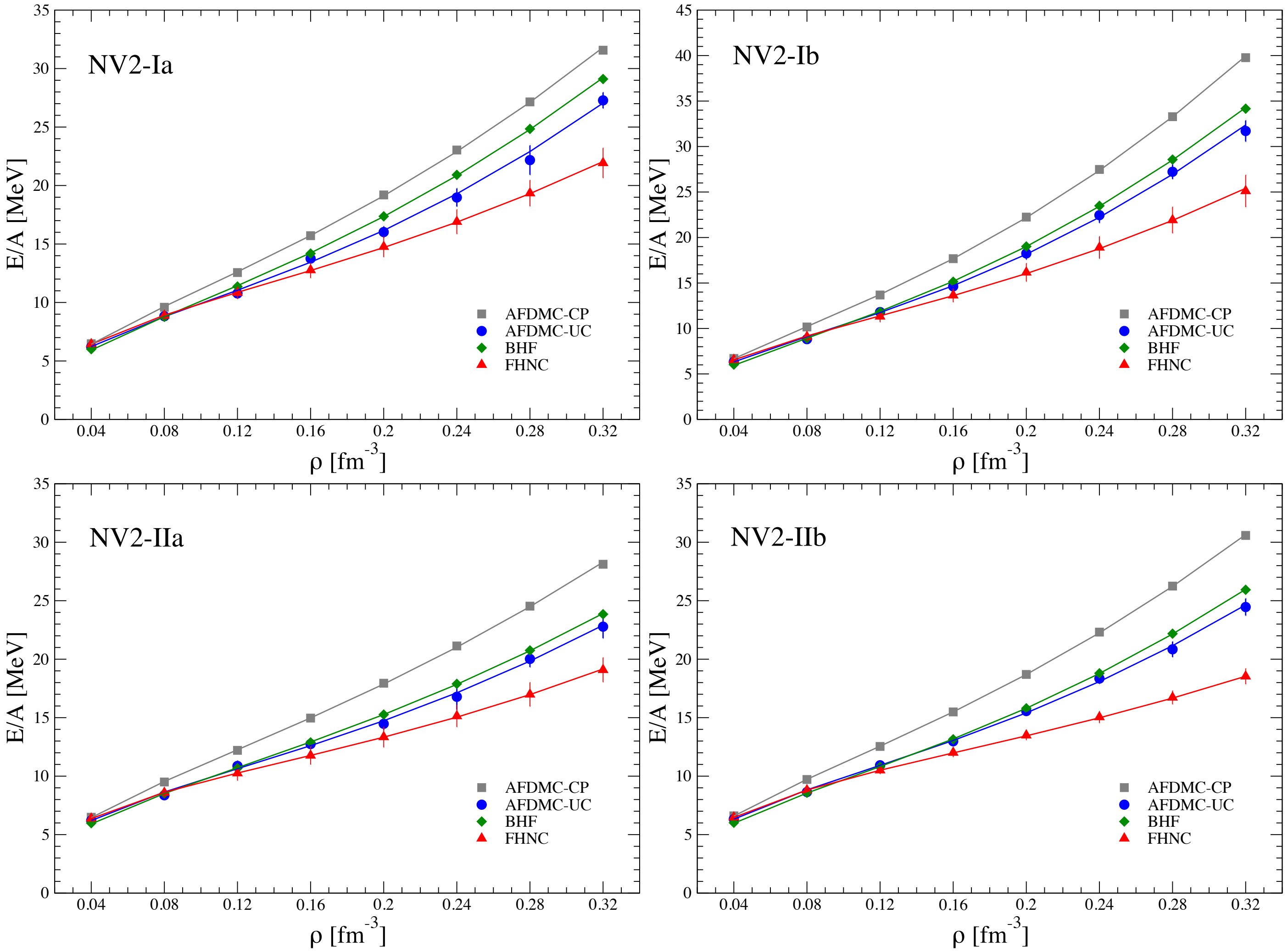
pp pairs

MP, S.Pastore, R.Wiringa in preparation



Working on the connection with Short Time Approximation (STA) to account for two-body currents (S.Pastore et al.)

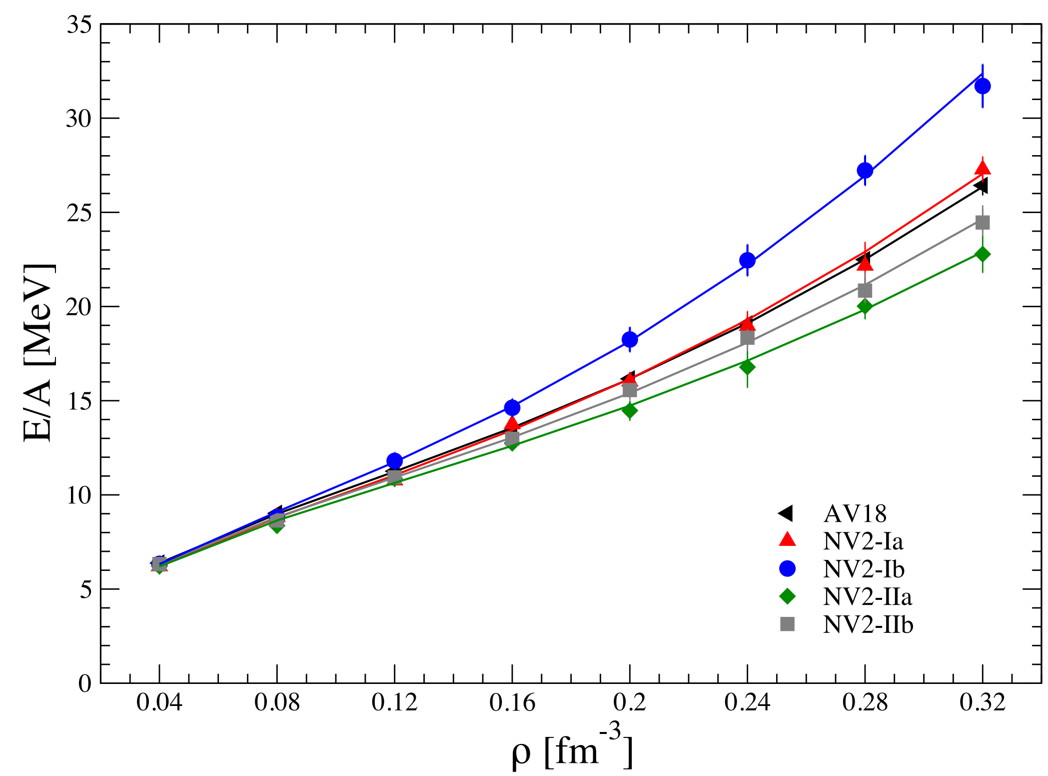
Multi-messenger Astronomy: EoS of Pure Neutron Matter



MP et al. Phys. Rev. C 101, 045801 (2020) Editors' Suggestion

- Benchmark calculations between BHF, FHNC/SOC, AFDMC(CP and UC)
- AFDMC-CP tends to overestimate the E/A compared to the AFDMC-UC: ~2-3MeV at $\rho = \rho_0$ and ~7-8MeV $\rho = 2\rho_0$
- AFDMC-UC, BHF, FHNC/SOC are very close to each other up to $\rho = \rho_0$ (~1 MeV)
- FHNC/SOC is below AFDMC-UC and BHF at higher density; due to limited three-body terms into the cluster expansion

- Model dependence of the EOS at two-body level; AFDMC-UC calculations
- The max spread between AV18, NV2-IIa/IIb (fit to higher NN scattering data) is ~4 MeV per particle at $\rho = 2\rho_0$
- Including NV2-Ia/Ib (fit to lower NN scattering data) the max spread is ~9MeV per particle at $\rho = 2\rho_0$



Model dependence very large in NV2+3 models: work in progress!

Optimization procedure for the LECs

- In EFT we inevitably end up with a model with parameters **a*** that we must fit to data

Least-square objective function for a set of observables

$$\chi^2(\mathbf{a}) = \sum_{i=1}^{N_{\rm data}} \left(\frac{o_i - t_i(\mathbf{a})}{\delta o_i}\right)^2$$

o_i : measured values
t_i : calculated values
δo_i: uncertainty observables

"Conventional" least-square minimization:

$$\mathbf{a}^* = \min_{\mathbf{a}} \chi^2(\mathbf{a})$$

- Take δo_i to be the experimental error (or same modification to take into account theoretical errors)
- Many optimization techniques suitable for this problem such as POUNDers, Newtons Methods,….
- UQ addressed as: Covariance methods, Bootstrapping, standard prescription truncation error, cutoff dependence,….
- over/under-fitting parameters,..

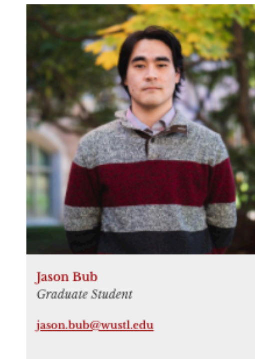
Bayesian parameter estimation:

$$\underbrace{\mathrm{pr}(\mathbf{a}|\mathrm{Data}, I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(\mathrm{Data}|\mathbf{a}, I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\mathbf{a}|I)}_{\text{prior}}$$

$$\propto e^{-\chi^2(\mathrm{a})/2}$$

- Particularly well suited for (any) EFT, but generally suited for theory errors
- Assumptions are made explicit (e.g. naturalness of LECs, truncation errors)
- Parameter estimation: conventional optimization recovered as special case
- Clear prescriptions for combining errors

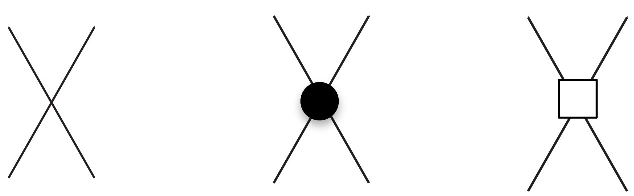
MCMC Implementation and its application



- With MCMC, we can efficiently sample the parameter space to extract the posterior distribution

- A general MCMC works by:
  1. initialize walkers in the parameter space
  2. propose a new location for the walker to move to
  3. accept or reject the move based on the posterior of the current and proposed locations
  4. repeat 2. And 3. until the walkers converge to the final posterior

- In order to get familiarity with MCMC , we choose (for now) to work with a simpler case: only local short-range interactions

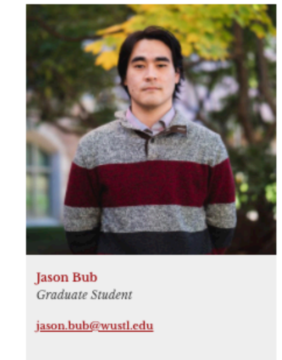


2 LECs   8 LECs   15 LECs

$$
\begin{aligned}
v_{\mathrm{LO}} &= v_{\mathrm{LO}}^{\mathrm{CI}} + v^{\mathrm{EM}} \\
v_{\mathrm{NLO}} &= v_{\mathrm{LO}}^{\mathrm{CI}} + v_{\mathrm{NLO}}^{\mathrm{CI}} + v_{\mathrm{NLO}}^{\mathrm{CD}} + v^{\mathrm{EM}} \\
v_{\mathrm{N3LO}} &= v_{\mathrm{LO}}^{\mathrm{CI}} + v_{\mathrm{NLO}}^{\mathrm{CI}} + v_{\mathrm{N3LO}}^{\mathrm{CI}} + v_{\mathrm{NLO}}^{\mathrm{CD}} + v_{\mathrm{N3LO}}^{\mathrm{CD}} + v^{\mathrm{EM}}
\end{aligned}
$$

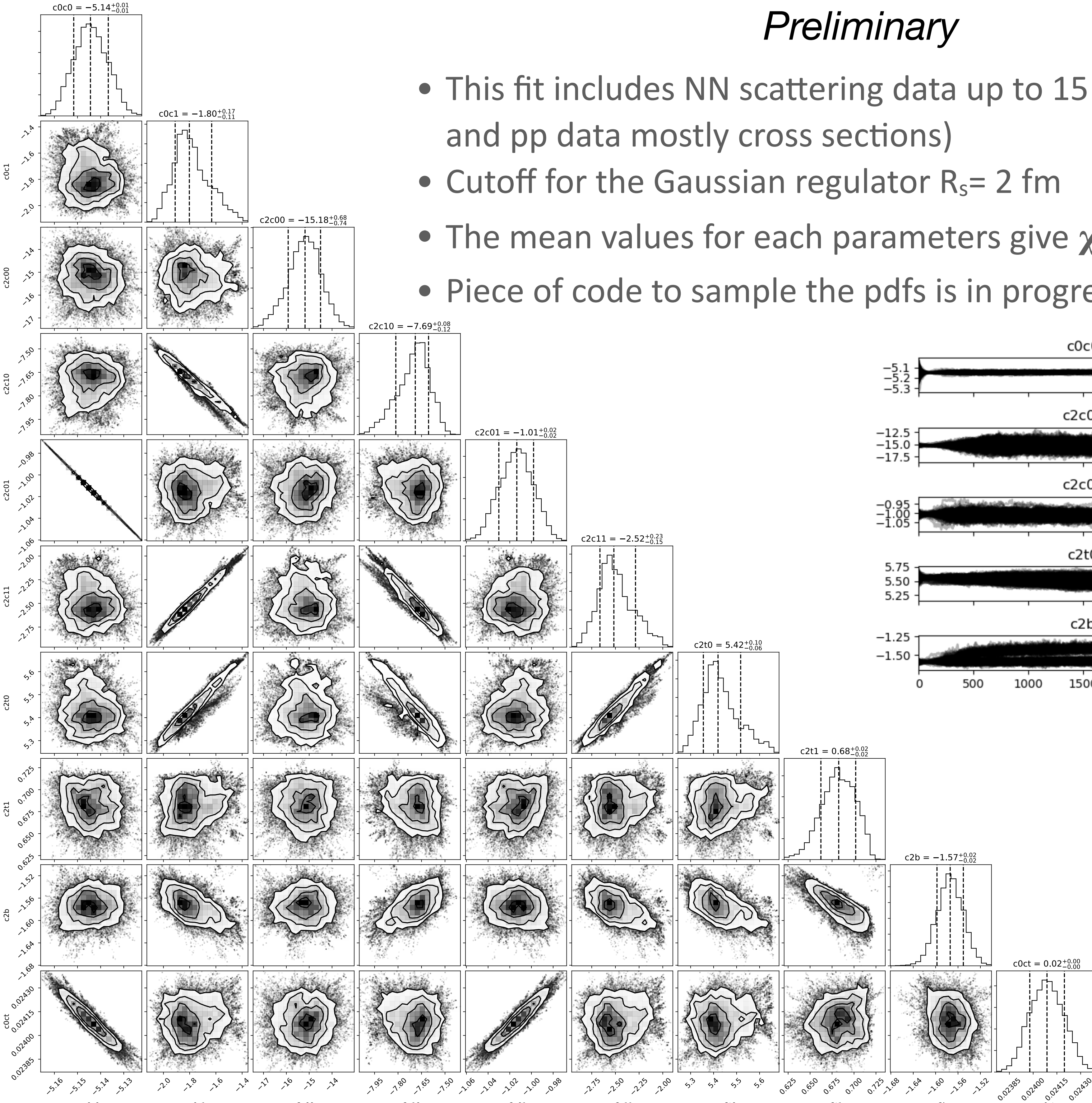
- To do so, we:
  - are using our existing codes written in Fortran to calculate the likelihood from NN scattering data
  - are using a pre-written MCMC package for the fitting: emcee package in Python
  - are using f2py to convert Fortan into a Python module

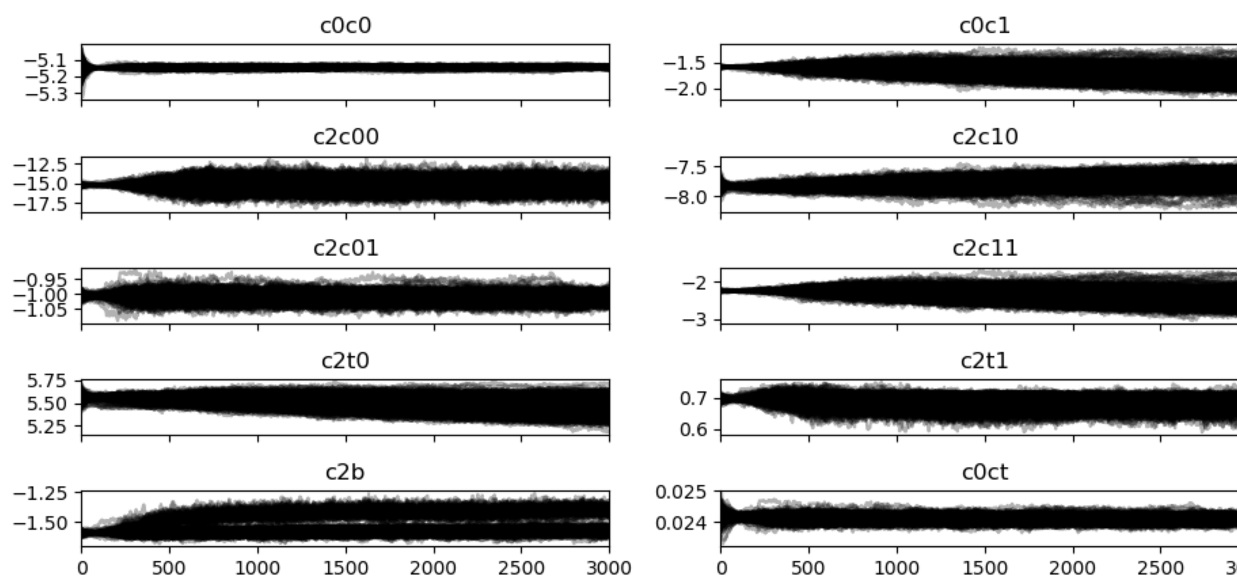
Results at NLO: Joint Probability Projections



Preliminary

- This fit includes NN scattering data up to 15 MeV lab energy (~770 np and pp data mostly cross sections)
- Cutoff for the Gaussian regulator R_S= 2 fm
- The mean values for each parameters give χ^2/datum ~1.6
- Piece of code to sample the pdfs is in progress





	Experiment	$R_S = 2\,\mathrm{fm}$
$^1a_{pp}$	-7.8063(26)	-7.7545
	-7.8016(29)	
$^1r_{pp}$	2.794(14)	2.667
	2.773(14)	
$^1a_{nn}$	-18.90(40)	-17.22
$^1r_{nn}$	2.75(11)	2.79
$^1a_{np}$	-23.740(20)	-23.741
$^1r_{np}$	2.77(5)	2.74
$^3a_{np}$	5.419(7)	5.424
$^3r_{np}$	1.753(8)	1.820
B_d (MeV)	2.224575(9)	2.224218
η	0.0256(4)	0.0357
P_D (%)		4.34

J.Bub, MP, S.Pastore in progress

Conclusion/Outlook

- We are testing our models of NN+3N interactions with Δ-isobar based on chiral EFT framework in both light-nuclei and infinite nuclear matter

- We mainly focus our attention on studying static and dynamic properties of nuclei up to A=12 and EoS of infinite neutron matter

- We are working on constructing a coherent picture of lepton-nucleus interactions with particular focus on neutrino-nucleus scattering in a wide rage of energy and momenta

- With the current Delta-full chiral interactions/currents we are planning to investigate muon capture, neutrino scattering, neutrinoless double beta decay, beta-decays for A>10

- Inclusion of the present Delta-full 3N in calculations of infinite nucleonic matter; sensitivity studies of the EoS

- We are working on improvements of our nuclear models using Bayesian analysis tools to better access theoretical error estimation

- Particularly emphasis needs to be devoted to the 3N force; the formulation we have is too simplistic if we want to have a good descriptions of spectra, properties of light-nuclei, infinite nuclear matter, three-body observables with a certain degree of accuracy