Applications of novel chiral interactions to quantum Monte Carlo methods

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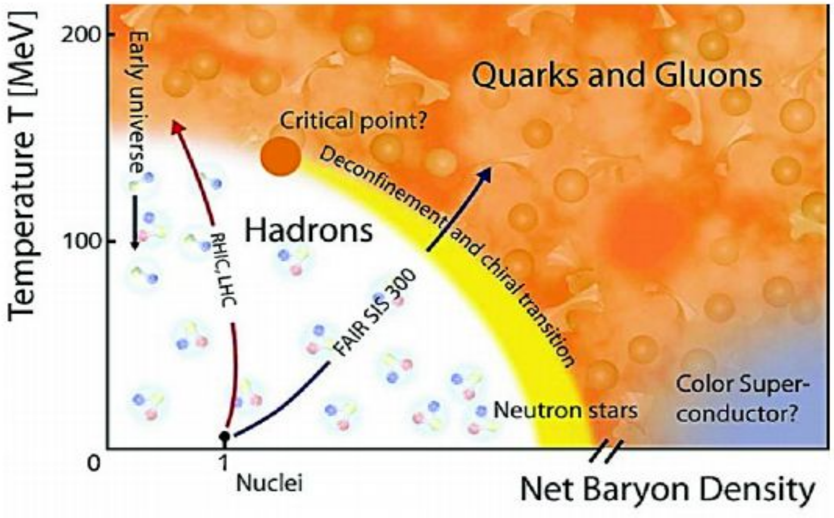
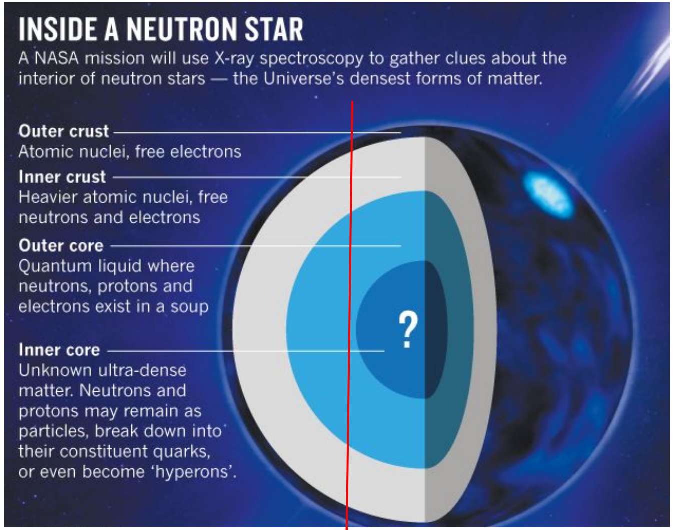
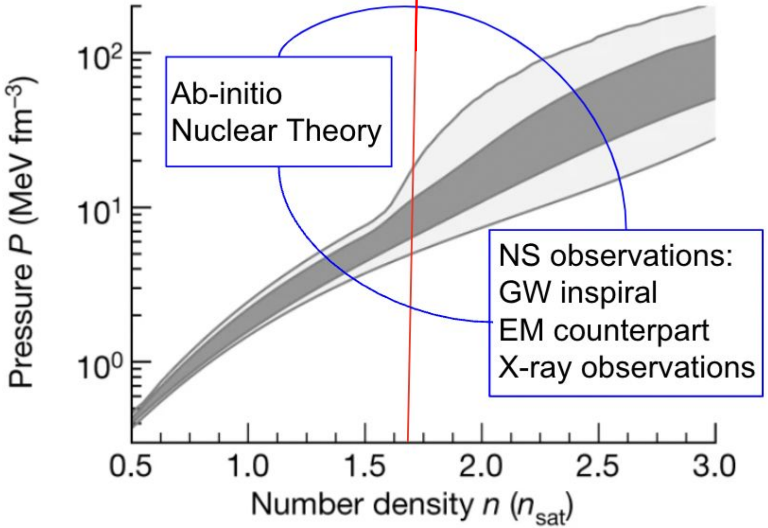
The Basic Question



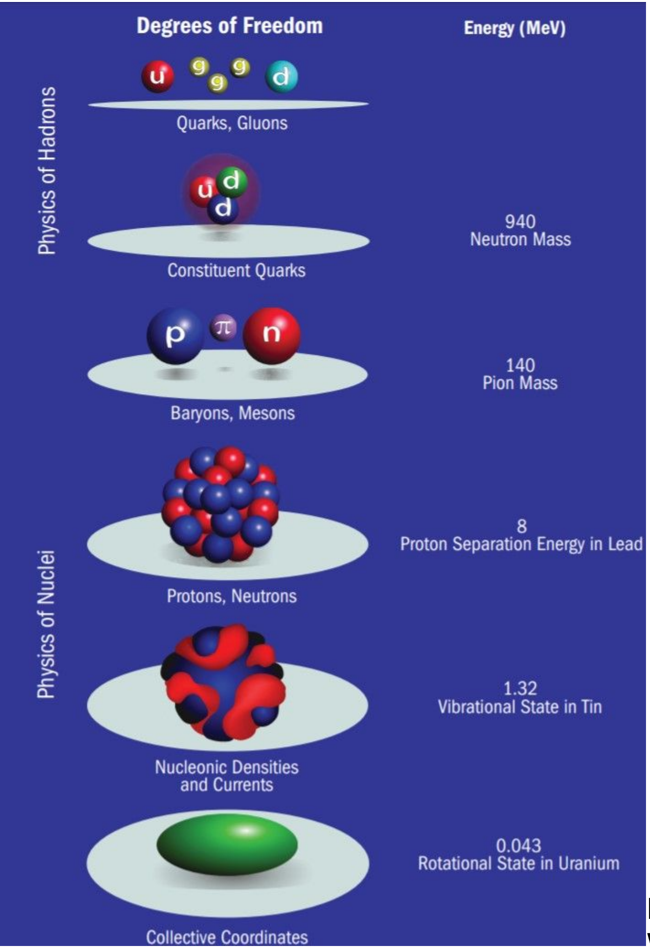
From http://nsmn1.uh.edu/cratti/

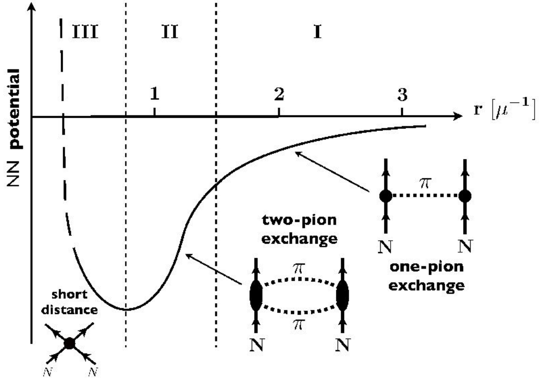
- What is the nature of the densest matter in the universe?
- How and when do new states of dense matter appear?
- How do neutrons and protons interact under extreme conditions of density and isospin asymmetry?



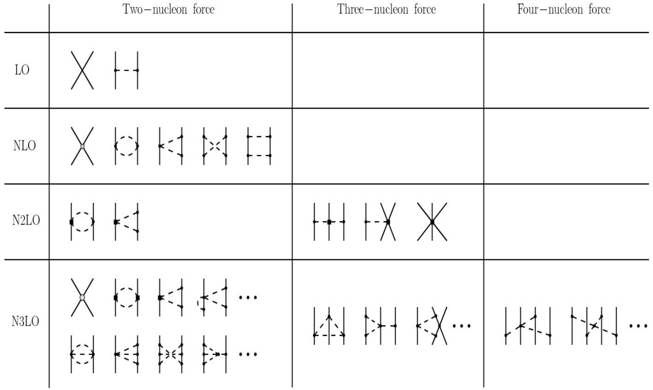


Nuclear Effective Field Theory





Holt et al., 10.1016/j.ppnp.2013.08.001



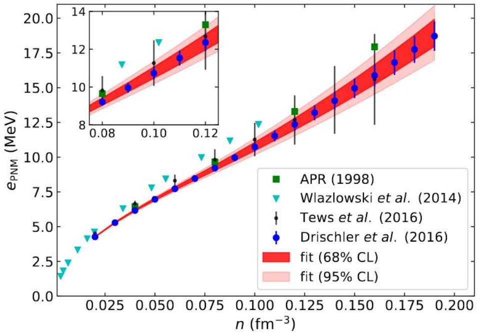
Bertsch et al., United States: N. p., 2007.
Web.

- The long-range component of the NN interaction is mediated by the pion which is constrained directly by the symmetries of QCD. Heavy mesons (ρ,ω) are ‘integrated out’ and are replaced with contact interactions.

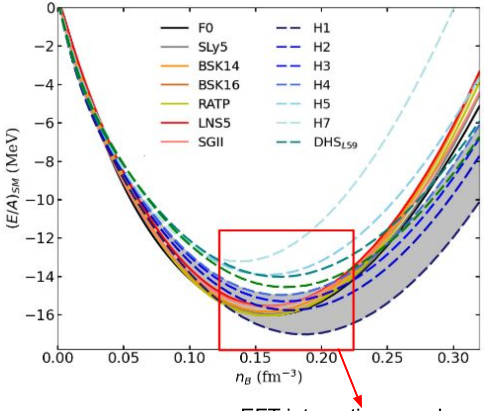
- The Lagrangian is an expansion $Q = p/\Lambda_b$, where Λ_b is the EFT breakdown scale (~600 MeV) and p is of the order of the pion mass (~140 MeV).

Applications of Chiral EFT (N^3LO + MBPT):

The Equation of State

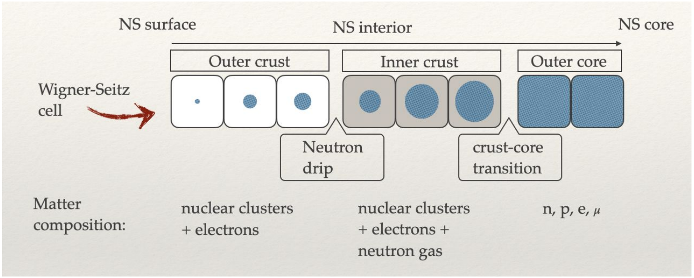


RS et al.,PRC 103 (2021) 4, 045803

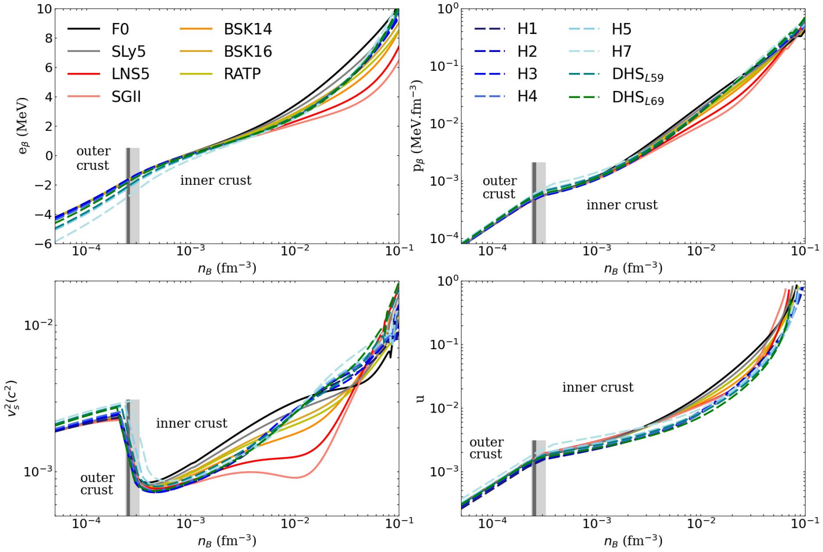


EFT interactions are broadly consistent with nuclear experiments and phenomenological interactions.

Modeling of the NS crust



G. Grams et al. [incl. Somasundaram], EPJA 58 (2022) 3, 56



EFT models perform significantly better than phenomenological interactions in the modeling of the inner crust.

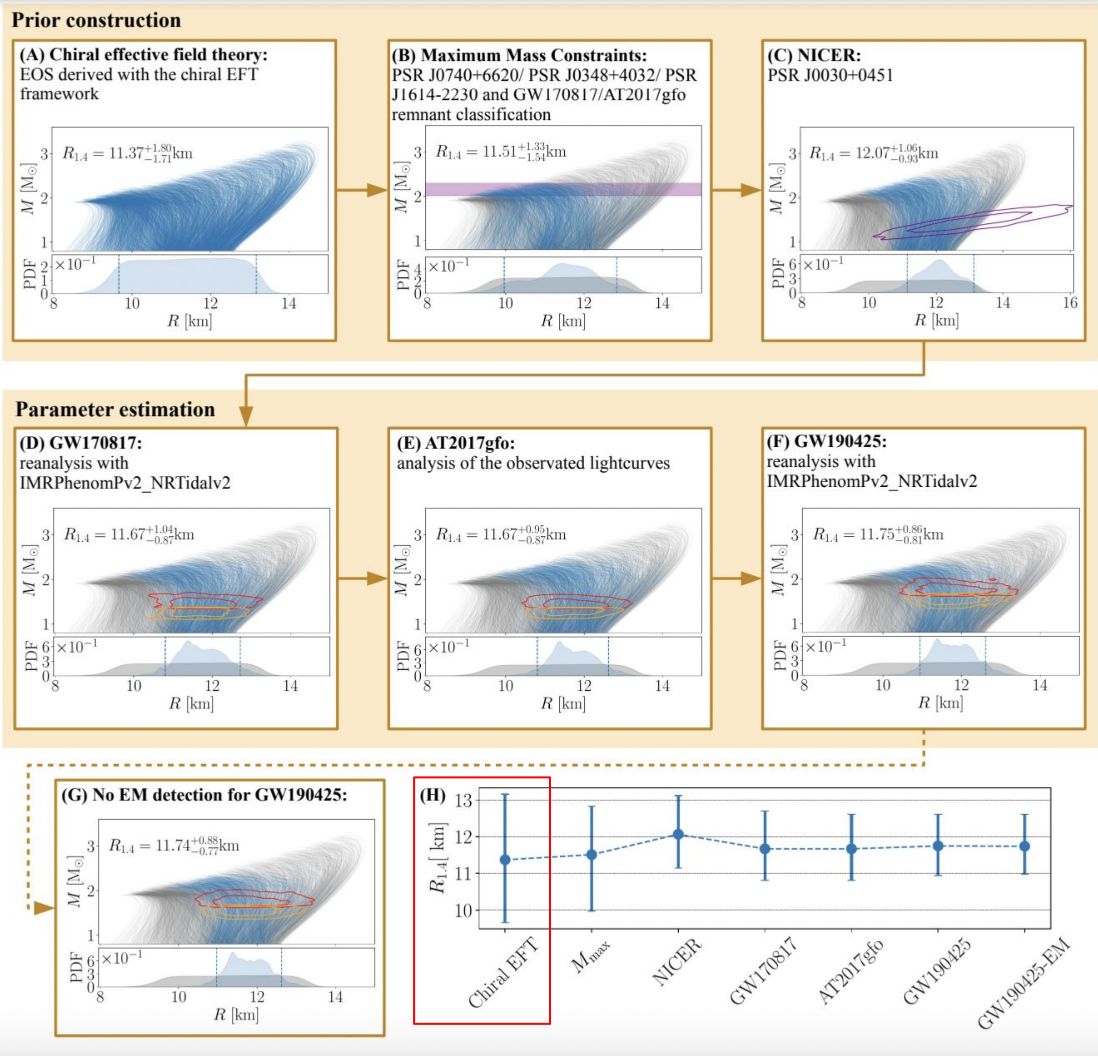
Results for the crust-core transition ($n \sim 0.08$ fm^{-3}) and the inner-outer crust transition ($n \sim 0.002$ fm^{-3}) are consistent with other approaches.

EFT input for the NS EOS

- EFT models breakdown at about $n \sim 2n_{sat}$. However, they provide valuable nuclear physics input to the analyses of multi-messenger astrophysical data.

- One way of improving uncertainties in EFT models is to perform higher calculations at higher orders in the EFT expansion.

- This needs to be coupled with robust methods to solve the many-body Schrodinger equation, such as quantum Monte Carlo (QMC)



Science 370 (2020) 6523, 1450-1453

Local chiral interactions

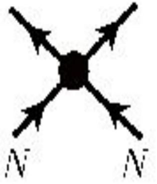
- Quantum Monte Carlo (QMC) methods are among the most accurate many-body methods to solve nuclear systems, but they require local interactions as input.

$$\lim_{\tau \to \infty} e^{-H\tau} |\Psi_T\rangle \to |\Psi_0\rangle$$

where H does not include derivative operators

- Chiral EFT is traditionally formulated in a nonlocal manner and has been developed upto N^3LO and beyond. Local EFT interactions have been introduced only in the past decade.

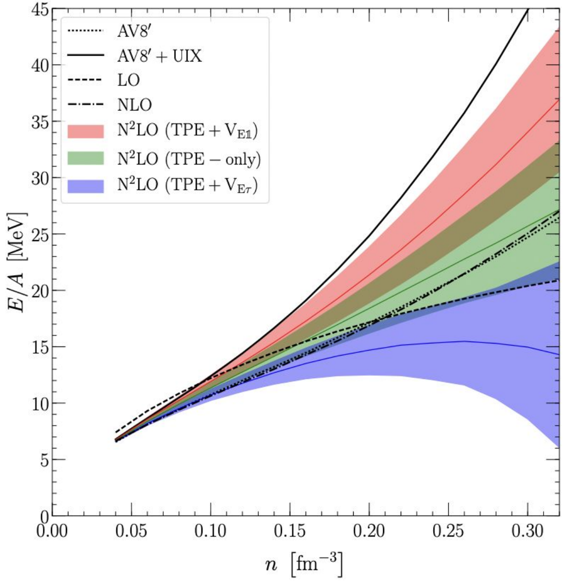
- We also need to regulate the interaction using local regulators:



$$= \quad \delta(r) \to f_{\text{short}}(r)$$

$$f_{\text{short}}(r) \sim \exp\left(-\left(\frac{r}{R_0}\right)^n\right)$$

EOS of neutron matter (N^2LO+QMC)

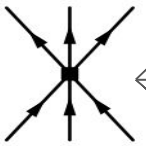


Tews et al., Astrophys.J. 860 (2018) 2, 149

<u>How can we decrease regulator artifacts?</u>

Local chiral interactions at N²LO: EFT at large cutoffs

- Local regulators violate the Fierz rearrangement freedom. This can have a drastic effect in the 3-body sector



c_E

$$V_{E\tau} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \delta_{R_{3N}}(\mathbf{r}_{kj}) \delta_{R_{3N}}(\mathbf{r}_{ij}),$$

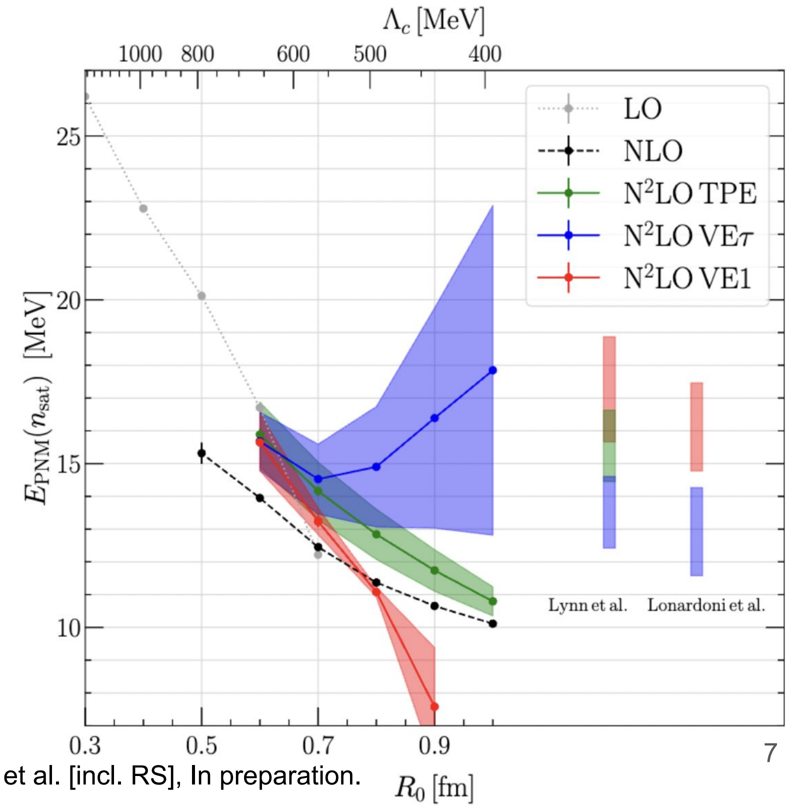
$$V_{E\mathbb{1}} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \delta_{R_{3N}}(\mathbf{r}_{kj}) \delta_{R_{3N}}(\mathbf{r}_{ij}),$$

$$V_{E\mathcal{P}} = \frac{c_E}{\Lambda_\chi F_\pi^4} \sum_{i<j<k} \sum_{\text{cyc}} \mathcal{P} \delta_{R_{3N}}(\mathbf{r}_{kj}) \delta_{R_{3N}}(\mathbf{r}_{ij}).$$

- Different operator structures are possible for the same 3N force, V_E. This ambiguity should vanish in the limit of infinite cutoff.

- QMC calculations of neutron matter for a wide range of cutoffs seem to confirm this, greatly improving the applicability of local chiral interactions to many-body systems.

QMC calculation of pure neutron matter



I. Tews et al. [incl. RS], In preparation.

Maximally local NN chiral interactions at N^3LO

- As the next step, we aim to construct chiral interactions at N^3LO that can be used for QMC calculations. However, the short-range part of the NN interaction contains pieces that are inevitably non-local.

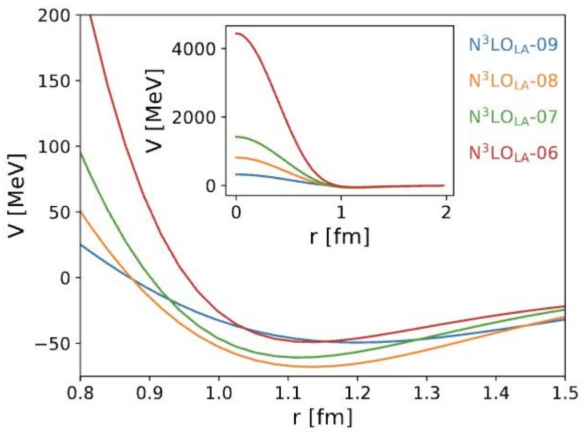
$$H^{\mathrm{N3LO}} = \underbrace{H^{\mathrm{local}}}_{\text{17 operators}} + \underbrace{H^{\text{non-local}}}_{\text{4 operators}}$$

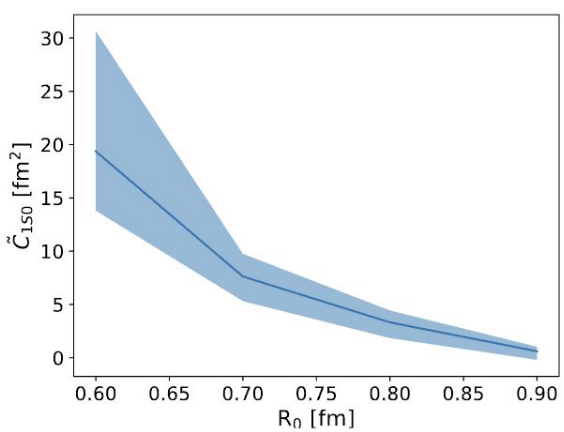
Our idea is to compute H^{local} exactly in QMC and treat $H^{\text{non-local}}$ perturbatively, $\Delta E = \langle \psi_0 | H^{\text{non-local}} | \psi_0 \rangle$

see Curry et al., arXiv:2302.07285

- Once again, we explore a wide range of cutoffs in the range ~440 MeV to ~660 MeV

- Going one order higher in the chiral expansion, as well as exploring high-cutoff interactions, is expected to decrease uncertainties by factor 2-3.

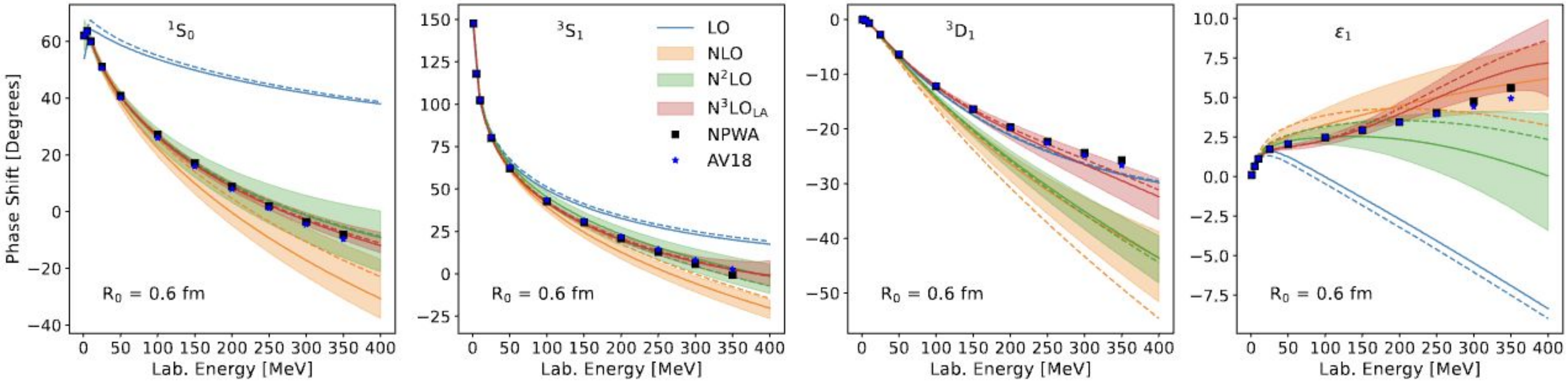




RS et al., arXiv:2306.13579

Maximally local NN chiral interactions at N^{3}LO: A Bayesian analysis

RS et al., arXiv:2306.13579



- The NN interaction is calibrated to scattering data using the method of Bayesian inference. This allows us to incorporate EFT truncation uncertainties using order-by-order calculations.

$$P = \frac{\mathcal{L} \times \Pi}{Z}, \qquad \mathcal{L} \propto \prod_i \exp\left\{ -\frac{1}{2} \left(\frac{X_i^{\rm exp} - X_i^{\rm theo}}{\sigma_i} \right)^2 \right\},$$

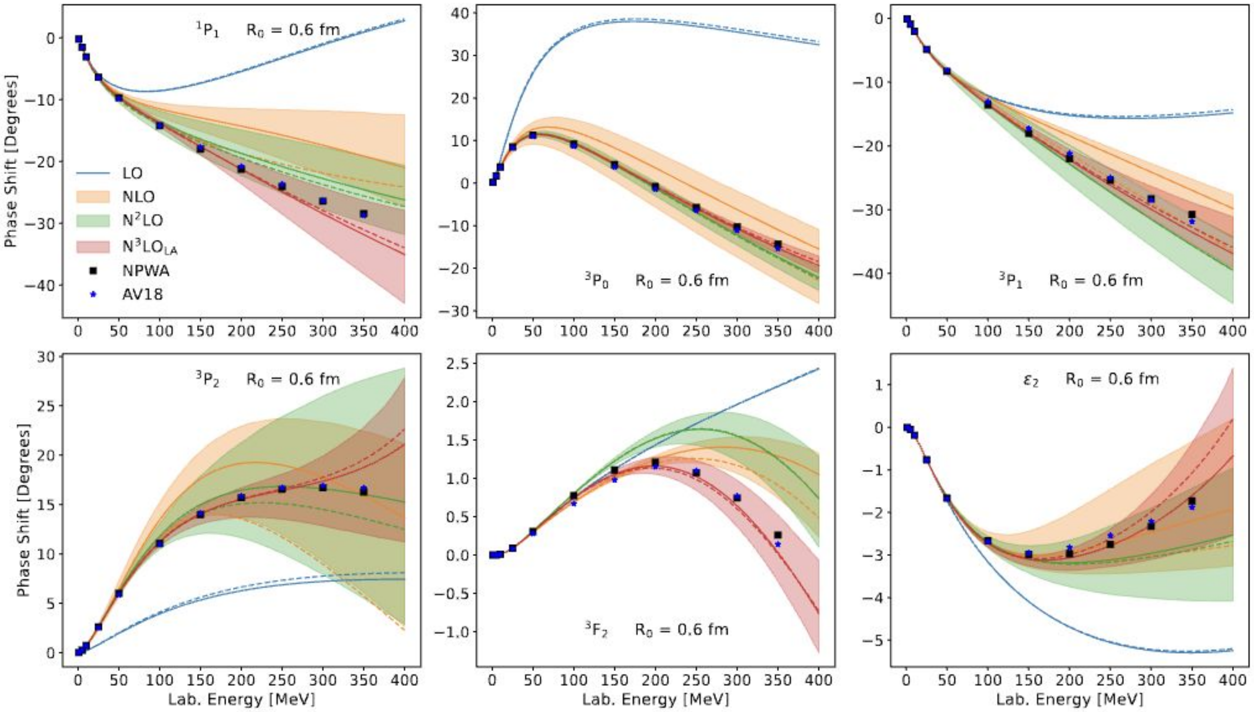
$$\sigma^2 = \sigma^2_{\rm exp} + \sigma^2_{\rm theo},$$

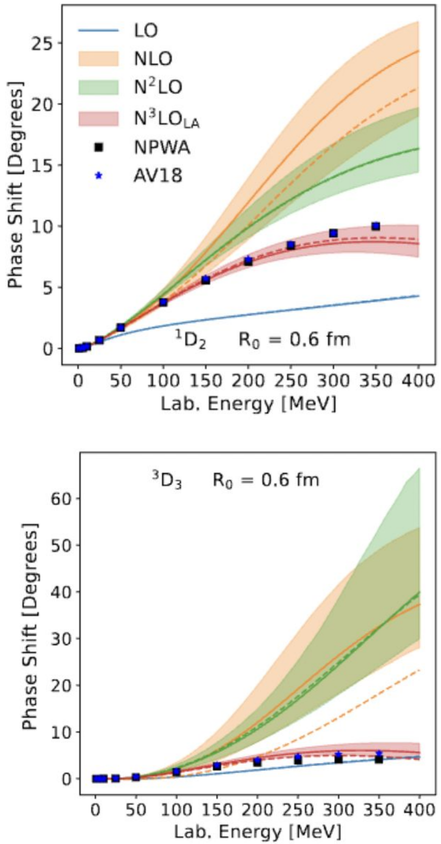
$$\Delta X^{{\rm N}^j{\rm LO}} = Q^{j+2} \max(|c_0|, |c_1|, \ldots, |c_{j+1}|),$$

$$\text{where } Q = \frac{\max(m_\pi, p)}{\min(\Lambda_c, \Lambda_B)} \text{ and } \Lambda_B = 600 \text{ MeV}$$

Maximally local NN chiral interactions at N^3LO: A Bayesian analysis

We clearly demonstrate the order-by-order convergence of the EFT, in terms of both agreement with experimental data and reduction of theoretical uncertainties.

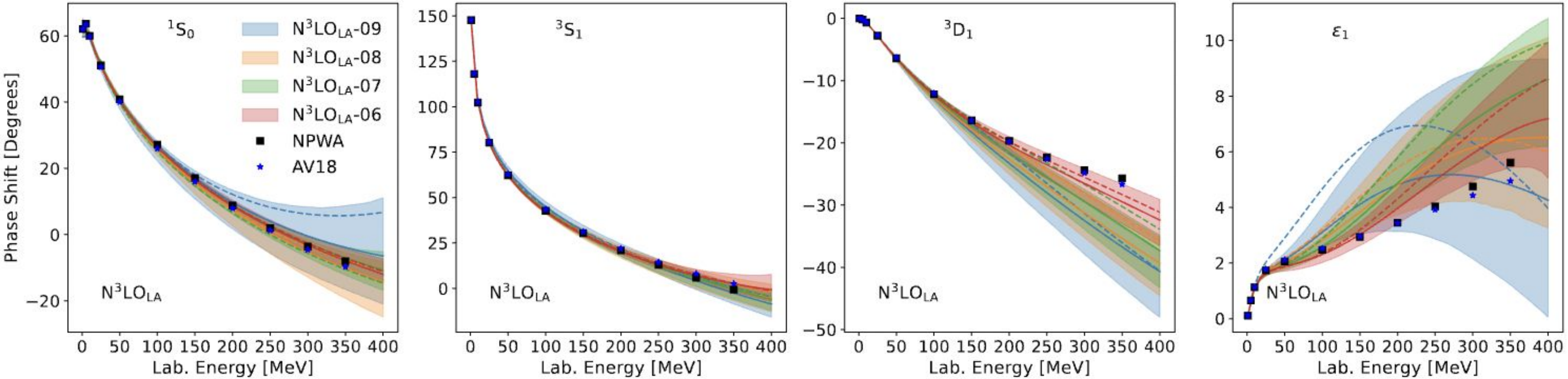




RS et al., arXiv:2306.13579

Maximally local NN chiral interactions at N³LO: A Bayesian analysis

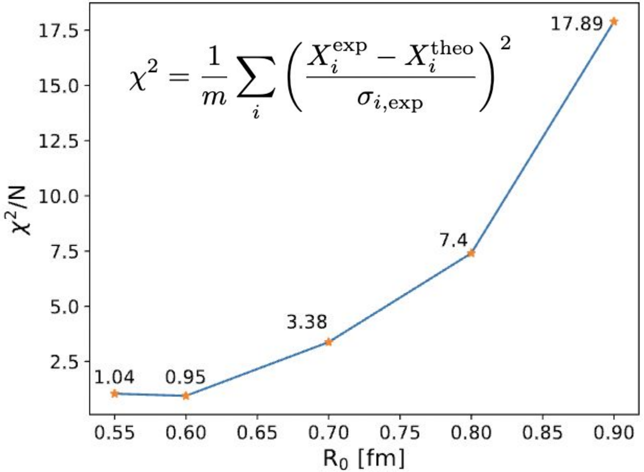
RS et al., arXiv:2306.13579



- We see that harder-core interactions exhibit significantly lower EFT truncation uncertainties.

- The more non-perturbative potentials are also better at reproducing NN scattering data.

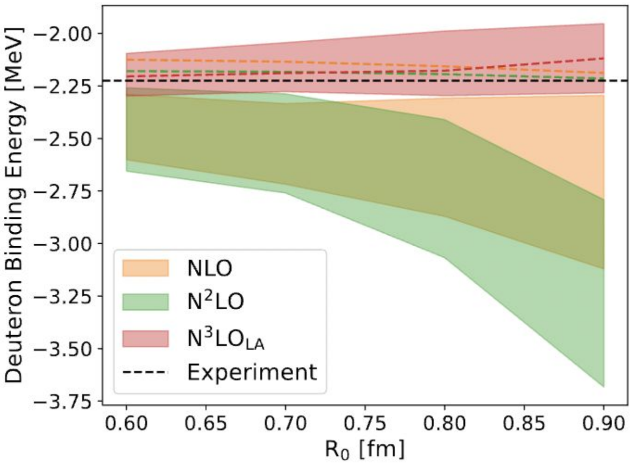
- By comparing with a simple least-squares fit, we see the importance of modeling truncation errors via Bayesian methods.



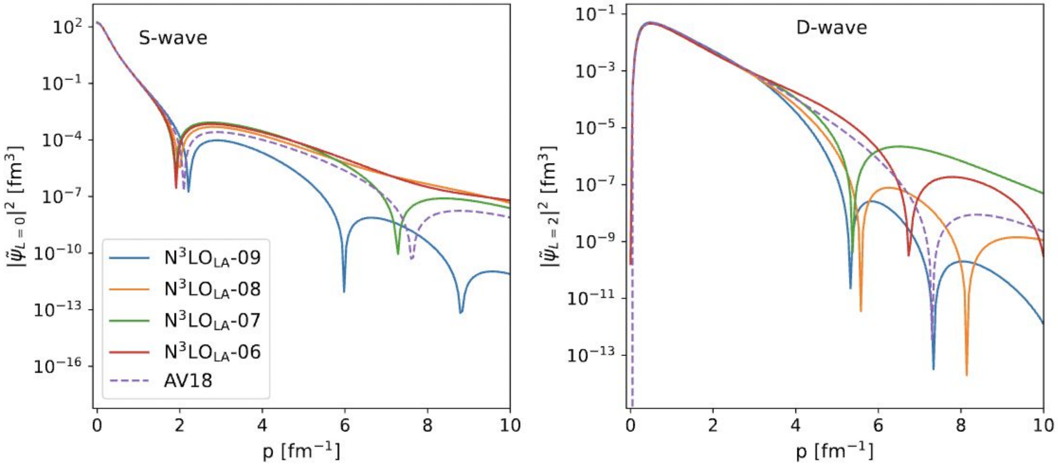
The Deuteron

- To make predictions for many-body systems, we need to incorporate (parameter free) 3N forces at N^3LO. This is our next step.

- For now, we benchmark against the properties of the deuteron. Our model predictions are in excellent agreement with data at the 95% CL.



RS et al., arXiv:2306.13579



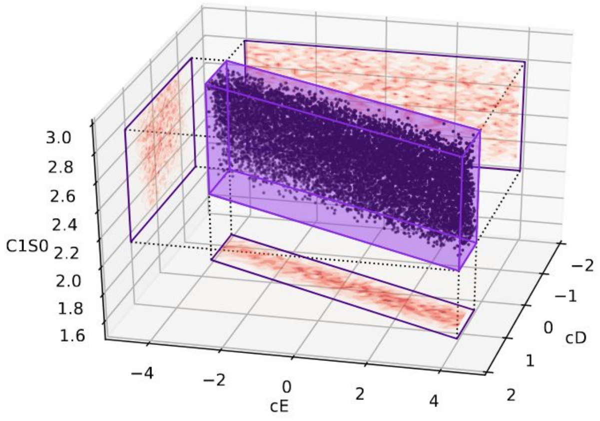
Our harder core interactions have certain unique properties, such as significant high-momentum tails that could have implications for electron scattering experiments.

Looking forward: Emulators for the NS EOS

- Complete propagation of nuclear physics uncertainties towards astrophysical NS observables requires the development of emulators.

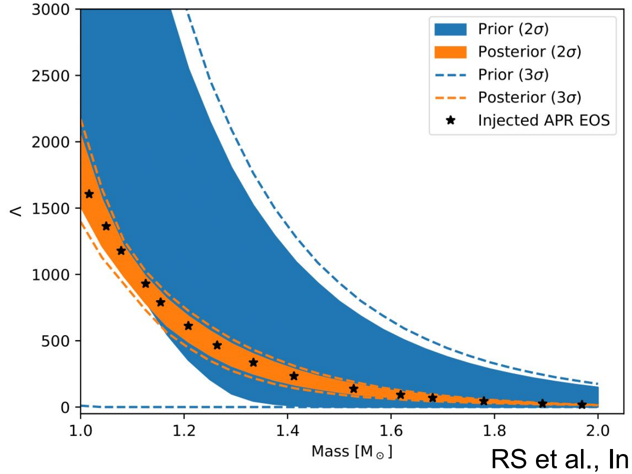
- Recently, emulators for the nuclear matter EOS have been developed based on the subspace-projected coupled-cluster method. The emulator employs a nonlocal Δ-full EFT interaction at N^2LO.

History matching to identify non-implausible domains for the LECs

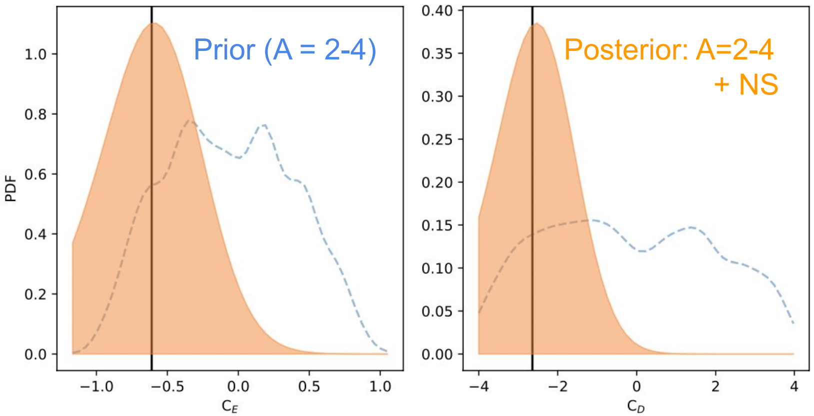


W.G. Jiang et al., 2212.13216

An Injection study of a year's worth of 3G GW detections



RS et al., In preparation



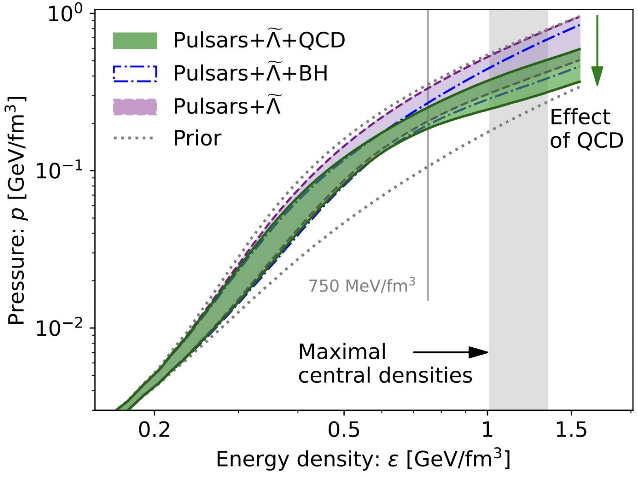
An aside: Does pQCD impact the EOS of NSs?

- Studies which use perturbative QCD calculations at high densities, claim to observe a ‘softening’ of the Eos relevant for NSs.

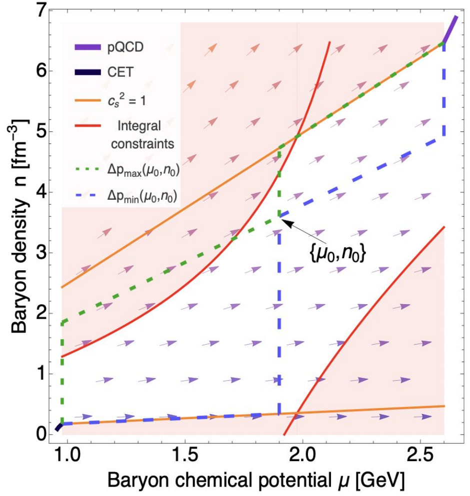
- We find that pQCD does not significantly constrain the EOS of NSs when uncertainties are taken into account.

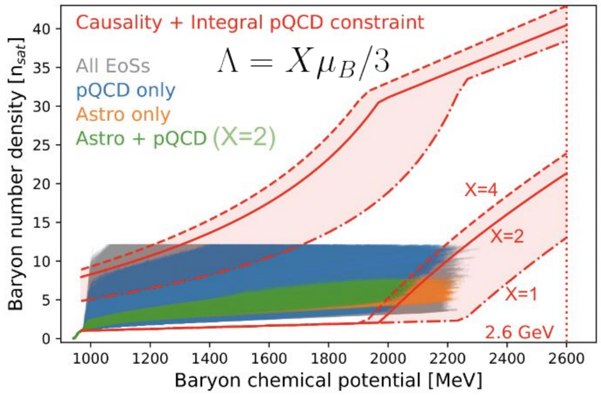
- It could however impact the EOS above the TOV limit.

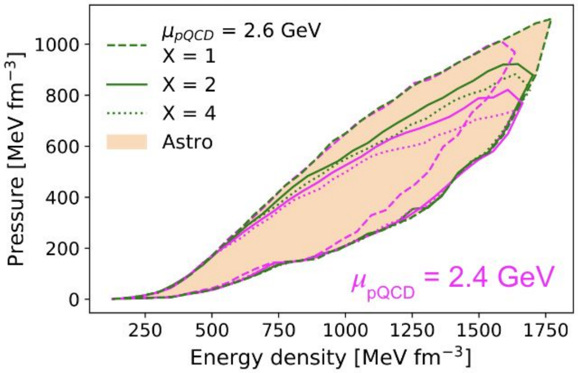
Tyler Gorda et al 2023 ApJ 950 107



Komoltsev et al,PRL. 128, 202701







RS et al., Phys.Rev.C 107 (2023) 5, L052801

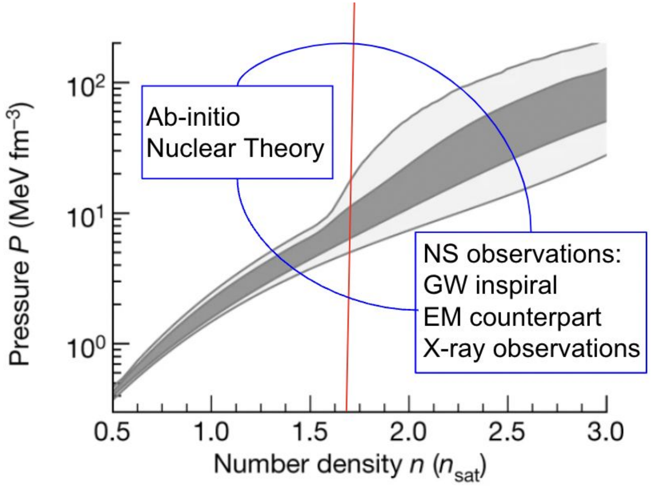
Conclusions and outlook

- We have developed novel chiral interactions for quantum Monte Carlo methods.

- Our new N^2LO interactions (NN+3N) explore a wide range of cutoffs. We showed how regulator artifacts can be drastically decreased for hard-core (non-perturbative) interactions.

- We have also developed maximally local N^3LO interactions (NN only) that incorporate Bayesian uncertainty quantification. The next step would be to include 3N forces at N^3LO, allowing for the complete QMC calculations of few and many body nuclear systems.

- Our work will allow for state-of-the-art computation of the NS EOS. Development of fast and efficient emulators for different many-body methods (such as QMC) is crucial for this research direction.



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Thank You!