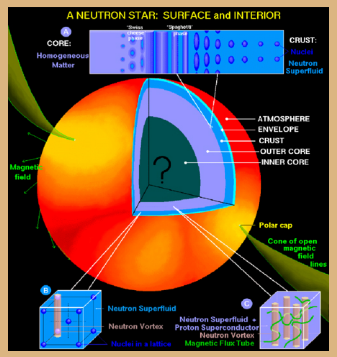
From microscopic to effective interactions using Quantum Monte Carlo

Alex Gezerlis

UNIVERSITY of GUELPH

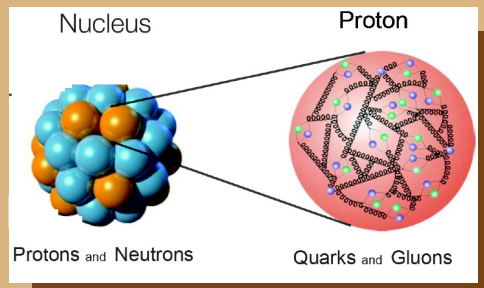
"New Ideas in Constraining Nuclear Forces"
ECT*, Trento, Italy
June 5, 2018

Outline

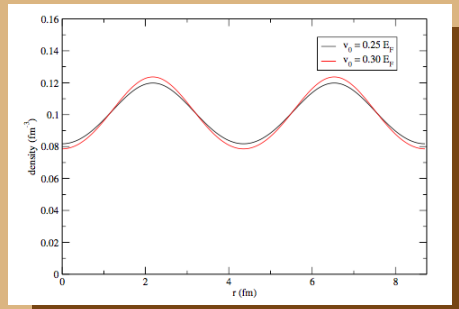


Credit: Dany Page

Motivation



Nuclear methods



Recent results

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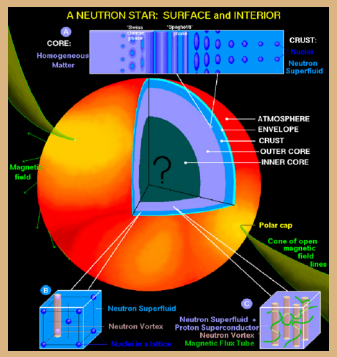

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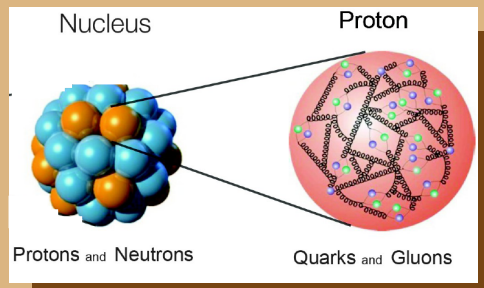

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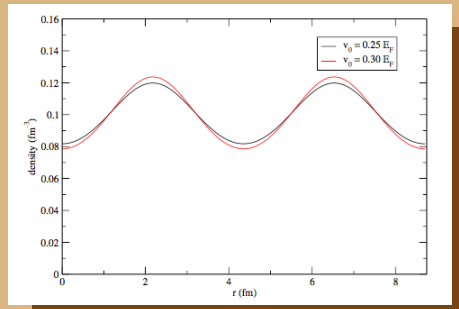

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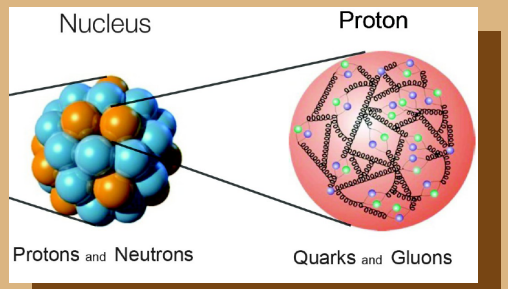
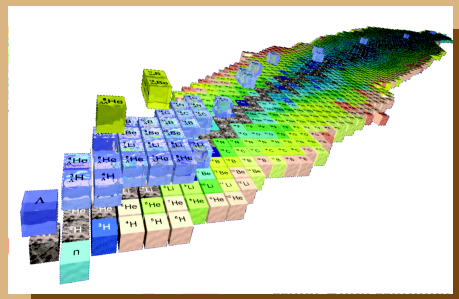
Physical systems studied

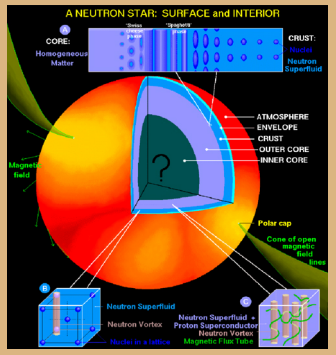
Nuclear forces



Nuclear structure



Nuclear astrophysics



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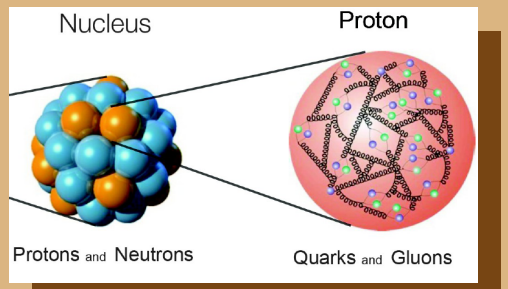

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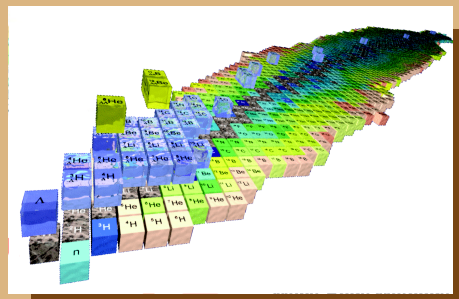

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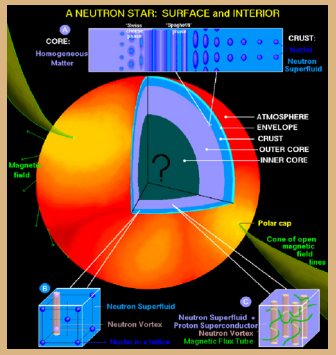

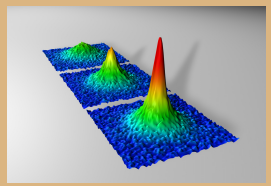

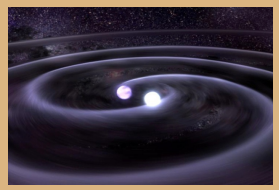

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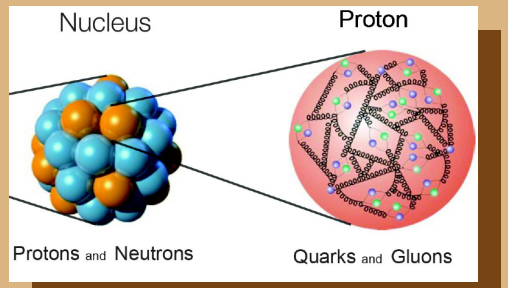
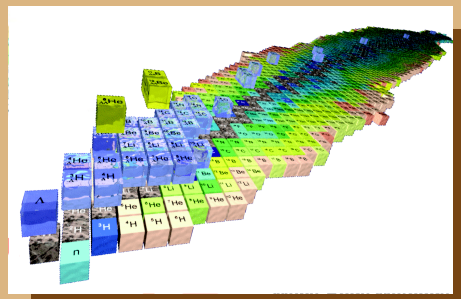


Many nucleons



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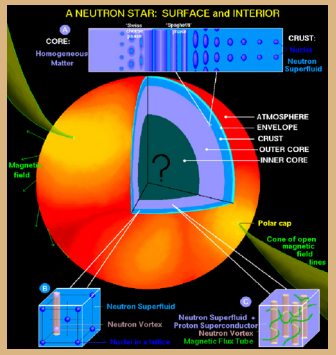

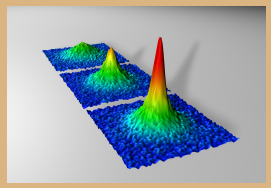

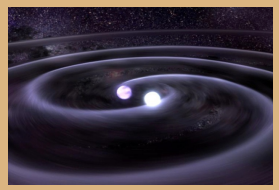

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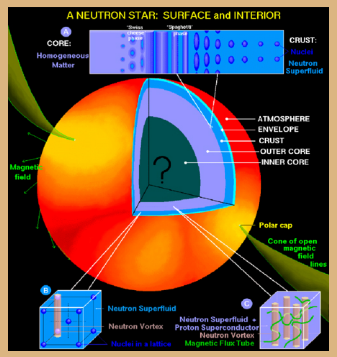

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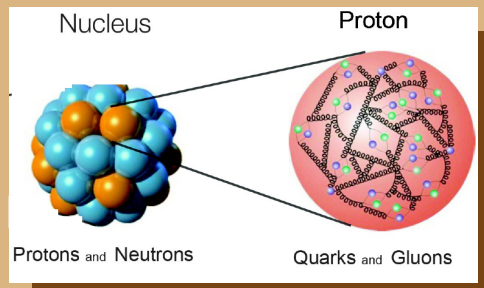

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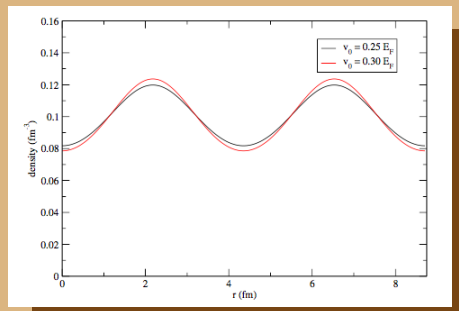

Recent results

Nuclear interactions 1

Historically

"Effective Interactions" were employed in the context of mean-field theory.

Phenomenological

NN interaction fit to N-body experiment

Non-microscopic

NN interaction does not claim to (and will not) describe np scattering

Nuclear physics is difficult

Scattering phase shifts: different “channels” have different behavior.

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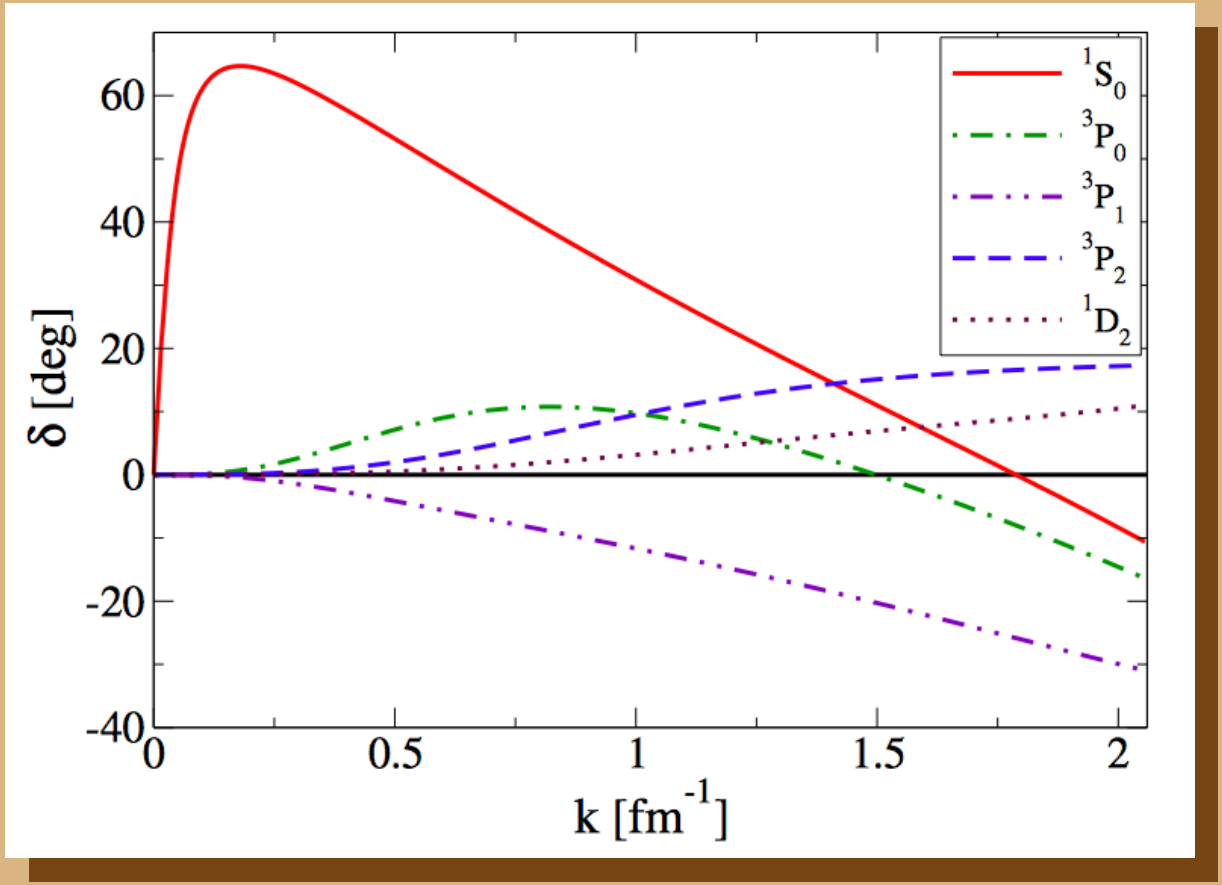

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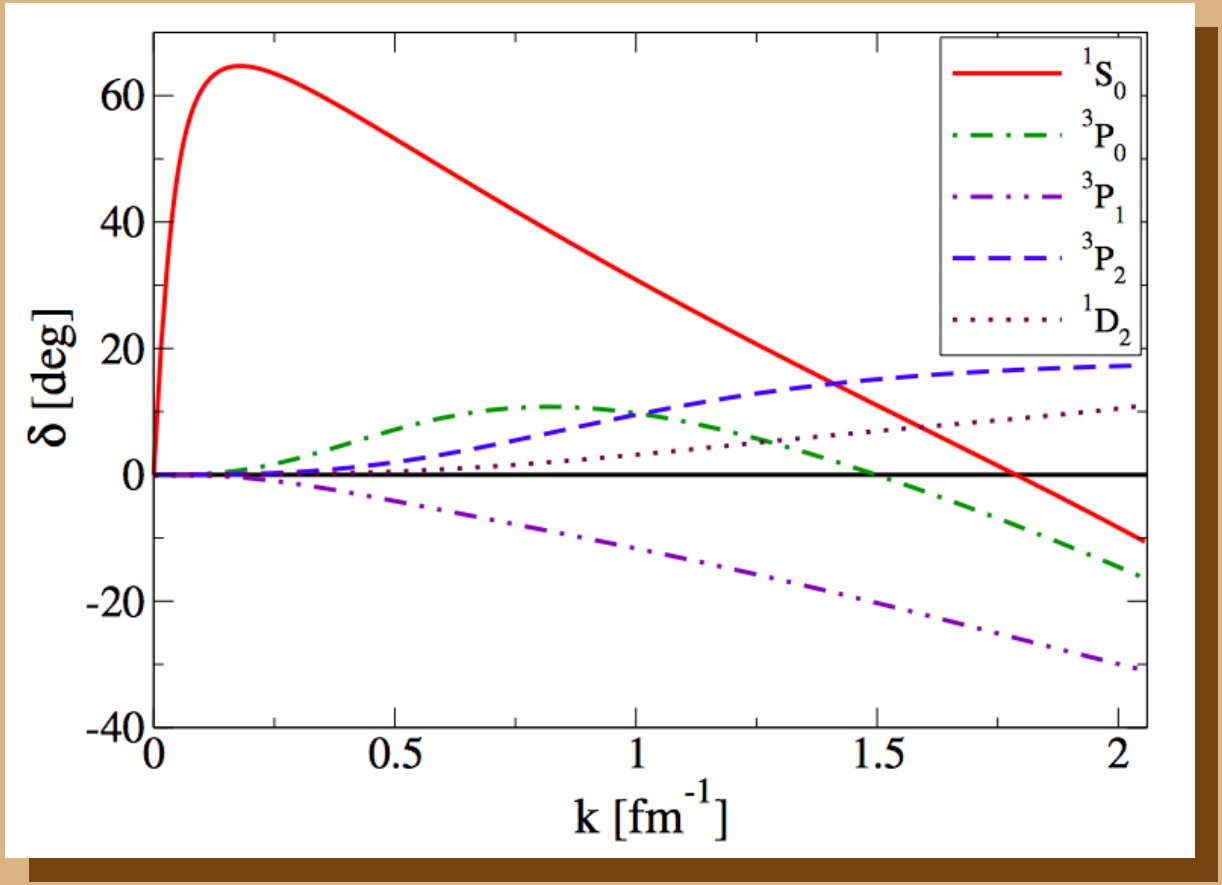
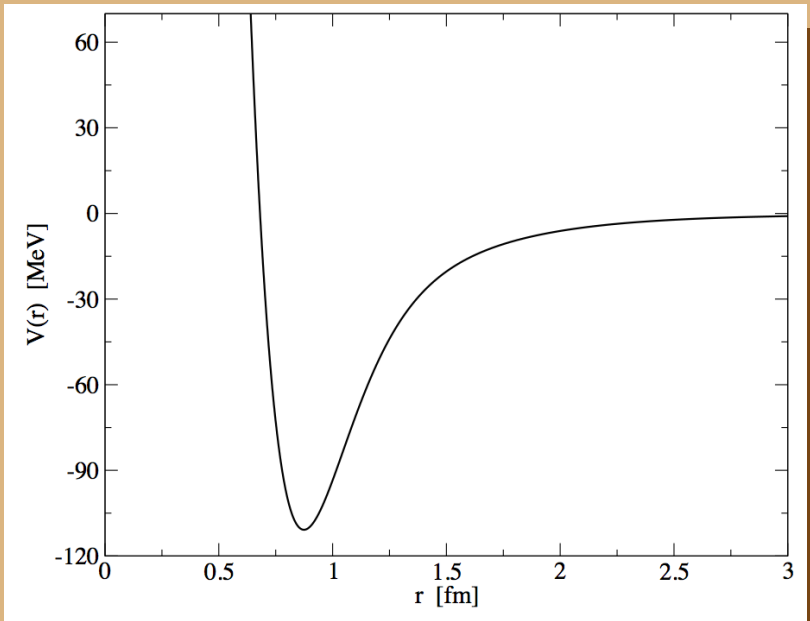


Any potential that reproduces them must be spin (and isospin) dependent

Nuclear interactions 2

Different approach: phenomenology treats NN scattering without connecting with the underlying level



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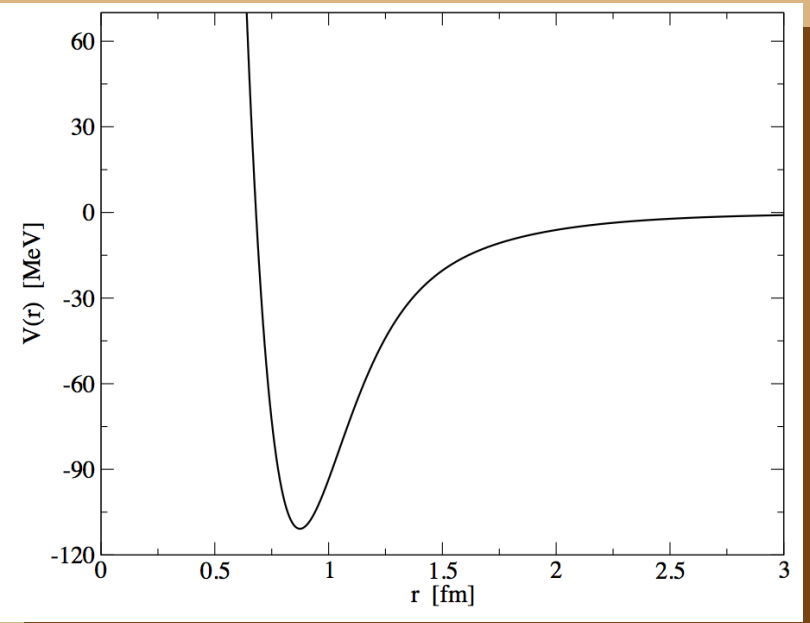
Different approach: phenomenology treats NN scattering without connecting with the underlying level

$$V_2 = \sum_{j<k} v_{jk} = \sum_{j<k} \sum_{p=1}^{8} v_p(r_{jk}) O^{(p)}(j,k)$$

$$O^{p=1,8}(j,k) = (1, \sigma_j \cdot \sigma_k, S_{jk}, \mathbf{L}_{jk} \cdot \mathbf{S}_{jk}) \otimes (1, \tau_j \cdot \tau_k)$$



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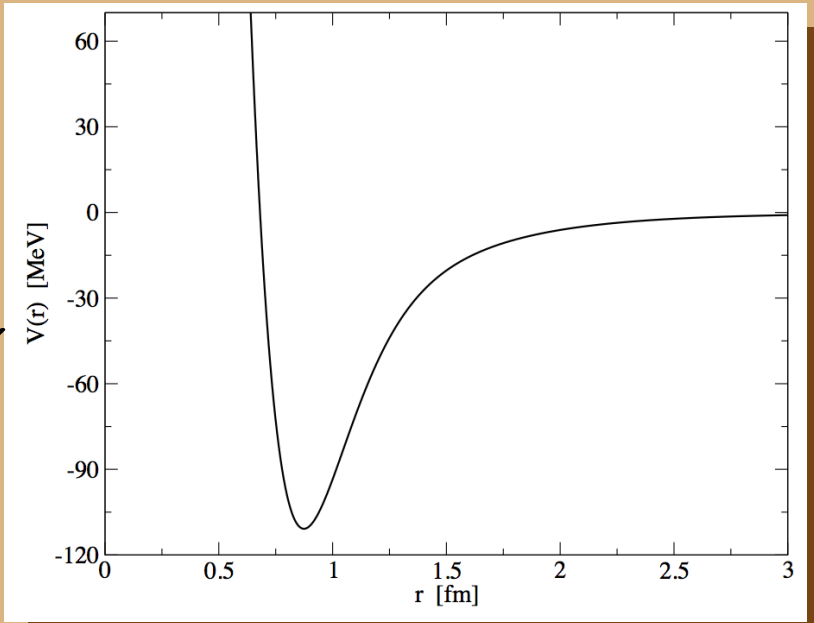

Such potentials are hard, making them non-perturbative at the many-body level (which is a problem for most methods on the market).

Softer, momentum-space formulations like CD-Bonn very popular

How to go beyond?

Historically, fit NN interaction to N-body experiment

Parallel approach, fit NN interaction to 2-body experiment, ignoring underlying level of quarks and gluons

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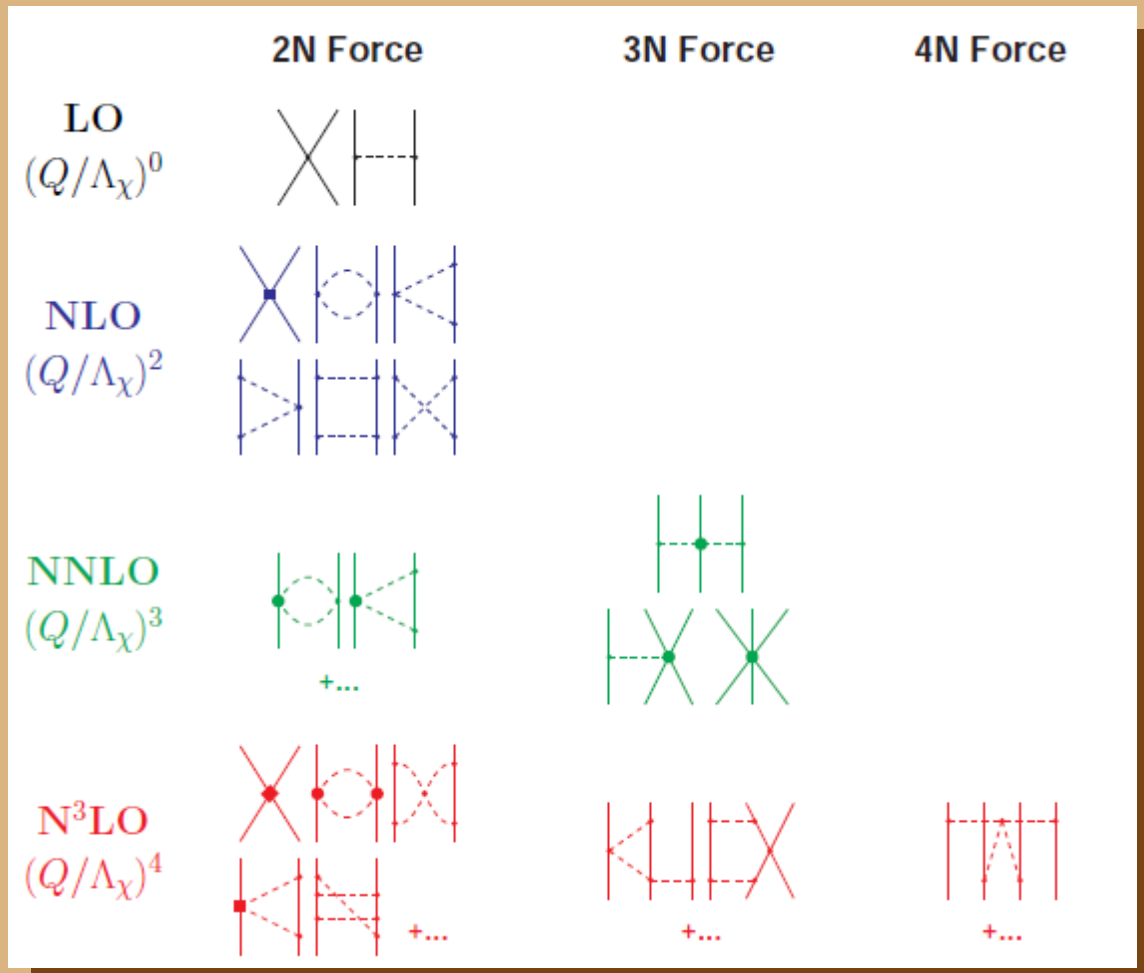
Historically, fit NN interaction to N-body experiment

Parallel approach, fit NN interaction to 2-body experiment, ignoring underlying level of quarks and gluons

Natural goal: fit NN interaction to 2-body experiment, without ignoring underlying level

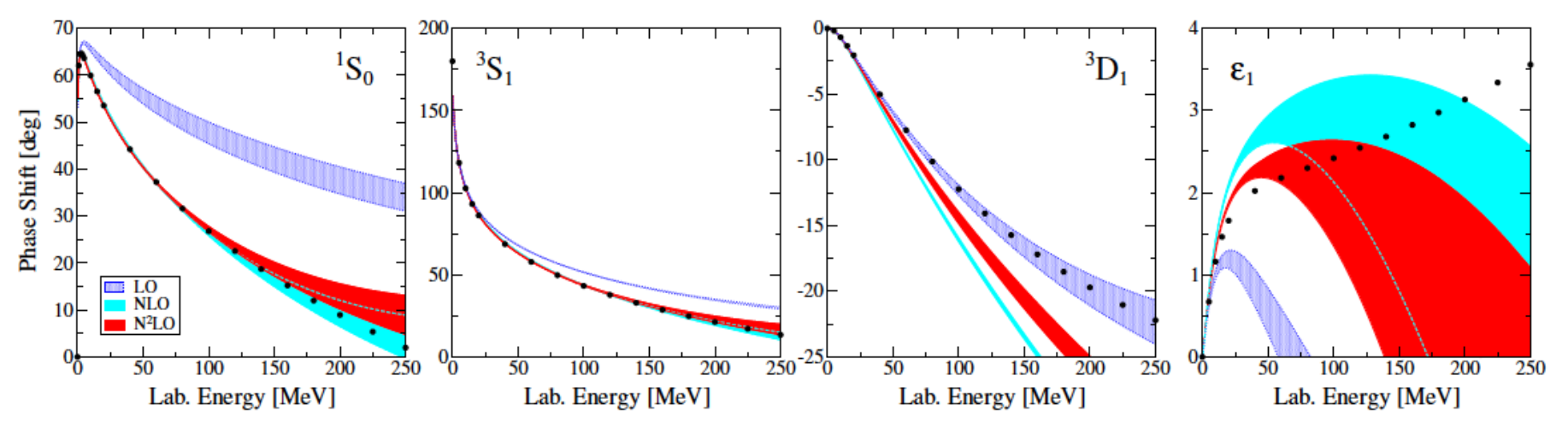
Effective field theory

Nuclear interactions 3



- Attempts to connect with underlying theory (QCD)
- Low-momentum expansion
- Naturally emerging many-body forces
- Low-energy constants from experiment or lattice QCD
- Now available in non-local, local, or semi-local varieties
- Power counting's relation to renormalization still an open question

Local chiral EFT



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I. Tews, S. Gandolfi, **A. Gezerlis**, A. Schwenk, Phys. Rev. C **93**, 024305 (2016)

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P. Klos, J. E. Lynn, I. Tews, S. Gandolfi, **A. Gezerlis**, H.-W. Hammer, and A. Schwenk, Phys. Rev. C, **94**, 054005 (2017)

But even with the interaction in place,
how do you solve the many-body problem?

Nuclear many-body problem

$$H\Psi = E\Psi$$

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so

$$H\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_A; s_1, \cdots, s_A; t_1, \cdots, t_A) = E\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_A; s_1, \cdots, s_A; t_1, \cdots, t_A)$$

i.e. $2^A \binom{A}{Z}$ complex coupled second-order differential equations

Main many-body methods employed (by me)

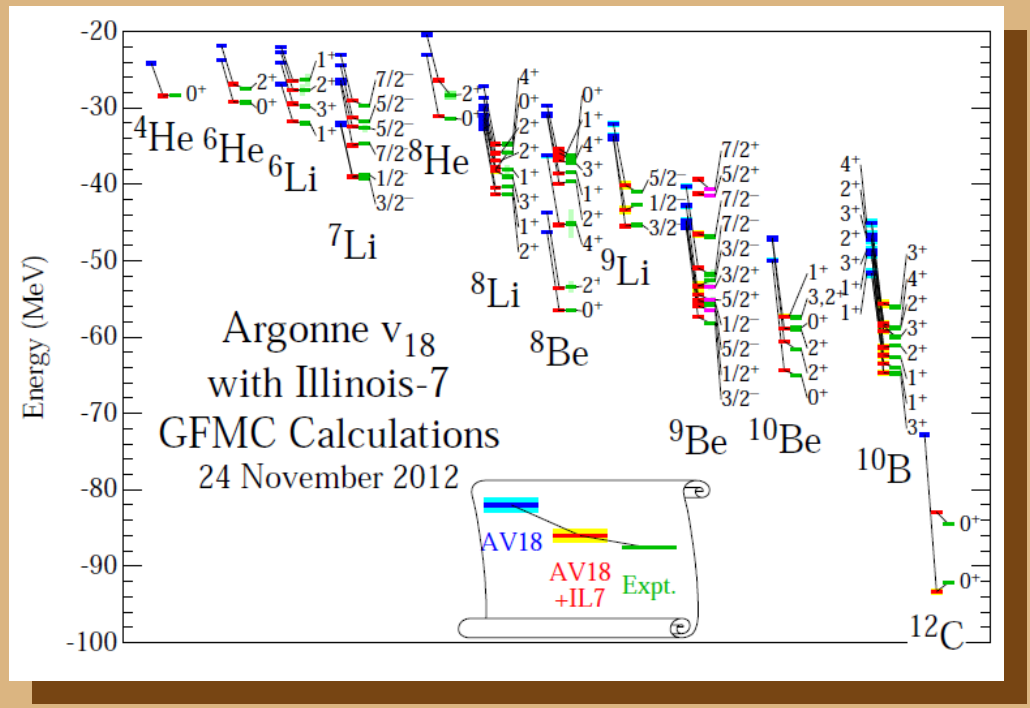
Two complementary methods

Quantum Monte Carlo

- Microscopic
- Computationally demanding (3N particle coordinates + spins)
- Limited to smallish N

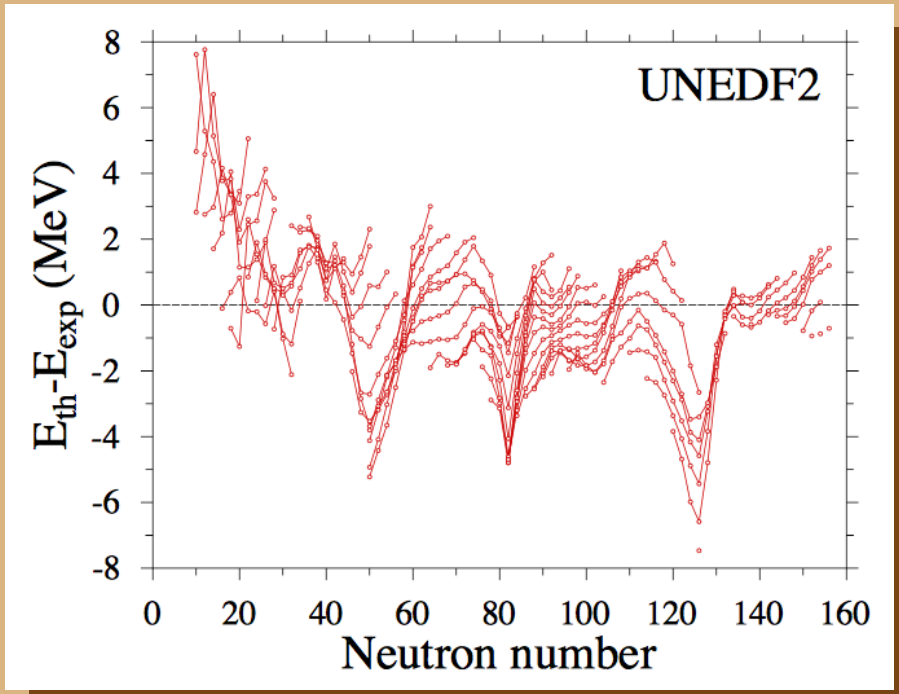
$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H} - E_T)\tau} \Psi_V$$

$$\to \alpha_0 e^{-(E_0 - E_T)\tau} \Psi_0$$



Credit: Steve Pieper

Two complementary methods



Credit: W. Nazarewicz

Density Functional Theory

- More phenomenological (to date, but see major developments)
- Easier in crude form (orbitals → density → energy density)
- Can do any large N

$$E = \int d^3r \, \{\mathcal{E}[\rho(\mathbf{r})] + \rho(\mathbf{r}) V_{\text{ext}}(\mathbf{r})\}$$

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Research Strategies

i) Use QMC as a benchmark with which to compare DFT results
ii) Constrain DFT with QMC, then use DFT to make predictions

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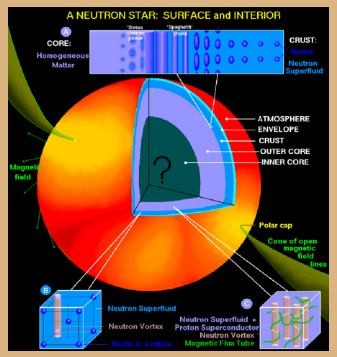

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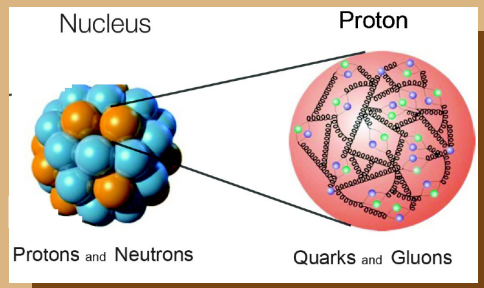
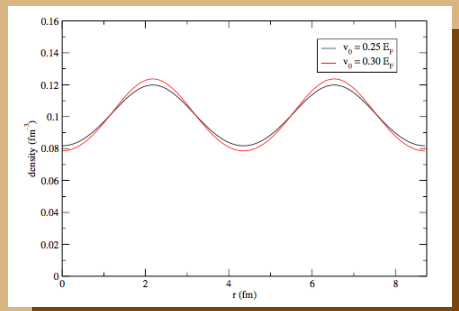


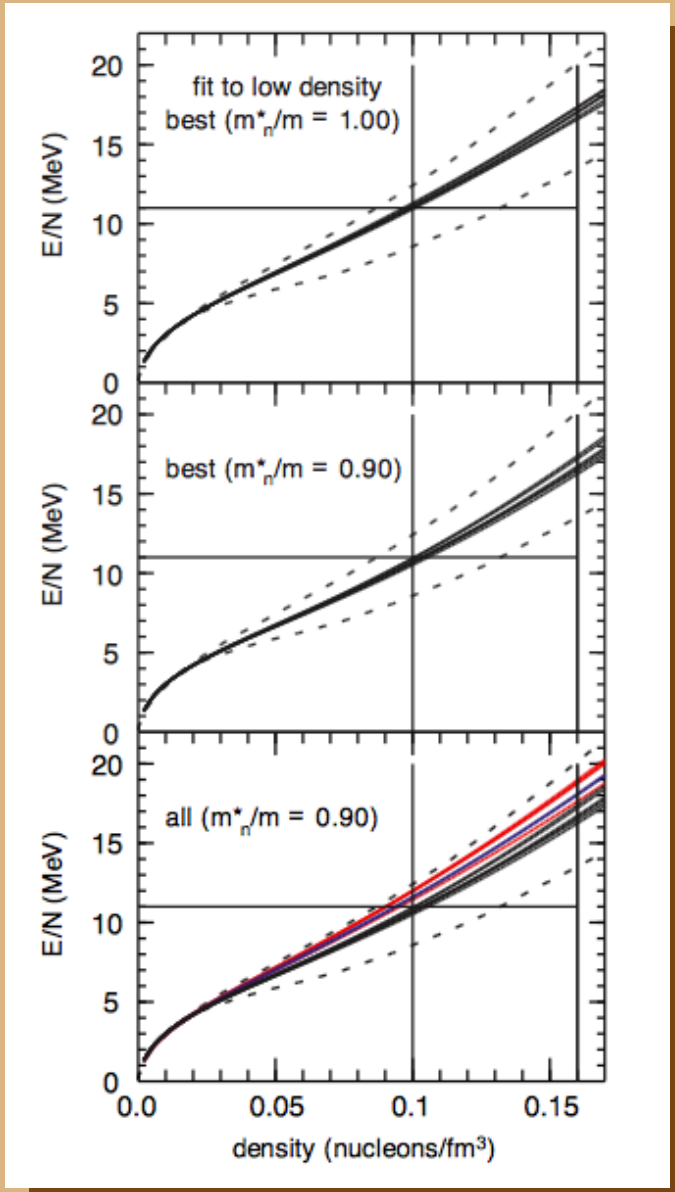
Nuclear background



Recent results

QMC with chiral EFT

From low to high density

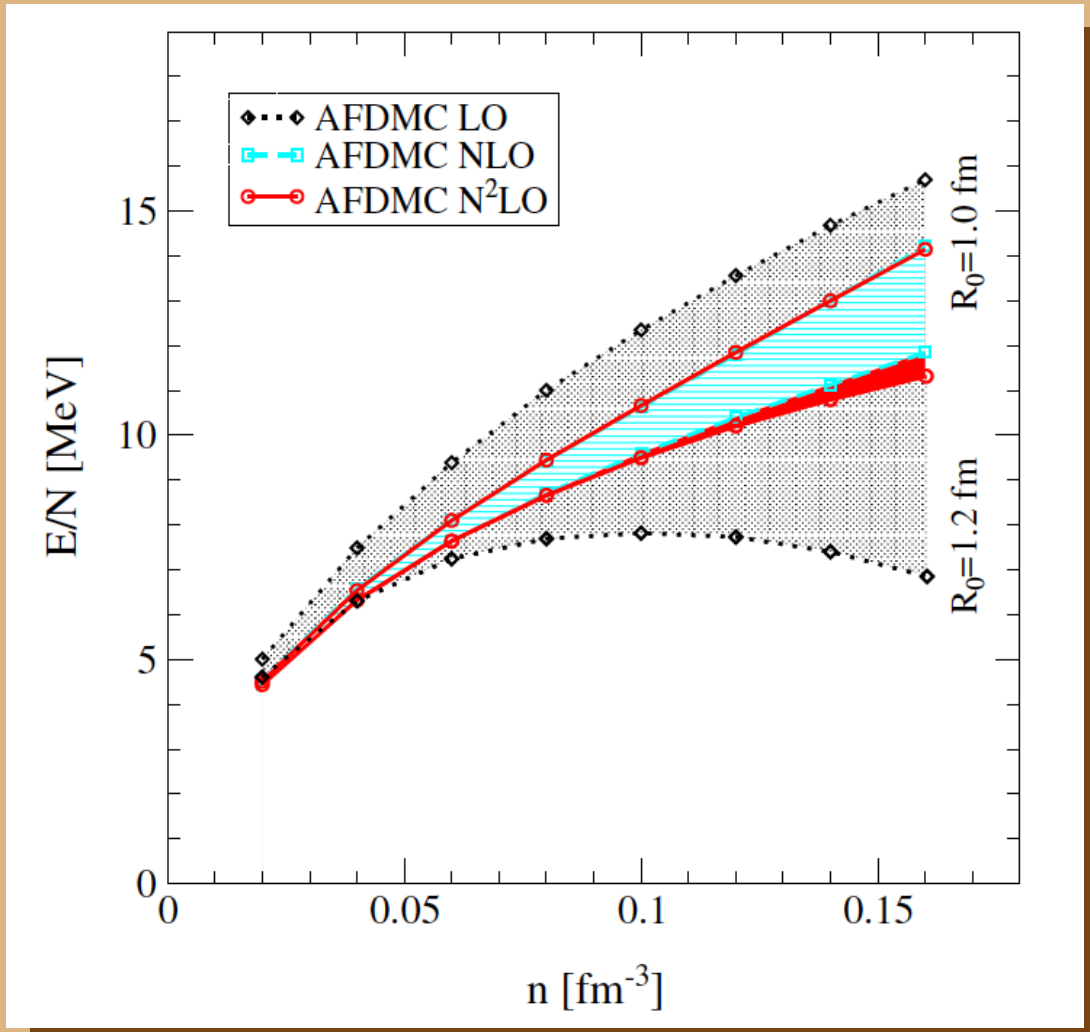


- Ab initio results for low-density matter under control
- Doubly-magic input better constrained at higher density

NEUTRONS

B. A. Brown and A. Schwenk, Phys. Rev. C 89, 011307 (2014)

Chiral EFT in QMC



- Use Auxiliary-Field Diffusion Monte Carlo to handle the full interaction
- First ever non-perturbative systematic error bands
- Band sizes to be expected
- Many-body forces will emerge systematically

NEUTRONS

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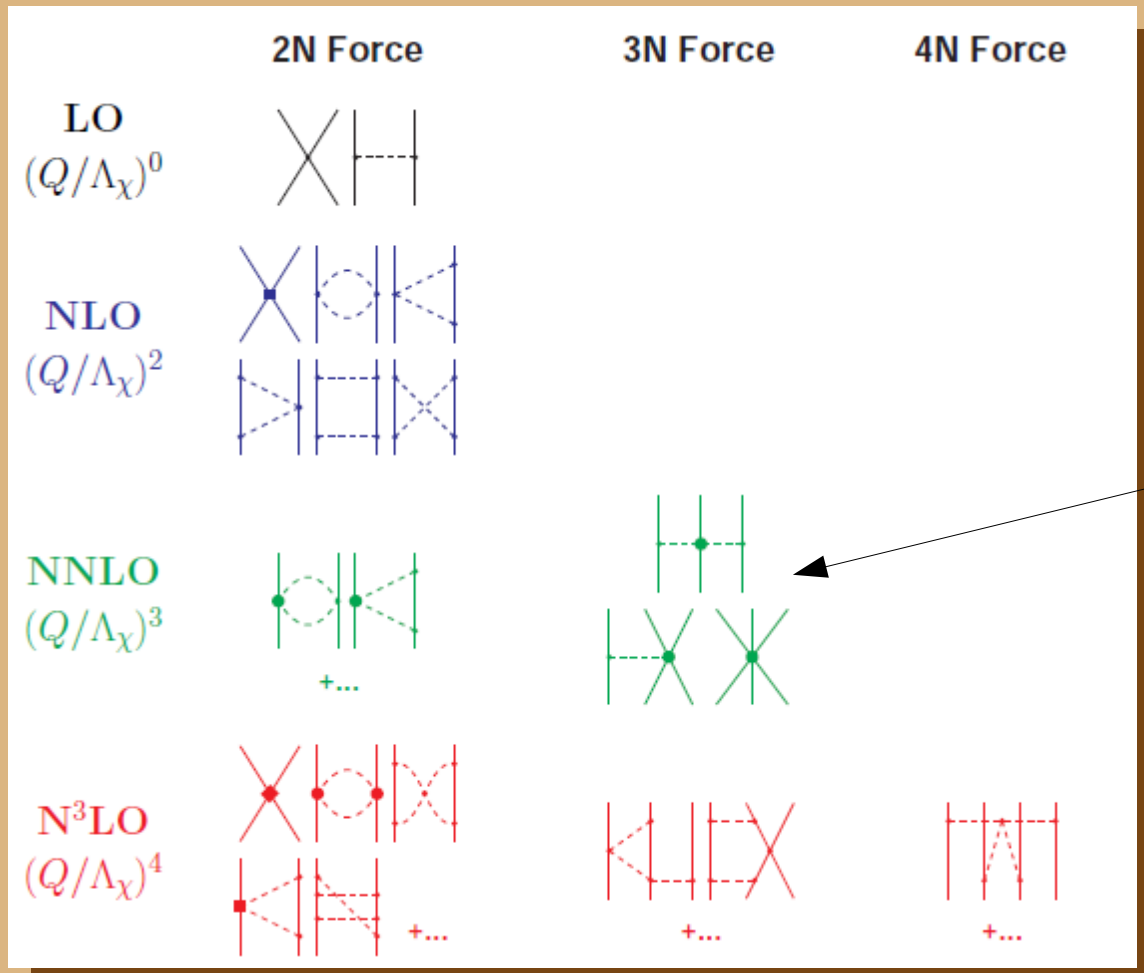
Nuclear Hamiltonian: chiral EFT

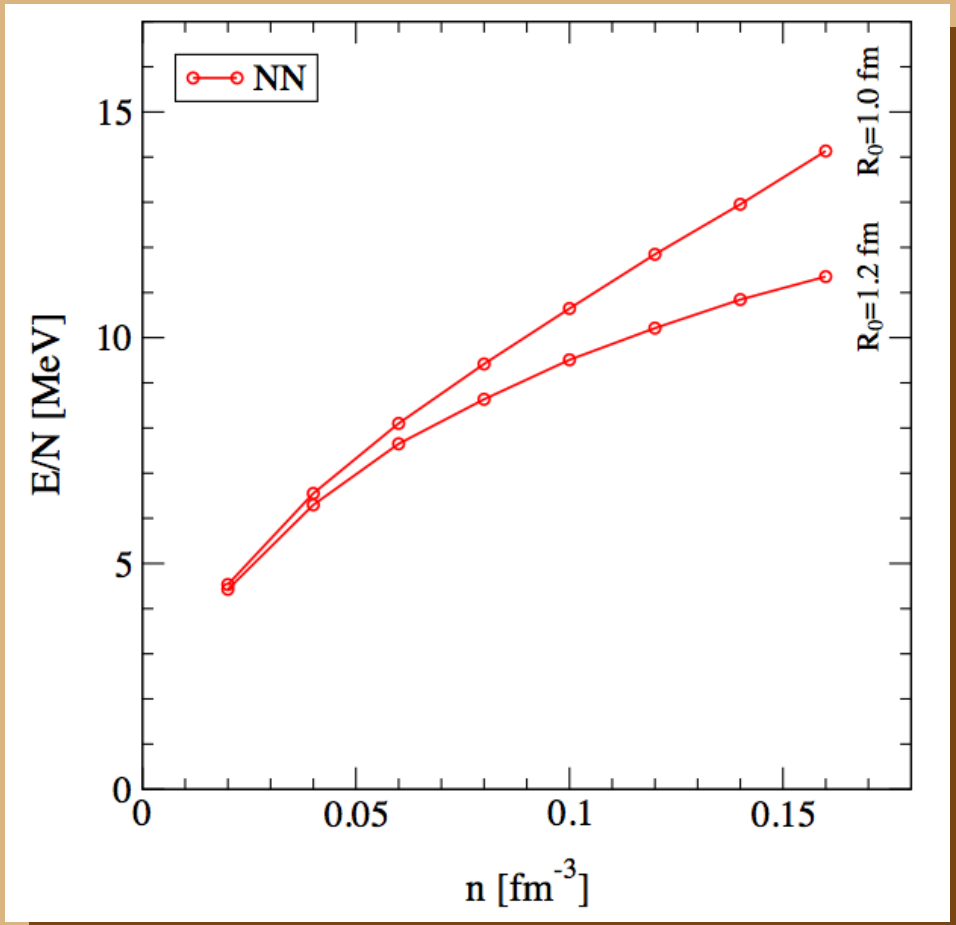


Leading three-nucleon force

- Two-pion exchange (parameter-free)
- One-pion exchange-contact (c_D)
- Three-nucleon contact (c_E)

3NF TPE in PNM

Overall error bands



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I. Tews, S. Gandolfi, A. Gezerlis, A. Schwenk, Phys. Rev. C **93**, 024305 (2016)

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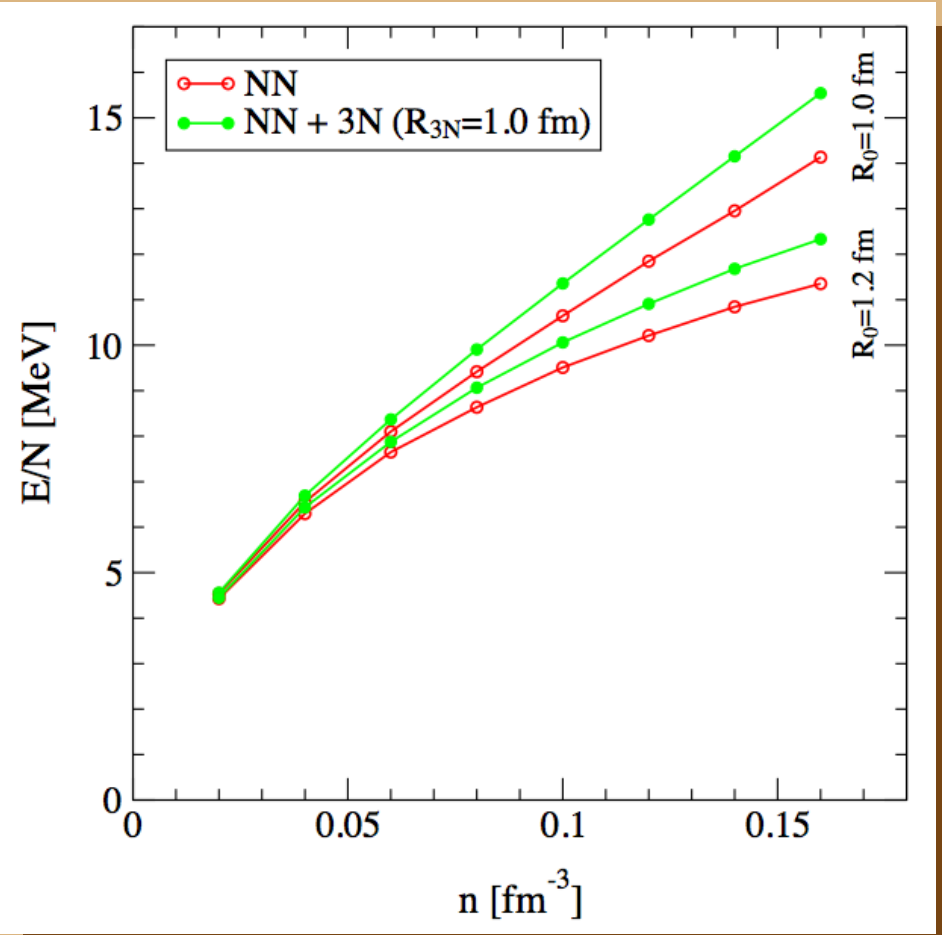

- NN error band already published
- Now vary 3NF cutoff within plateau

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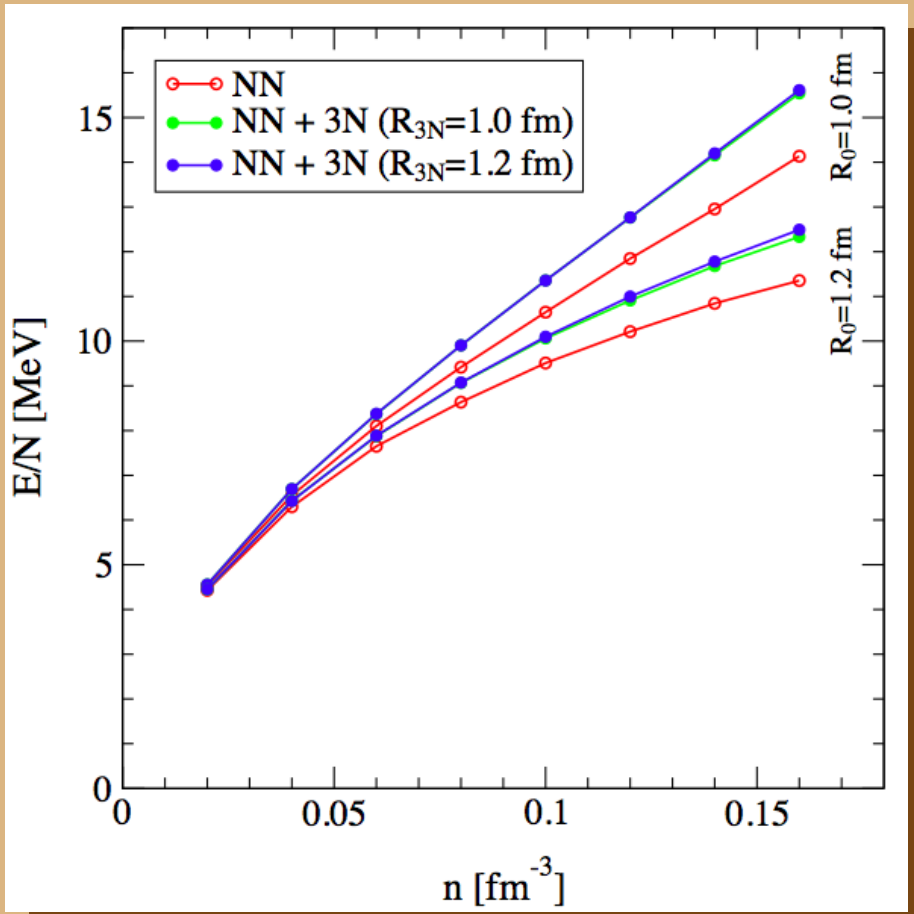

- NN error band already published
- Now vary 3NF cutoff within plateau
- 3NF cutoff dependence tiny in comparison with NN cutoff one
- 3NF contribution 1-1.5 MeV, cf. with MBPT 4 MeV with EGM

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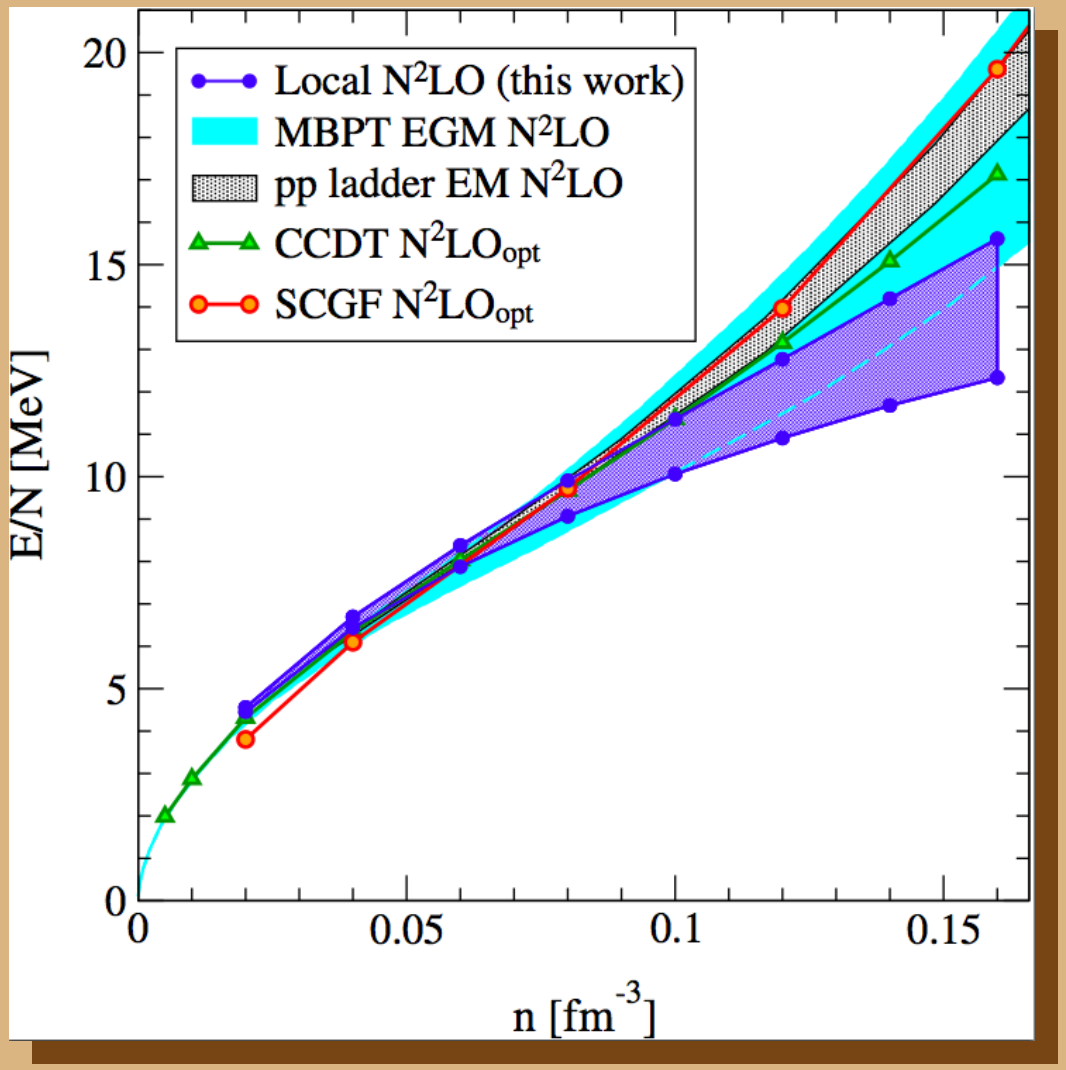
Compare with other calculations at N2LO

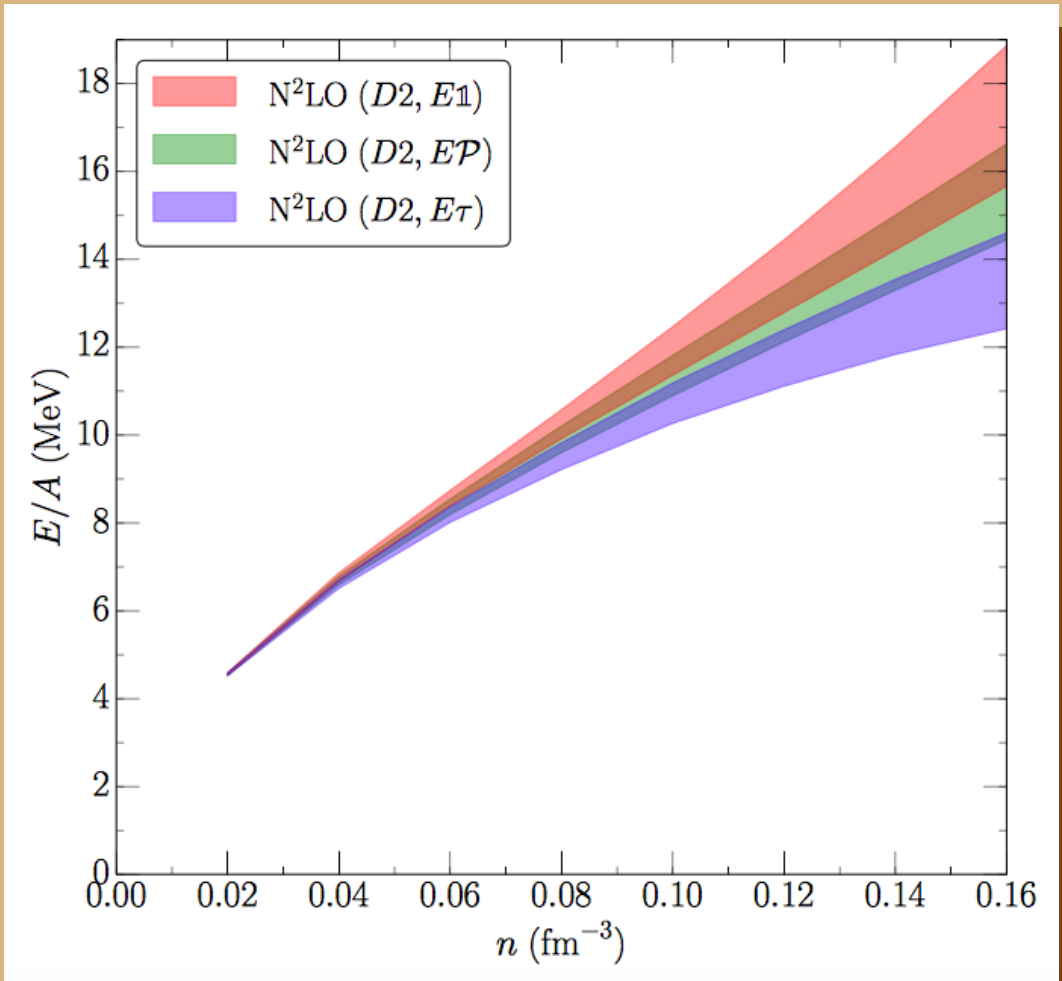


- Overall agreement across methods
- QMC band result of using more than one cutoff
- Band width essentially understood

NEUTRONS

I. Tews, S. Gandolfi, A. Gezerlis, A. Schwenk, Phys. Rev. C **93**, 024305 (2016)

Overall error bands



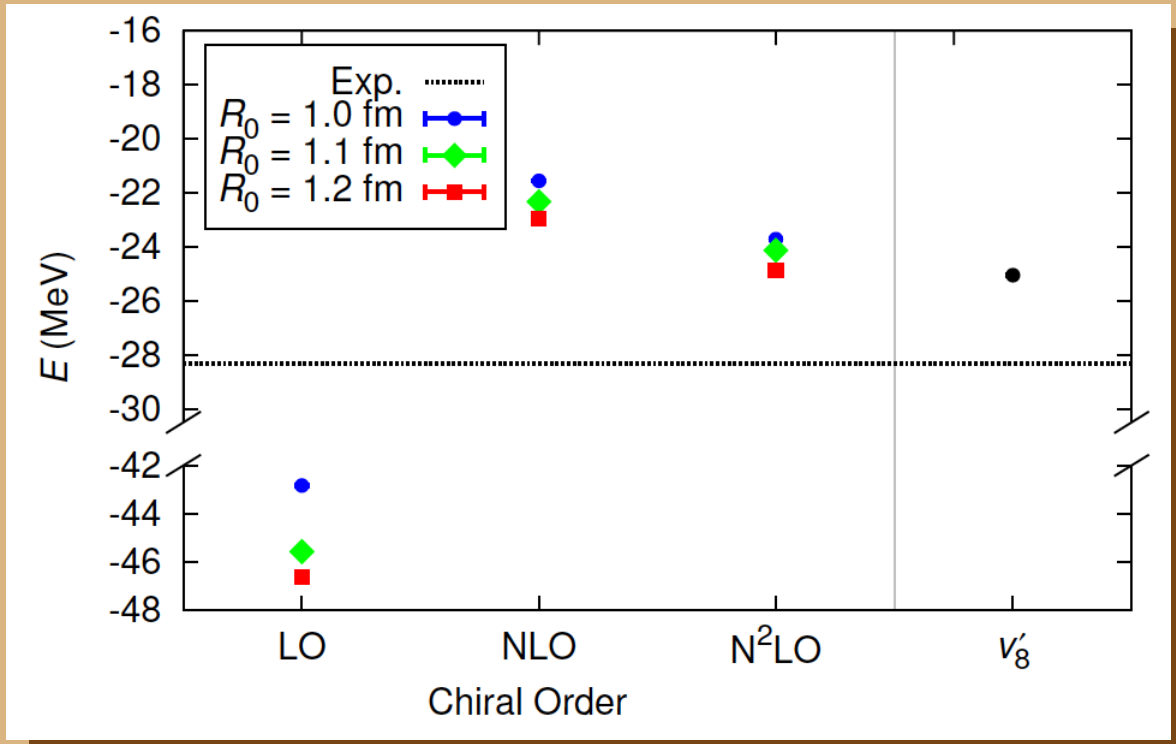
- Updated way of producing error estimate (using LO, NLO, NNLO)
- Fierz ambiguity also in 3NF

NEUTRONS

J. E. Lynn, I. Tews, J. Carlson, S. Gandolfi, A. Gezerlis, K. E. Schmidt, A. Schwenk, I. Tews, Phys. Rev. Lett. **116**, 062501 (2016)

Now turn to light nuclei

Nuclear GFMC with chEFT: 4He

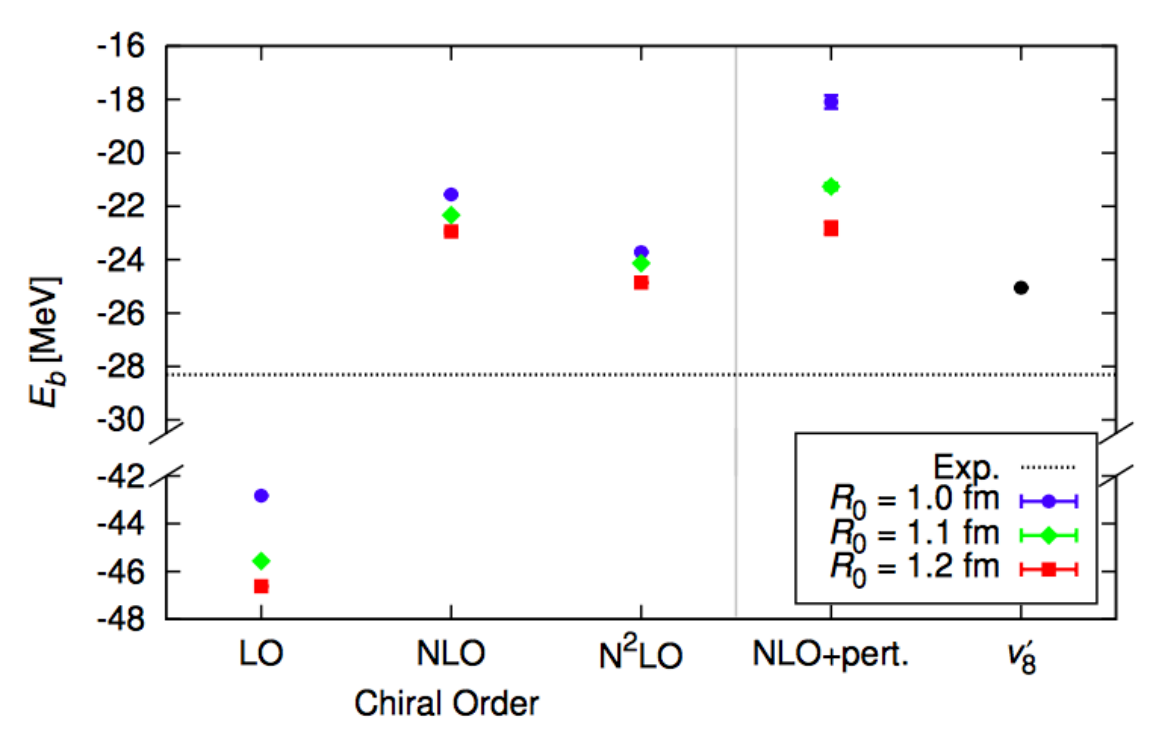


- Binding energy of ^{4}He
- Non-perturbative systematic error bands
- All results are strong force + Coulomb, no NNN

NUCLEONS

J. E. Lynn, J. Carlson, E. Epelbaum, S. Gandolfi, A. Gezerlis, A. Schwenk, Phys. Rev. Lett. **113**, 192501 (2014)

Nuclear GFMC with chEFT: 4He

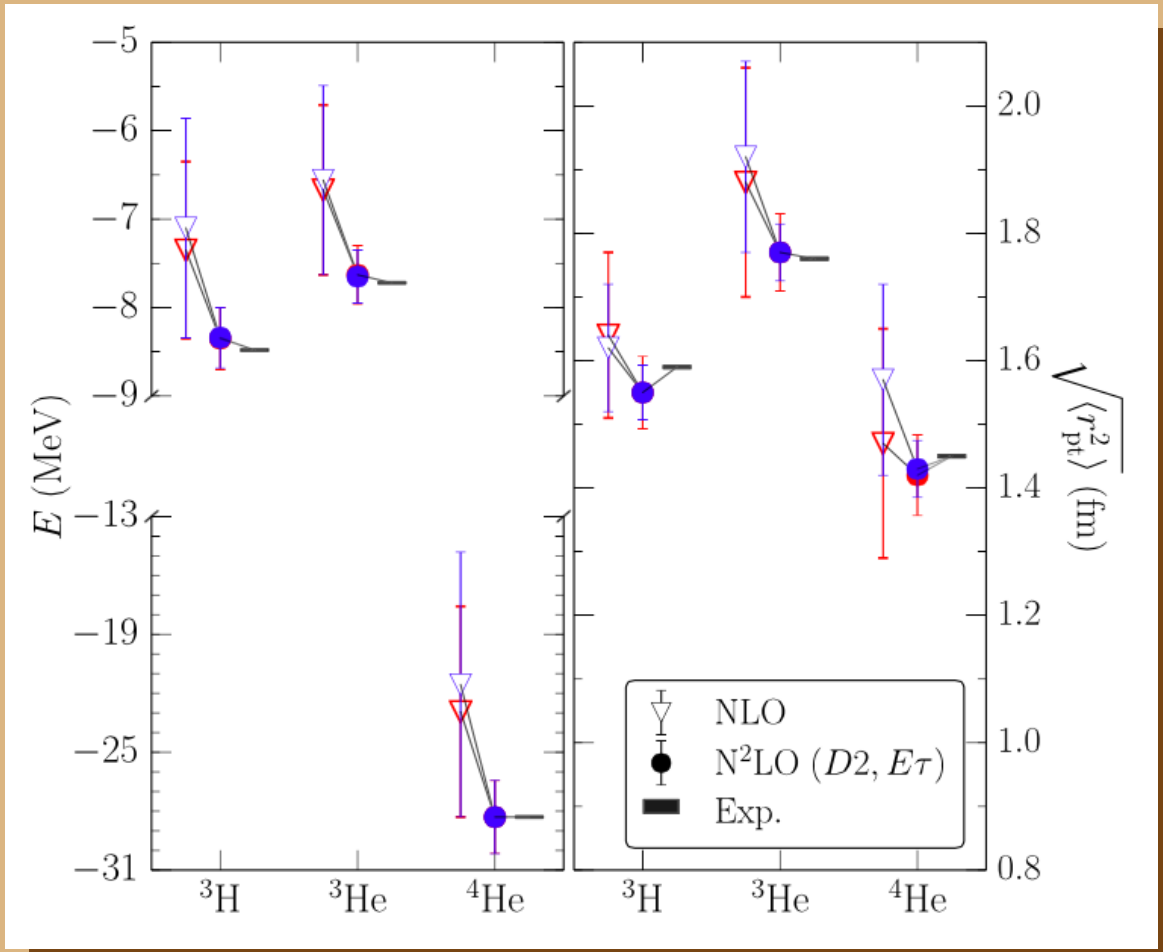


- Binding energy of ^{4}He
- All results are strong force + Coulomb, no NNN
- Example of doing one interaction perturbatively and another one non-perturbatively

NUCLEONS

J. E. Lynn, J. Carlson, E. Epelbaum, S. Gandolfi, A. Gezerlis, A. Schwenk, Phys. Rev. Lett. **113**, 192501 (2014)

Nuclear GFMC with chEFT: NN+3NF



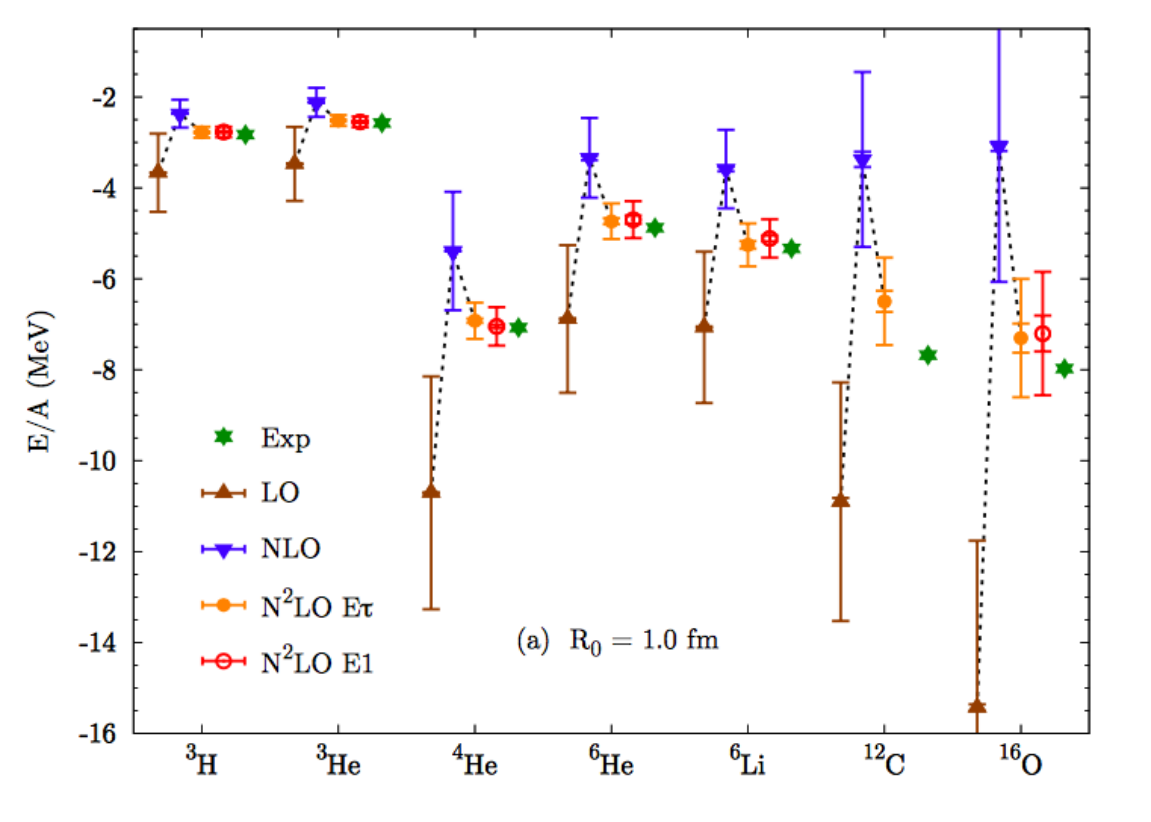
- Use c_D and c_E we fit
- Shown are both binding energies and point proton radii
- Things look reasonably good

NUCLEONS

J. E. Lynn, I. Tews, J. Carlson, S. Gandolfi, A. Gezerlis, K. E. Schmidt, A. Schwenk, I. Tews, Phys. Rev. Lett. **116**, 062501 (2016)

J. E. Lynn, I. Tews, J. Carlson, S. Gandolfi, A. Gezerlis, K. E. Schmidt, A. Schwenk, I. Tews, Phys. Rev. C **96**, 054007 (2017)

AFDMC with chEFT: NN+3NF

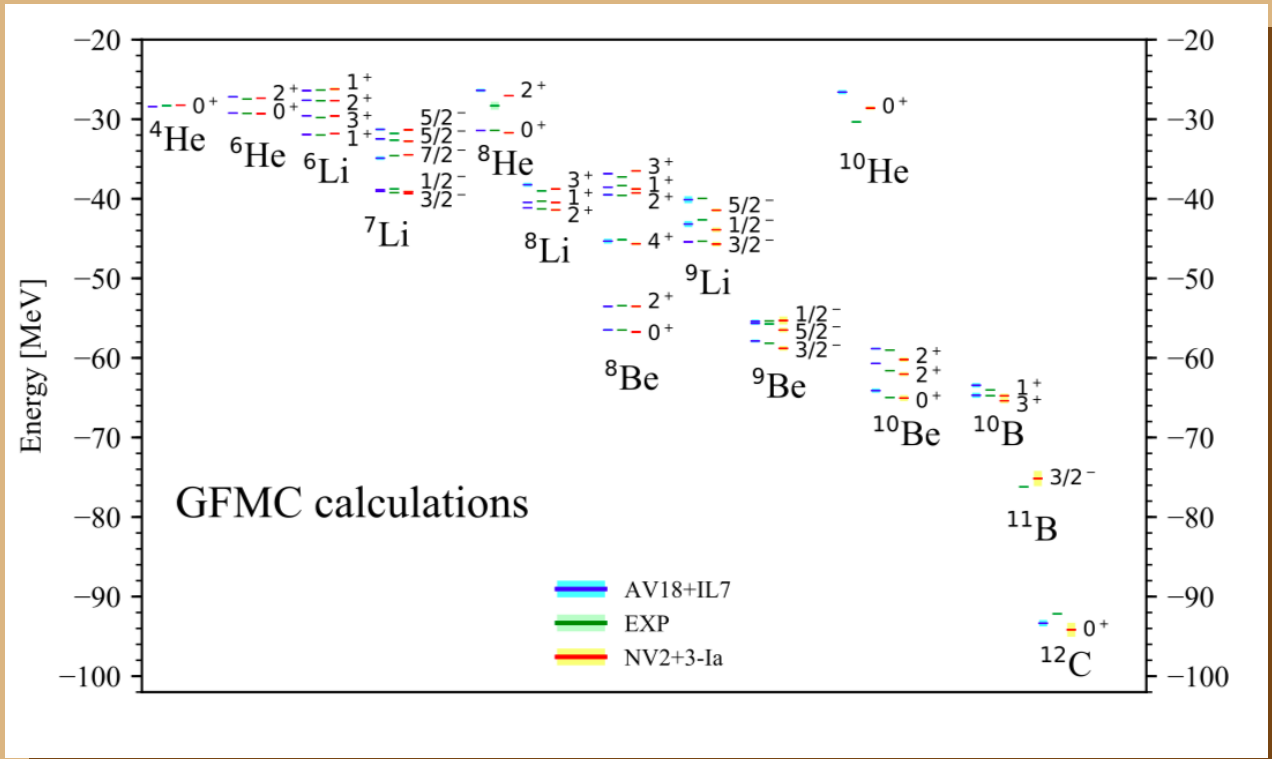


- AFDMC with better wave function
- Same local chiral EFT interactions as above
- Can be pushed to heavier masses

NUCLEONS

D. Lonardoni et al, Phys. Rev. C **97**, 044318 (2018)

Nuclear GFMC with chEFT



- GFMC with very good wave functions
- Different local chiral EFT interactions than above
- 37 states shown, with 60 more probed

NUCLEONS

M. Piarulli et al, Phys. Rev. C **120**, 052503 (2018)

AFDMC with pionless EFT

4He

Λ	m_π = 140 MeV
2 fm^{-1}	−23.17 ± 0.02
4 fm^{-1}	−23.63 ± 0.03
6 fm^{-1}	−25.06 ± 0.02
8 fm^{-1}	−26.04 ± 0.05
$\rightarrow \infty$	$-30^{\pm 0.3\,(\mathrm{sys})}_{\pm 2\,(\mathrm{stat})}$
Exp.	−28.30

16O

Λ	m_π = 140 MeV
2 fm^{-1}	−97.19 ± 0.06
4 fm^{-1}	−92.23 ± 0.14
6 fm^{-1}	−97.51 ± 0.14
8 fm^{-1}	−100.97 ± 0.20
$\rightarrow \infty$	$-115^{\pm 1\,(\mathrm{sys})}_{\pm 8\,(\mathrm{stat})}$
Exp.	−127.62

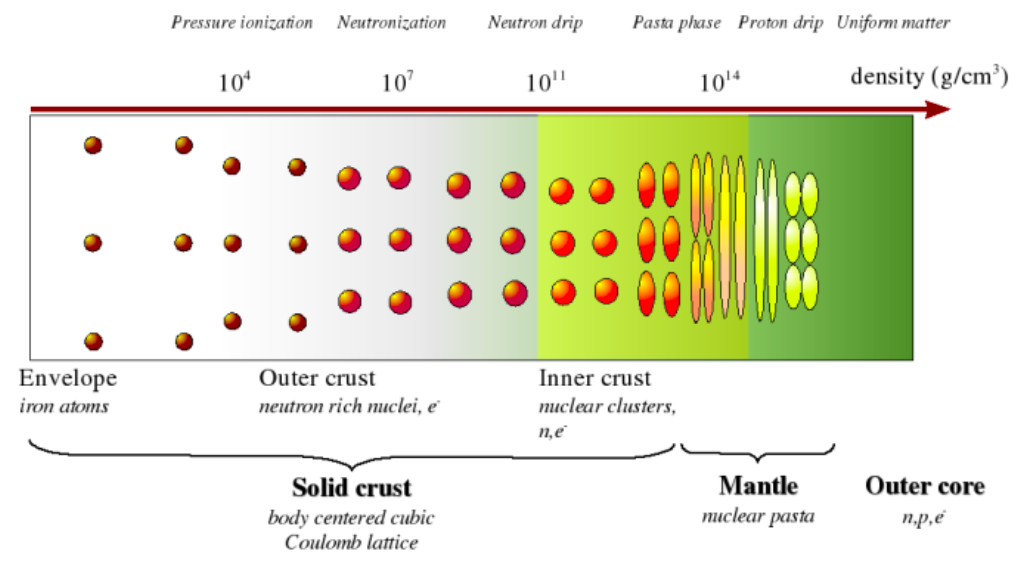
- AFDMC with simple wave function
- LO pionless EFT interaction (with 3NF
- 16O tends to break up into 4He clusters

NUCLEONS

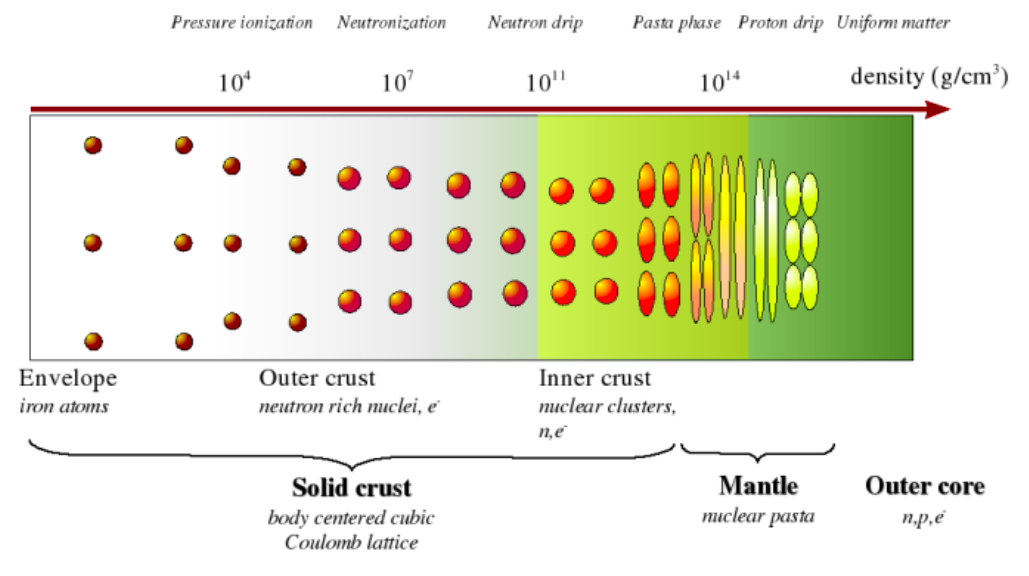
L. Contessi, A. Lovato, F. Pederiva, A. Roggero, J. Kirscher, U. van Kolck, Phys. Lett. **B 07**, 048 (2017)

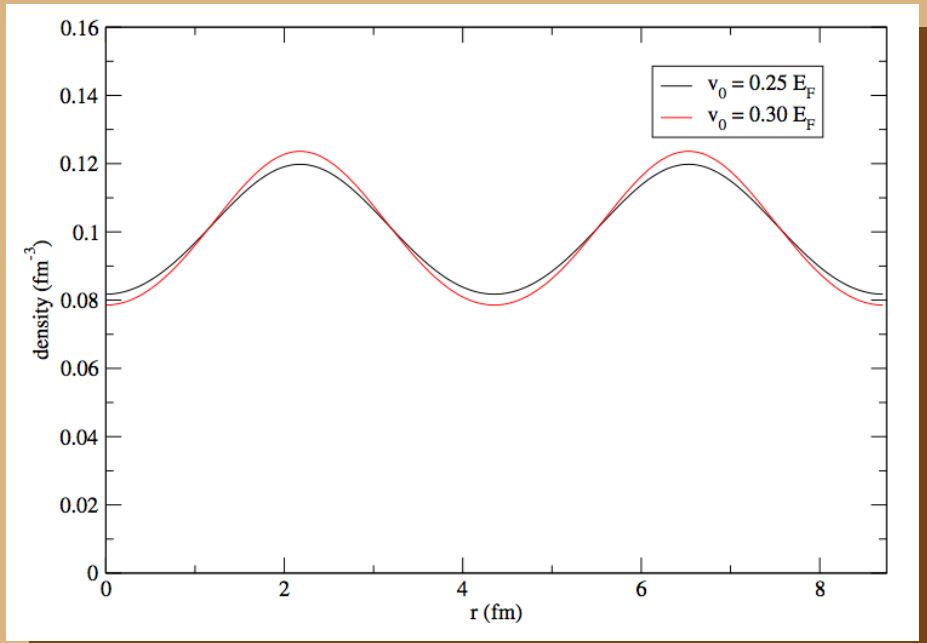
Inhomogeneous matter

Neutron star crusts inhomogeneous

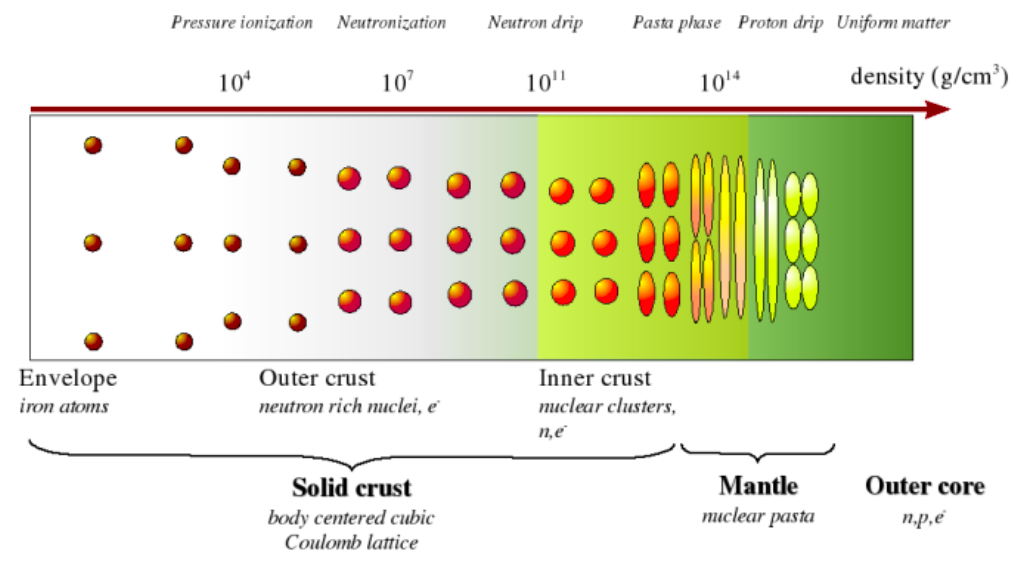


Neutron star crusts inhomogeneous

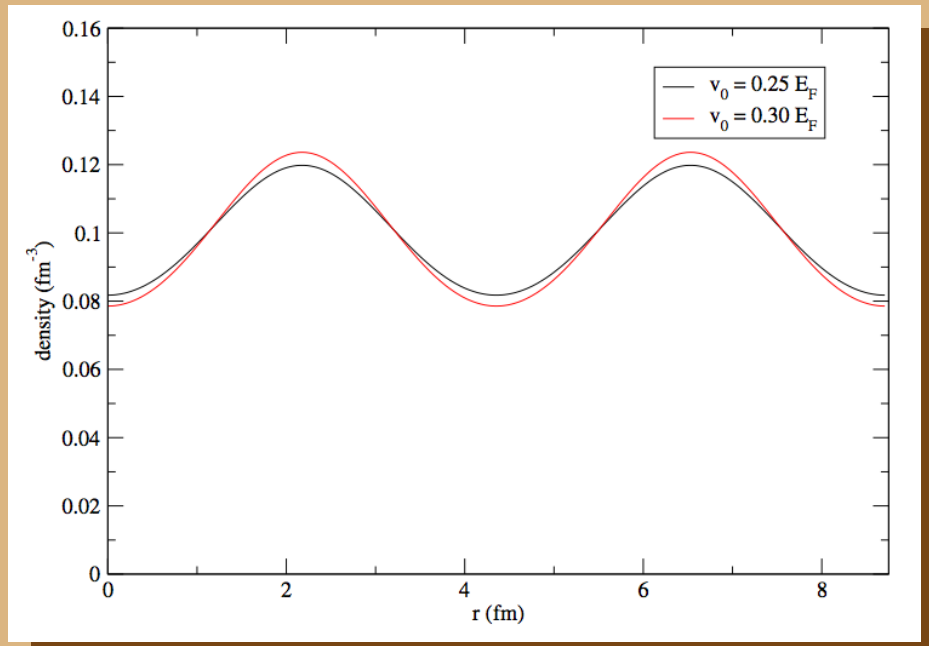




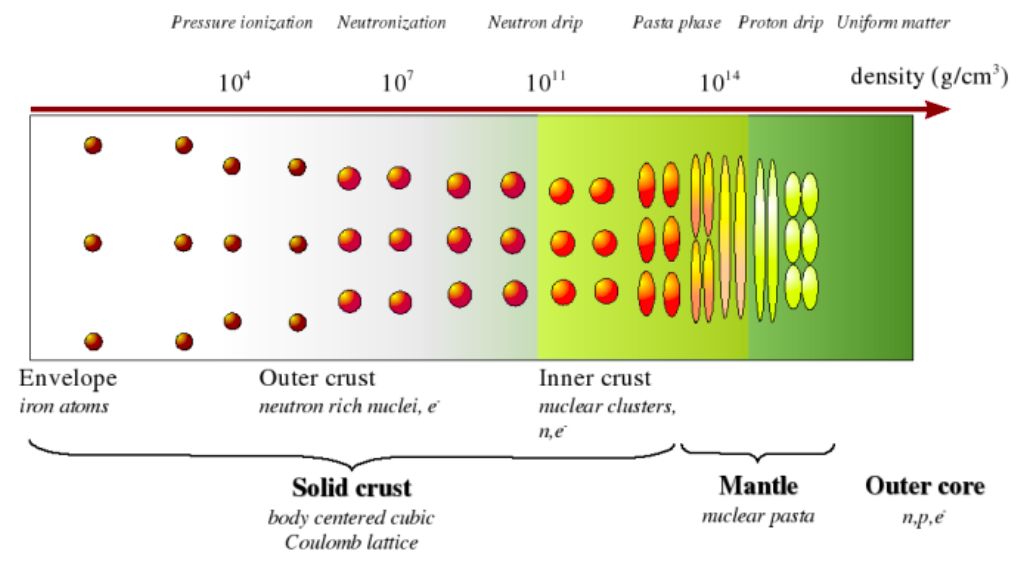
Neutron star crusts inhomogeneous



M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016)

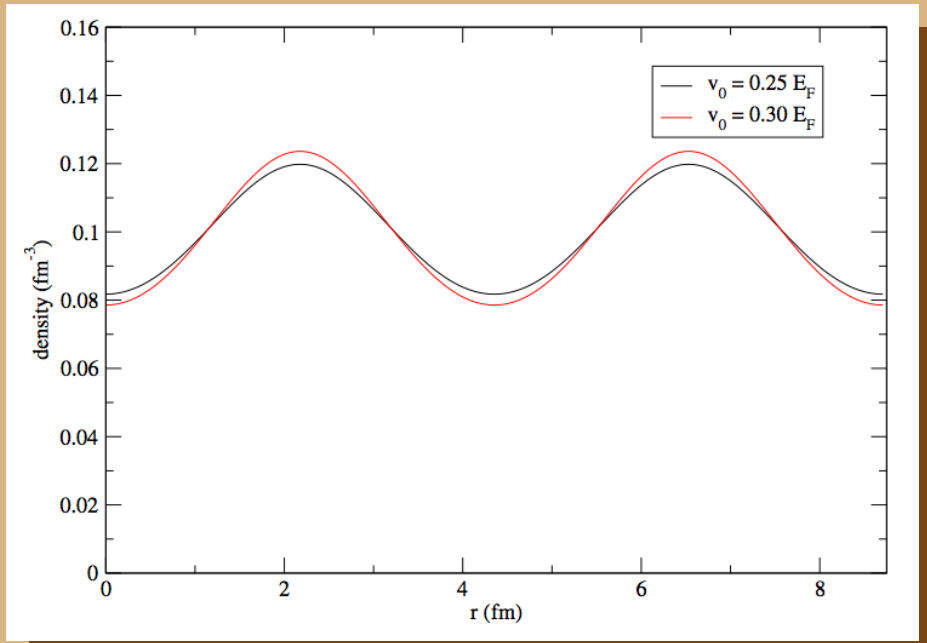


Neutron star crusts inhomogeneous



Situation identical to electrons in solids or atoms in optical lattices

M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016)



Problem setup

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \sum_i 2v_q \cos(\mathbf{q}\cdot\mathbf{r}_i)$$

Problem setup

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \sum_i 2v_q \cos(\mathbf{q}\cdot\mathbf{r}_i)$$

non-relativistic kinetic energy

two-nucleon interaction

three-nucleon interaction

single-particle external potential

Problem setup

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \sum_i 2v_q \cos(\mathbf{q}\cdot\mathbf{r}_i)$$

Trial wave function

$$|\Psi_T\rangle = \prod_{i<j} f(r_{ij})\ \mathcal{A}\left[\prod_i |\phi_i, s_i\rangle\right]$$

Problem setup

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \sum_i 2v_q \cos(\mathbf{q}\cdot\mathbf{r}_i)$$

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single-particle orbitals:
- plane waves
- Mathieu functions

Problem setup

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \sum_i 2v_q \cos(\mathbf{q}\cdot\mathbf{r}_i)$$

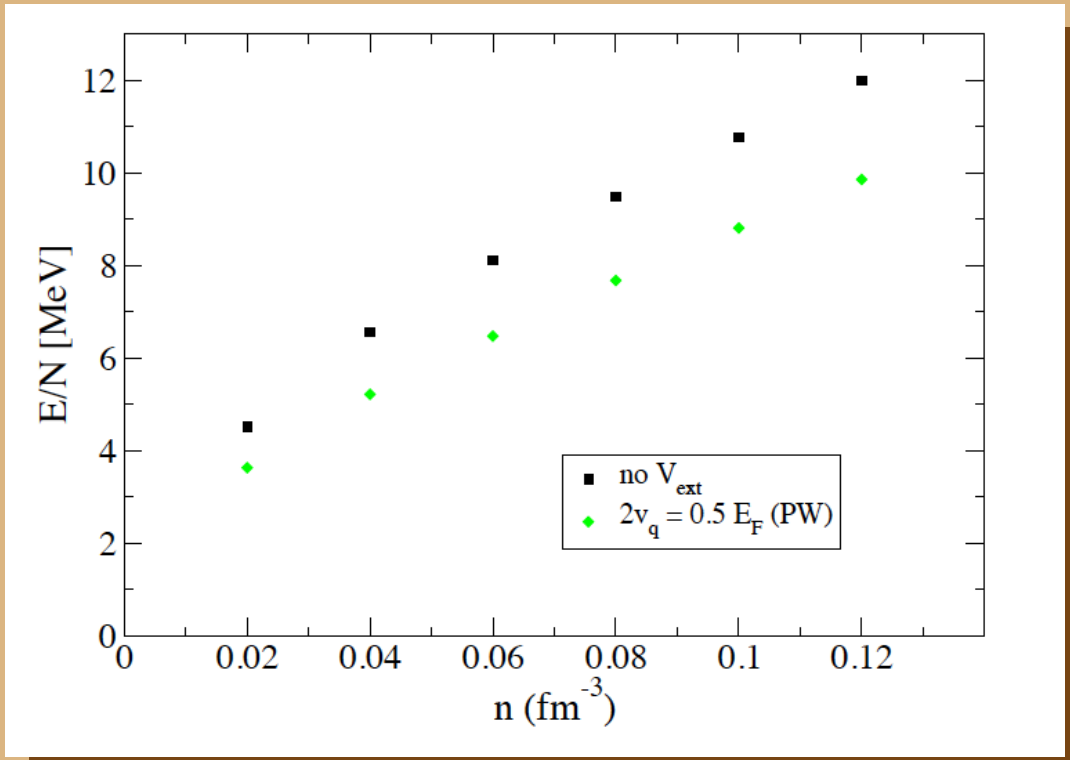
Trial wave function

$$|\Psi_T\rangle = \prod_{i<j} f(r_{ij})\ \mathcal{A}\left[\prod_i |\phi_i, s_i\rangle\right]$$

single-particle orbitals:
- plane waves
- Mathieu functions

Approach: Carry out microscopic QMC calculations for ~100 particles

One periodicity, one strength

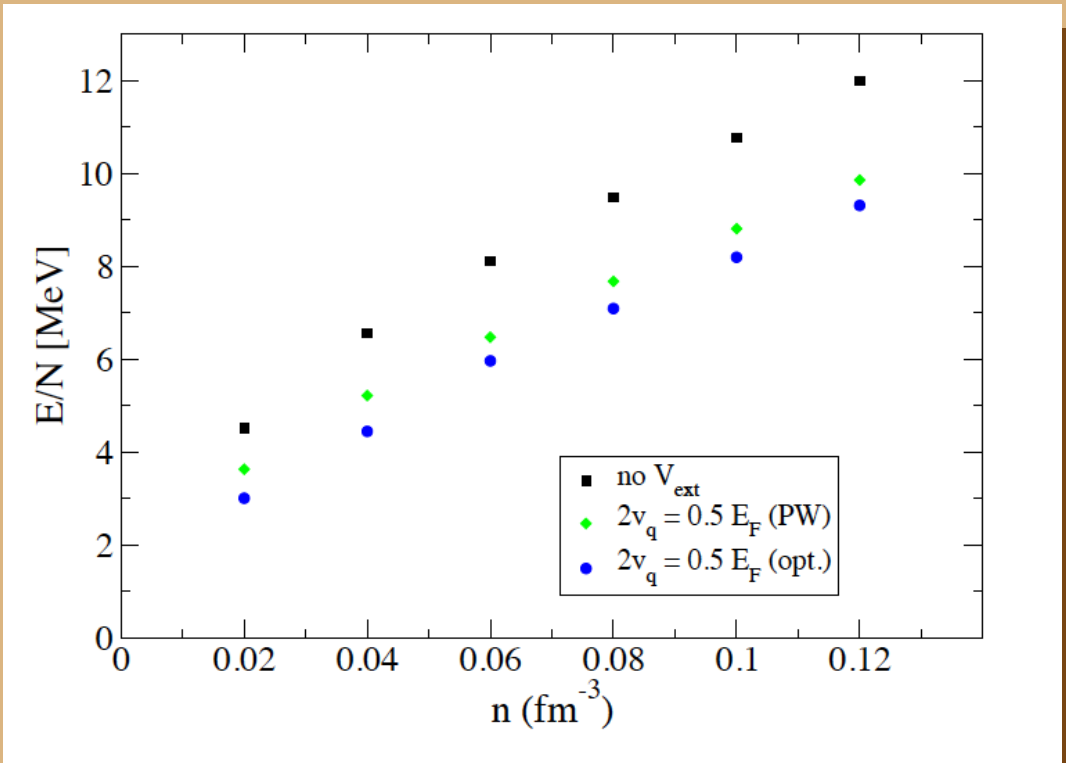


- Periodic potential in addition to nuclear forces
- Energy trivially decreased

M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016)

NEUTRONS

One periodicity, one strength



- Periodic potential in addition to nuclear forces
- Energy trivially decreased
- Considerable dependence on wave function (physics input)
- Microscopic input for energy-density functionals

M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016)

NEUTRONS

Background on DFT

Standard functional in PNM

$$\mathcal{E} = \frac{\hbar^2}{2m}\tau + s_1 n^2 + s_2 n^{\sigma+2} + s_3 n\tau + s_4(\nabla n)^2$$

Background on DFT

Standard functional in PNM

$$\mathcal{E} = \frac{\hbar^2}{2m}\tau + s_1 n^2 + s_2 n^{\sigma+2} + s_3 n\tau + s_4(\nabla n)^2$$

Skyrme functional in isospin representation

$$\mathcal{E}_{\text{Skyrme}} = \sum_{T=0,1}\left[(C_T^{n,a} + C_T^{n,b} n_0^{\sigma})n_T^2 + C_T^{\Delta n}(\nabla n_T)^2 + C_T^{\tau} n_T \tau_T\right]$$

Background on DFT

Standard functional in PNM

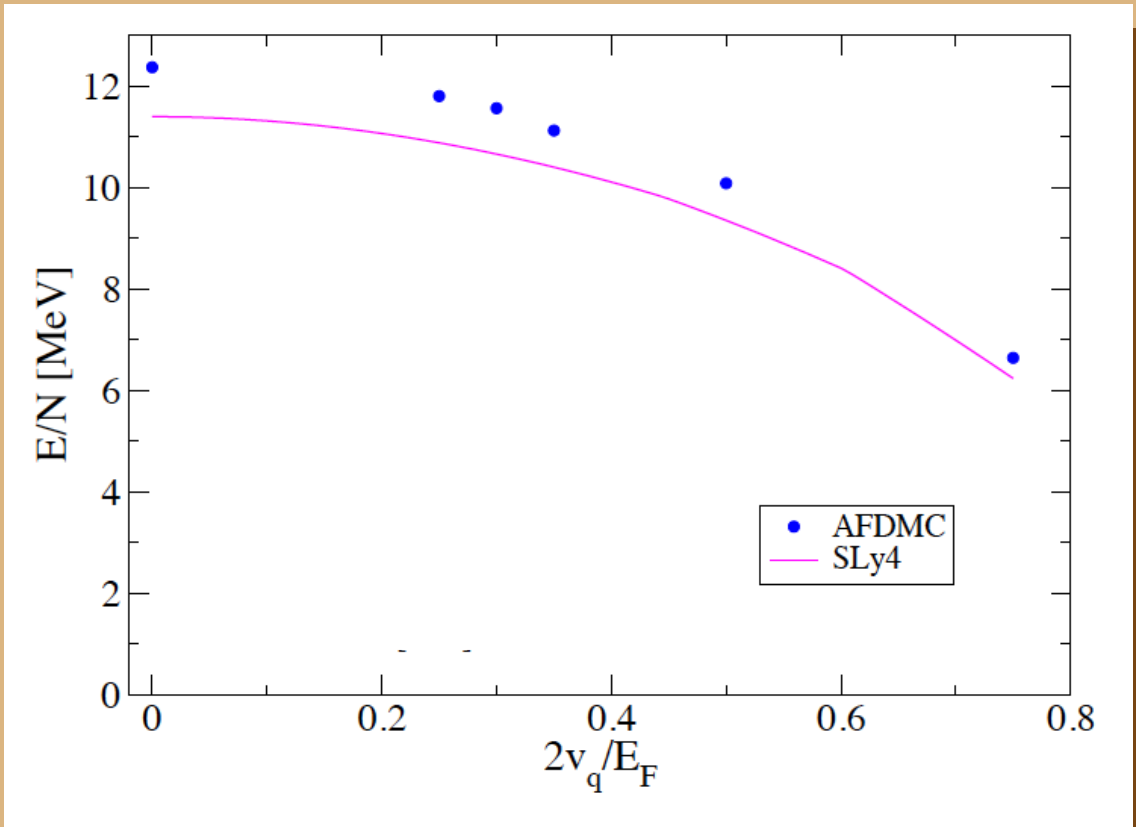
$$\mathcal{E} = \frac{\hbar^2}{2m}\tau + s_1 n^2 + s_2 n^{\sigma+2} + s_3 n\tau + s_4(\nabla n)^2$$

Skyrme functional in isospin representation

$$\mathcal{E}_{\text{Skyrme}} = \sum_{T=0,1}\left[(C_T^{n,a} + C_T^{n,b} n_0^{\sigma})n_T^2 + C_T^{\Delta n}(\nabla n_T)^2 + C_T^{\tau} n_T \tau_T\right]$$

Approach: Use QMC results to constrain DFT gradient term(s)
(which then apply to terrestrial nuclei and neutron-stars more broadly)

One periodicity, many strengths



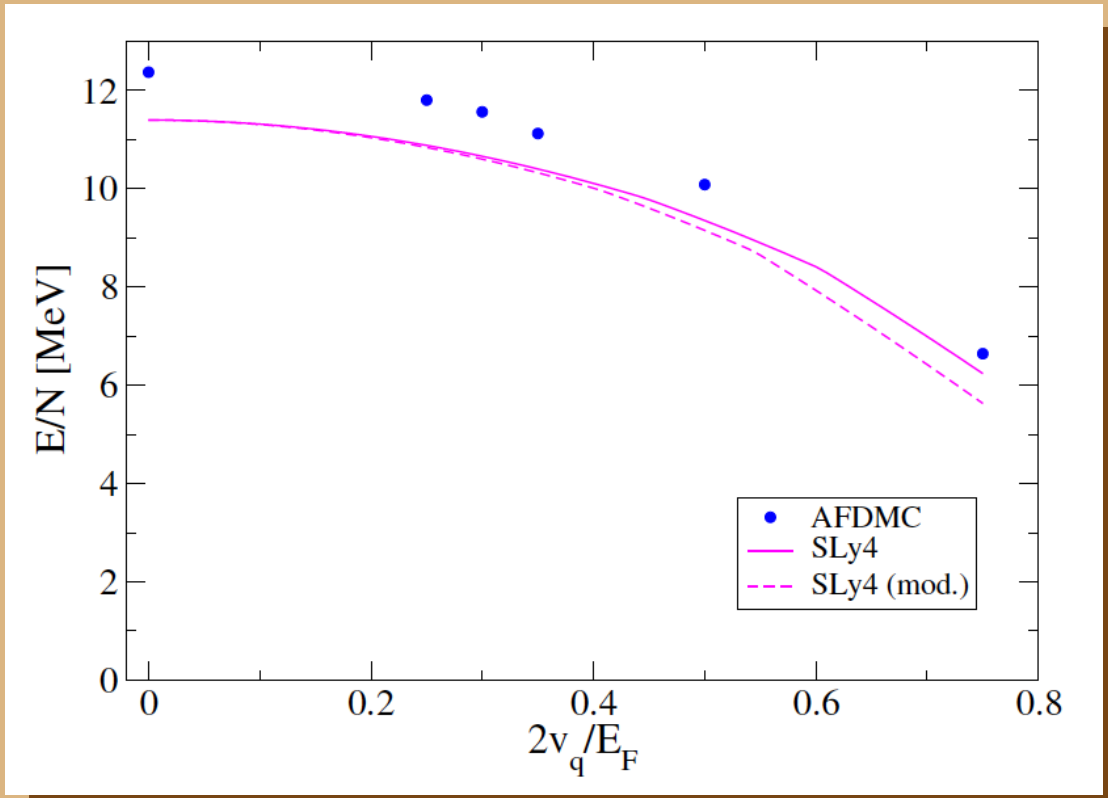
$n = 0.10$ fm^{-3}

- Try to disentangle bulk from isovector gradient contribution

M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016)

NEUTRONS

One periodicity, many strengths



$n = 0.10$ fm^{-3}

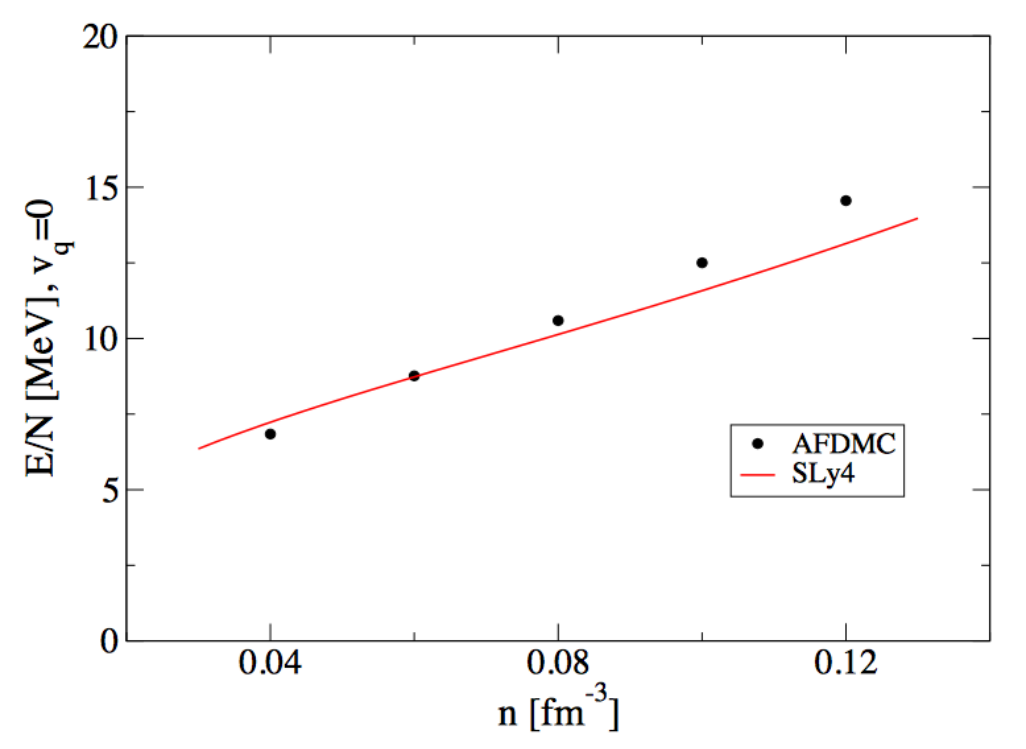
- Try to disentangle bulk from isovector gradient contribution (homogeneous EOSs also differ)

M. Buraczynski and A. Gezerlis,
Phys. Rev. Lett. **116**, 152501 (2016)

NEUTRONS

One periodicity, many strengths

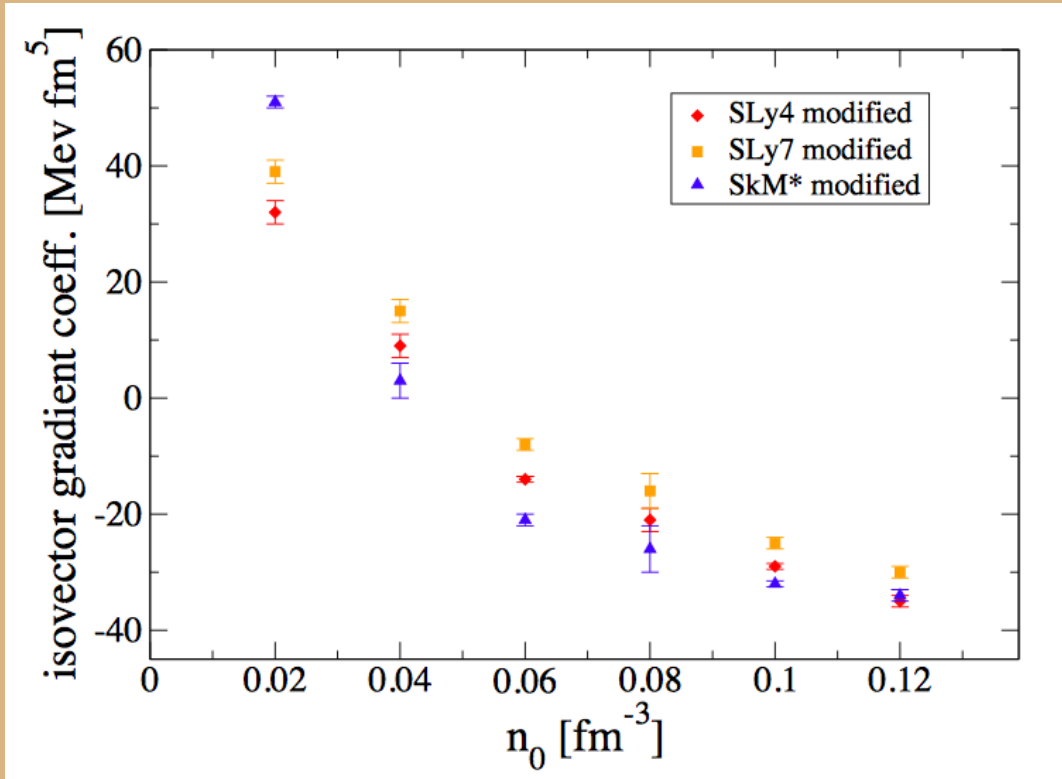
Relationship between homogeneous EOSs depends on the density



NEUTRONS

M. Buraczynski and A. Gezerlis, Phys. Rev. C **95**, 034012 (2017)

One periodicity, many strengths



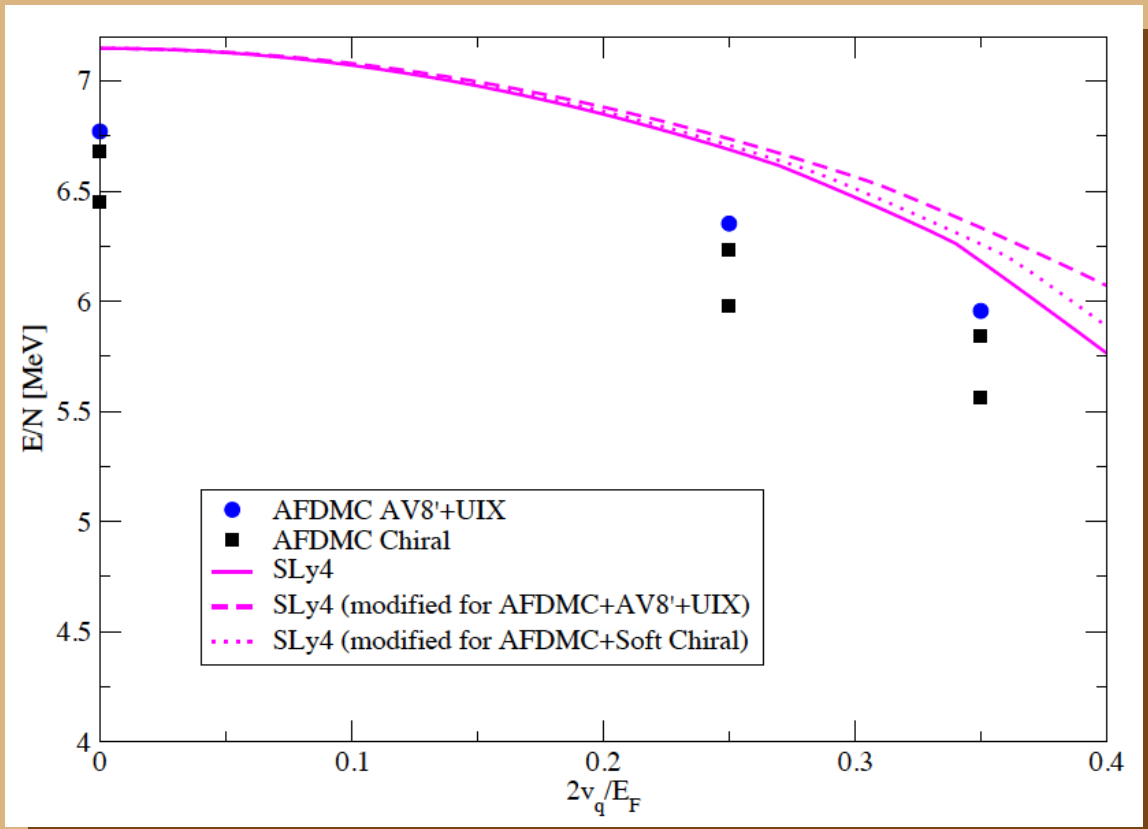
Many densities

- Repeat exercise at lower density
- Homogeneous relation is reversed
- Find density-dependent isovector coefficient, analogously to what is seen with DME (Holt, Kaiser)

NEUTRONS

M. Buraczynski and A. Gezerlis, Phys. Rev. C **95**, 034012 (2017)

One periodicity, many strengths



preliminary

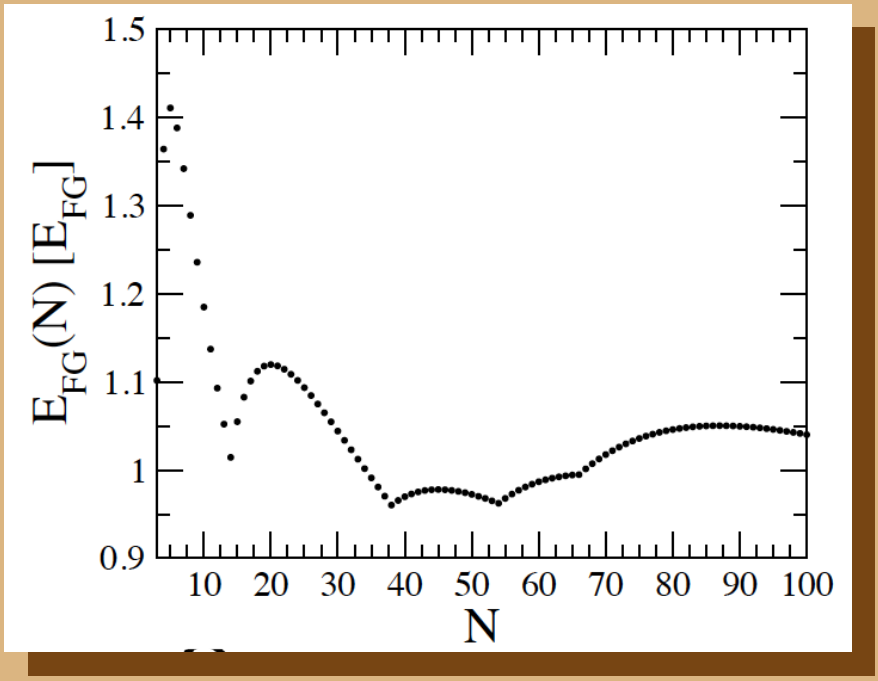
$n = 0.10$ fm^{-3}

- Using chiral EFT interactions as input to AFDMC (and from there to the Skyrme fitting)

NEUTRONS

Finite-size effects

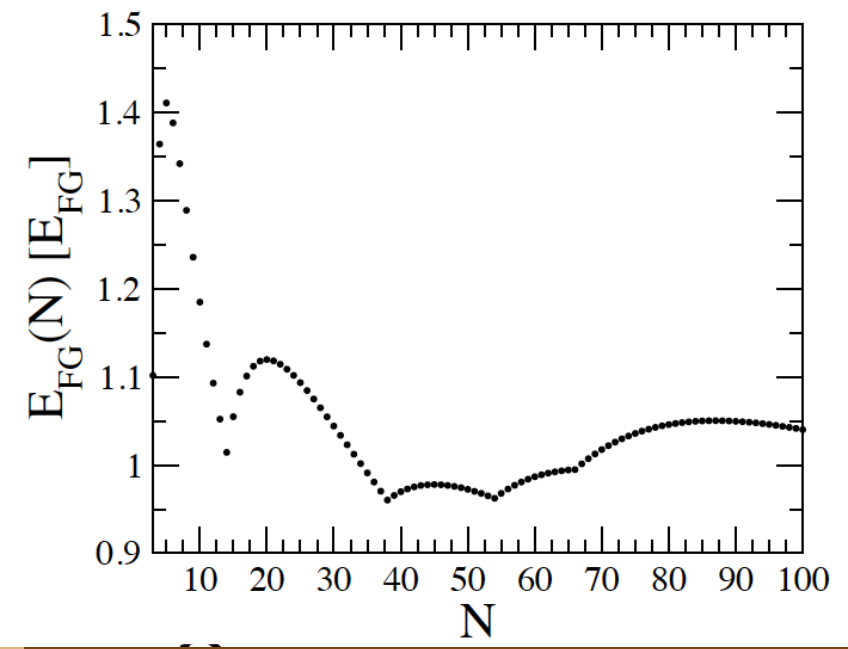
Free non-interacting gas



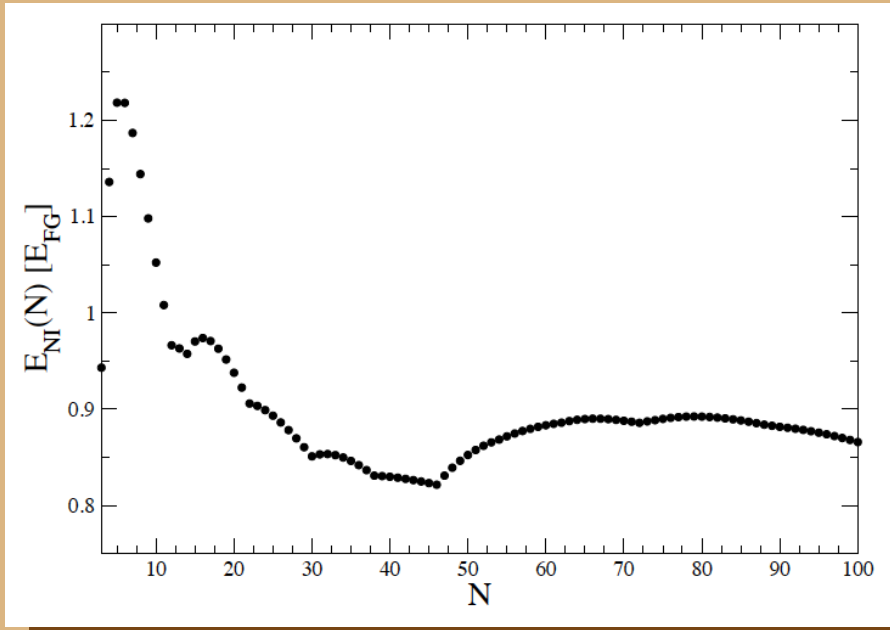
M. Buraczynski and A. Gezerlis, Phys. Rev. C **95**, 034012 (2017)

Finite-size effects

Free non-interacting gas



Modulated non-interacting gas



M. Buraczynski and A. Gezerlis, Phys. Rev. C **95**, 034012 (2017)

Neutron matter density response

Non-interacting gas: Lindhard function

$$\chi_L = -\frac{m q_F}{2\pi^2\hbar^2}\left[1 + \frac{q_F}{q}\left(1 - \left(\frac{q}{2q_F}\right)^2\right)\ln\left|\frac{q+2q_F}{q-2q_F}\right|\right]$$

Neutron matter density response

Non-interacting gas: Lindhard function

$$\chi_L = -\frac{m q_F}{2\pi^2\hbar^2}\left[1 + \frac{q_F}{q}\left(1 - \left(\frac{q}{2q_F}\right)^2\right)\ln\left|\frac{q+2q_F}{q-2q_F}\right|\right]$$

$$\frac{E_{\rm tot}}{N} = \frac{E_0}{N} + \frac{\chi(q)}{n_0}v_q^2 + C_4 v_q^4 + \cdots$$

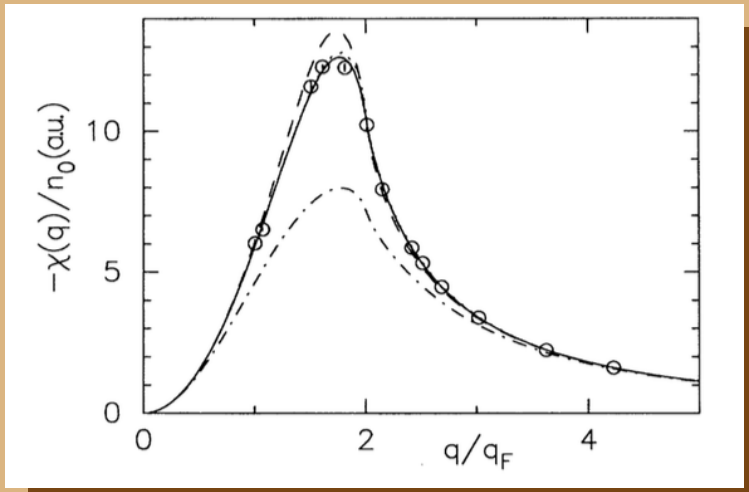
Neutron matter density response

Non-interacting gas: Lindhard function

$$\chi_L = -\frac{m q_F}{2\pi^2\hbar^2}\left[1+\frac{q_F}{q}\left(1-\left(\frac{q}{2q_F}\right)^2\right)\ln\left|\frac{q+2q_F}{q-2q_F}\right|\right]$$

Three-dimensional electron gas

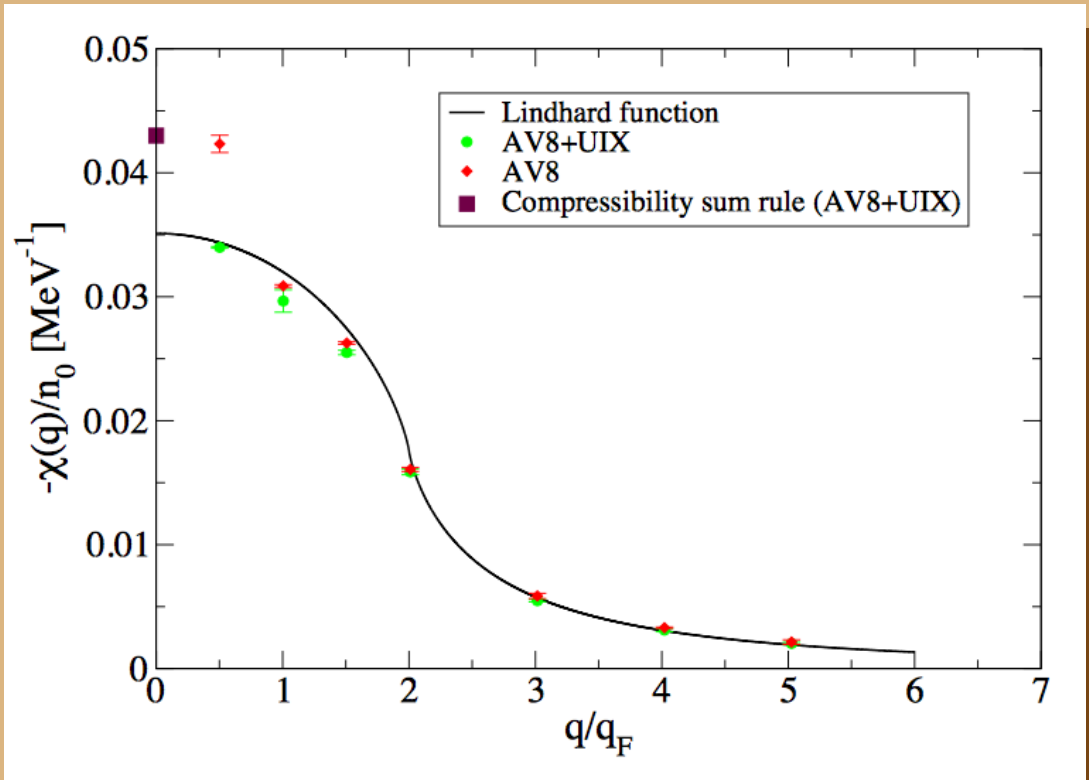
$$\frac{E_{\rm tot}}{N} = \frac{E_0}{N} + \frac{\chi(q)}{n_0}v_q^2 + C_4 v_q^4 + \cdots$$



S. Moroni, D. M. Ceperley, G. Senatore, Phys. Rev. Lett. **75**, 689 (1995)

Many periodicities, many strengths

$n = 0.10\ \mathrm{fm}^{-3}$



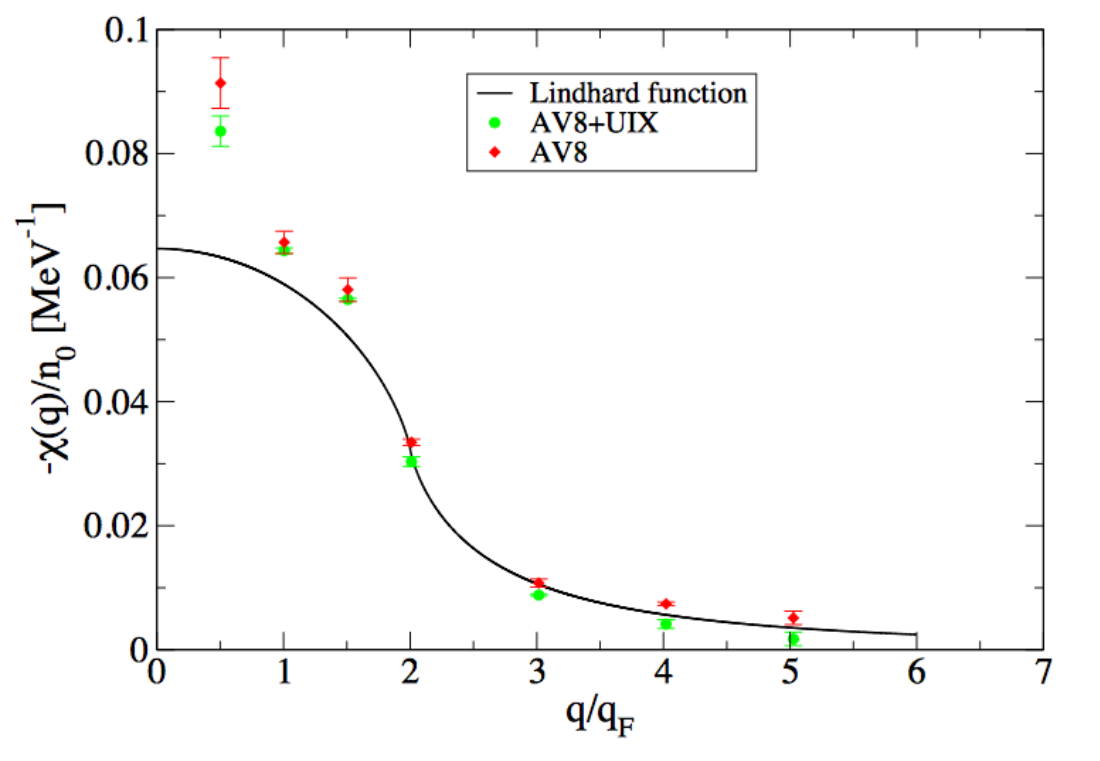
- First ever ab initio density-density response for neutron matter
- Neither Lindhard nor Coulomb
- Results on this plot derived from several strengths and periodicities

NEUTRONS

M. Buraczynski and A. Gezerlis, Phys. Rev. Lett. **116**, 152501 (2016)

M. Buraczynski and A. Gezerlis, Phys. Rev. C **95**, 034012 (2017)

Many periodicities, many strengths



$n = 0.04$ fm^{-3}

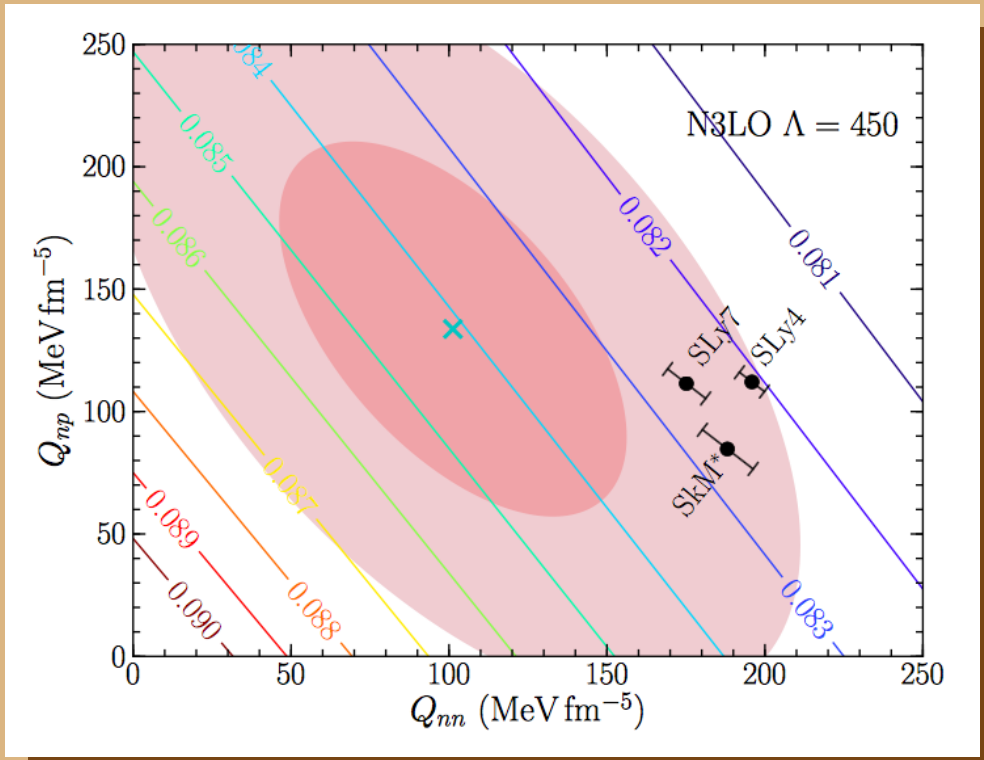
- First ever ab initio density-density response for neutron matter
- Neither Lindhard nor Coulomb
- Results on this plot derived from several strengths and periodicities

NEUTRONS

M. Buraczynski and A. Gezerlis, Phys. Rev. Lett. **116**, 152501 (2016)

M. Buraczynski and A. Gezerlis, Phys. Rev. C **95**, 034012 (2017)

Impact on neutron stars



Core-crust boundary

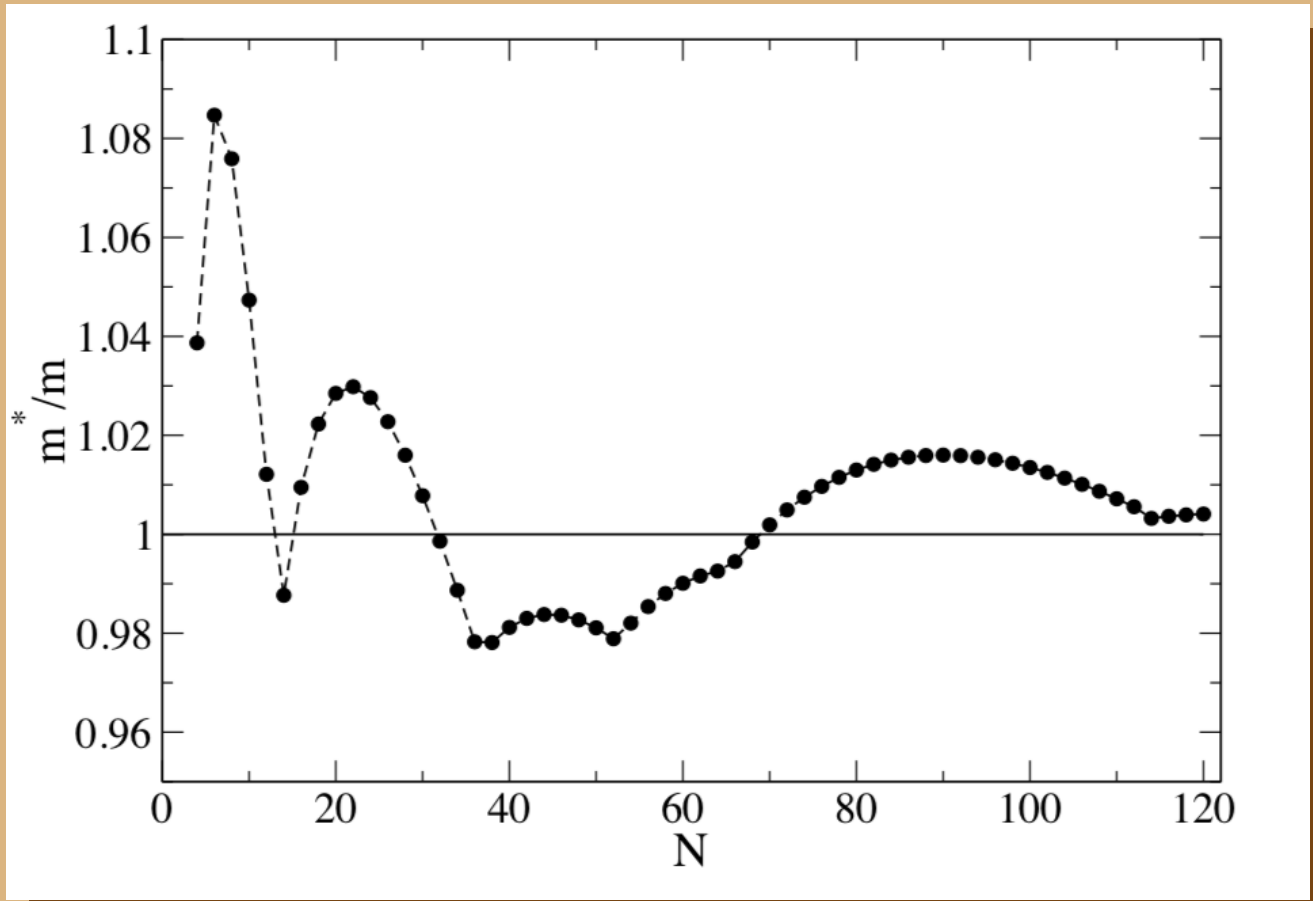
- Thermodynamic instability determines transition from inhomogeneous to homogeneous matter
- Modified isovector coefficients compared with large class of other results

Y. Lim and J. W. Holt, Phys. Rev. C **95**, 065805 (2017)

Quasiparticle energy dispersion

Finite-size effects

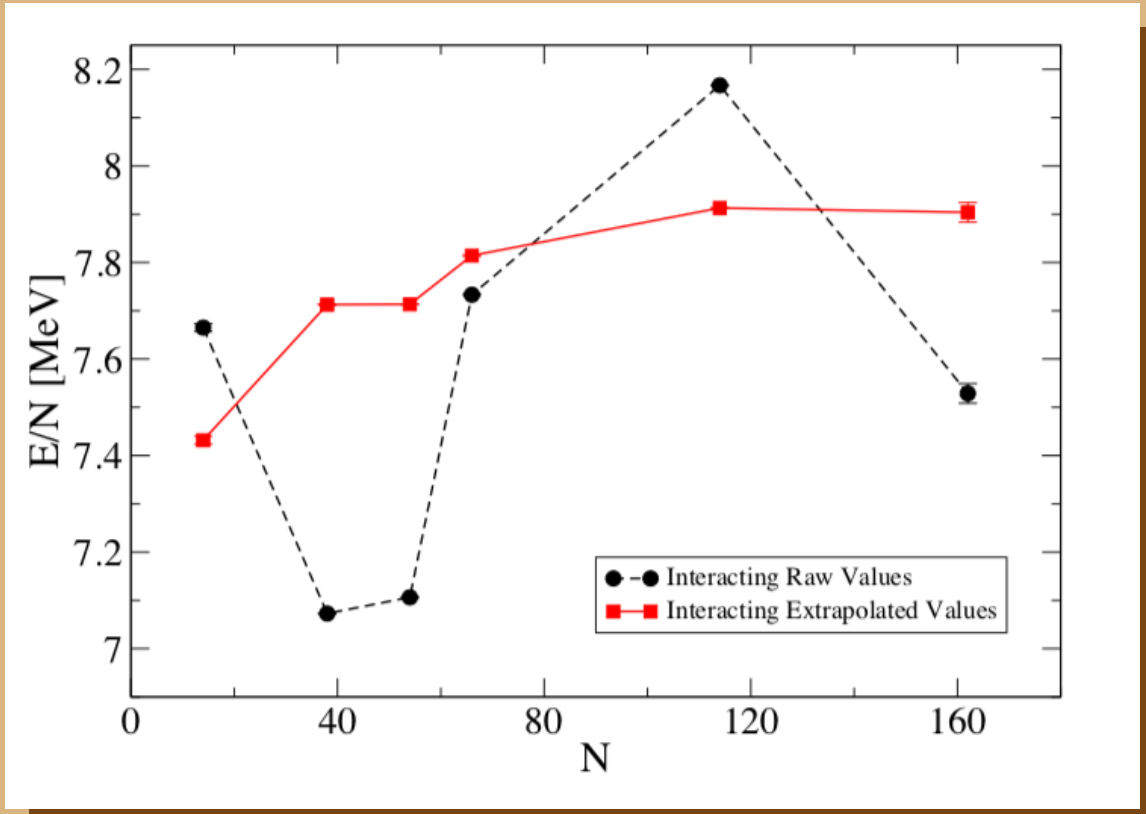
Effective mass for non-interacting gas for finite N



preliminary

Interacting gas results

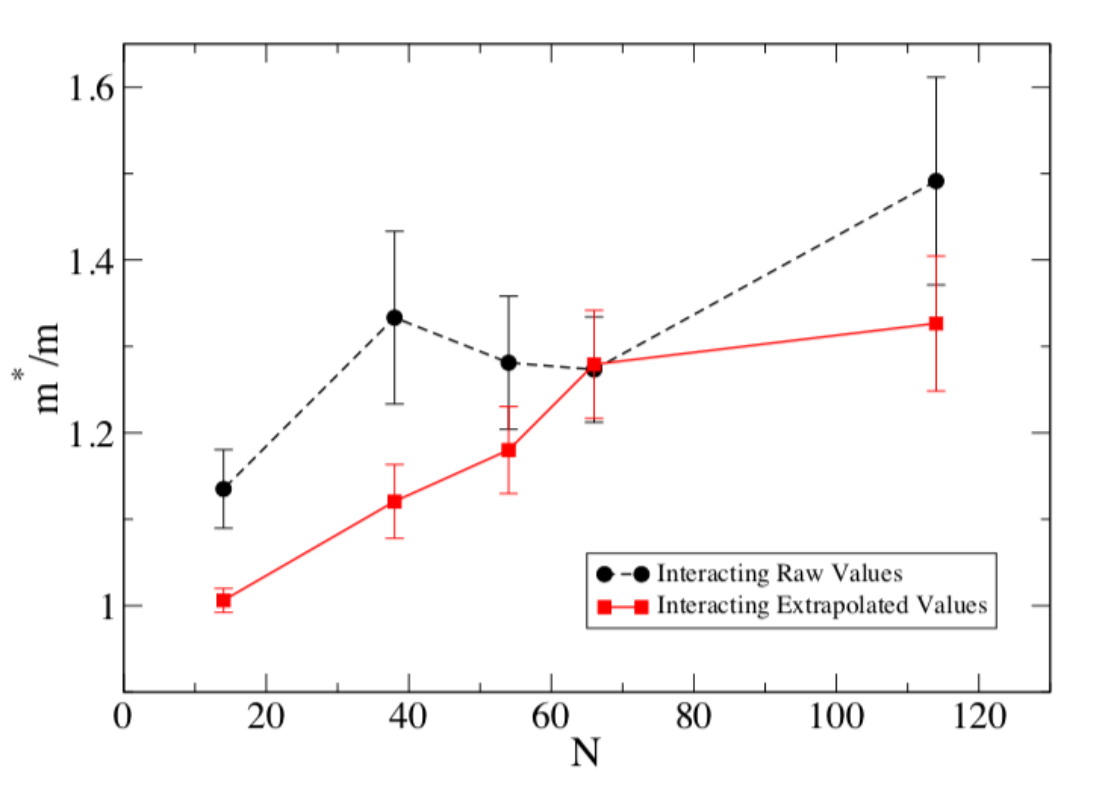
Novel prescription to reach thermodynamic limit when subtracting



preliminary

Interacting gas results

Study imbalanced gas with extra particle placed at different excitation energies



preliminary

Conclusions

- Rich connections between physics of nuclei and that of compact stars
- Exciting time in terms of interplay between nuclear interactions, QCD, and many-body approaches
- Ab initio and phenomenology are mutually beneficial

Acknowledgments

Collaborators

Guelph

- Mateusz Buraczynski
- Will Dawkins
- Nawar Ismail
- Nicholas van Heijst

Darmstadt

- Joel Lynn
- Achim Schwenk

INT

- Ingo Tews

LANL

- Joe Carlson
- Stefano Gandolfi

IPN Orsay

- Denis Lacroix

Acknowledgments

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IPN Orsay

- Denis Lacroix

Extra slide 1

Big-picture questions

- Functionals tailored to neutron stars or universal density functional theory?

- Functional fit only to *ab initio* (as per Fayans and Orsay) or fit to any available data point?

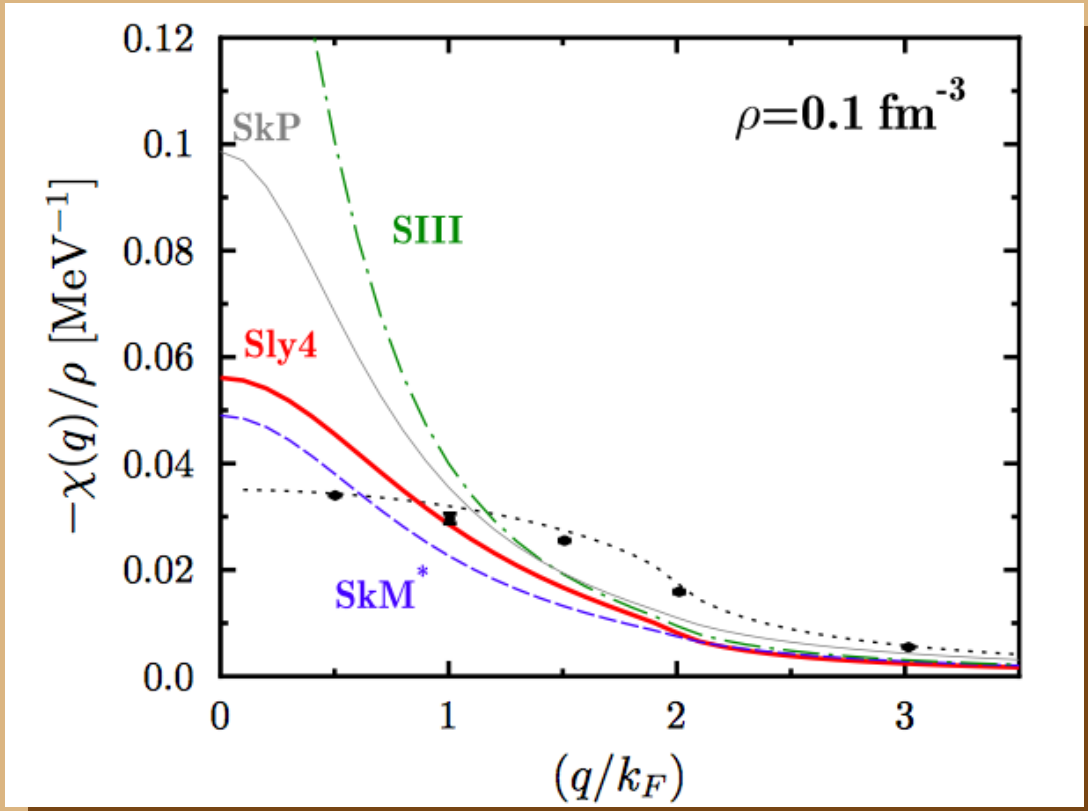
- How will LIGO data constrain functionals? How will this propagate to *ab initio* and nuclear forces?

Extra slide 2

Little-picture questions

Extra slide 2a

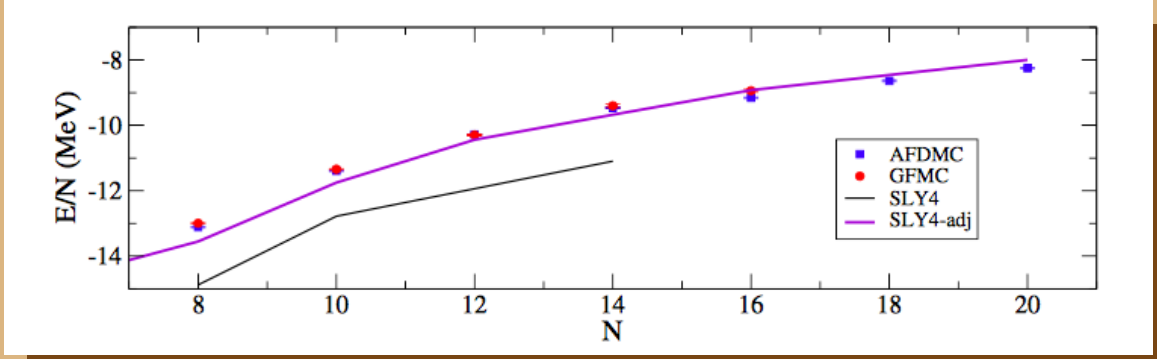
Something wrong with Skyrme response?



A. Boulet and D. Lacroix, Phys. Rev. C 97, 014301 (2017)

Extra slide 2b

Isovector coefficient density-dependent or not?



S. Gandolfi, J. Carlson, S. Pieper, Phys. Rev. Lett. 106, 012501 (2011)

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