Quantum Monte Carlo
with chiral two- and three-neutron forces

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UNIVERSITY of GUELPH

ICNT Workshop: Theory for open-shell nuclei
East Lansing, MI
May 14, 2015

ICNT

International Collaborations in Nuclear Theory

2015 Approved and Supported Programs

International Collaborations in Nuclear Theory: Theory for open-shell nuclei near the limits of stability (May 11 - 29, 2015 MSU, East Lansing, MI) organized by S. K. Bogner, M. Hjorth-Jensen and J. D. Holt

2013 Approved and Supported Programs

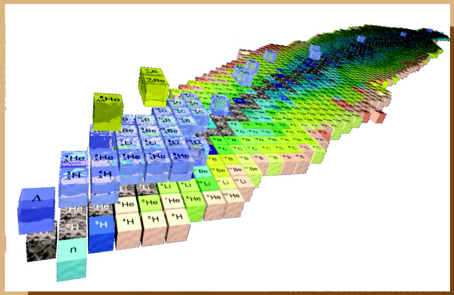
Halo Physics at the Neutron Dripline: Combining Ab Initio Nuclear Theory with Halo Effective Field Theory (GSI, Feb/Mar 2014)

ICNT workshop "Physics of exotic nuclei: Theoretical advances and challeges" (Tokyo, June 9-13, 2014)

2012 Approved and Supported Programs

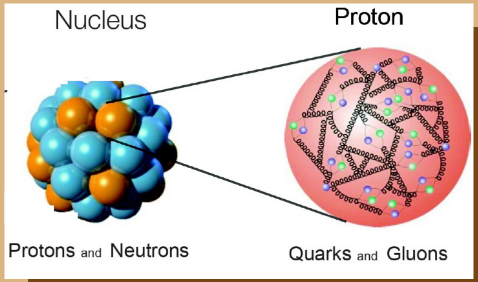
Symmetry Energy in the Context of New Radioactive Beam Facilities and Astrophysics (NSCL, July 15-August 9 2013)

Outline



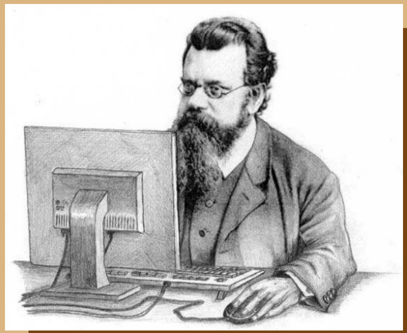
Many neutrons

- Neutron-rich nuclei
- Neutron stars



Nuclear forces

- Chiral Effective Field Theory
- Local chiral EFT



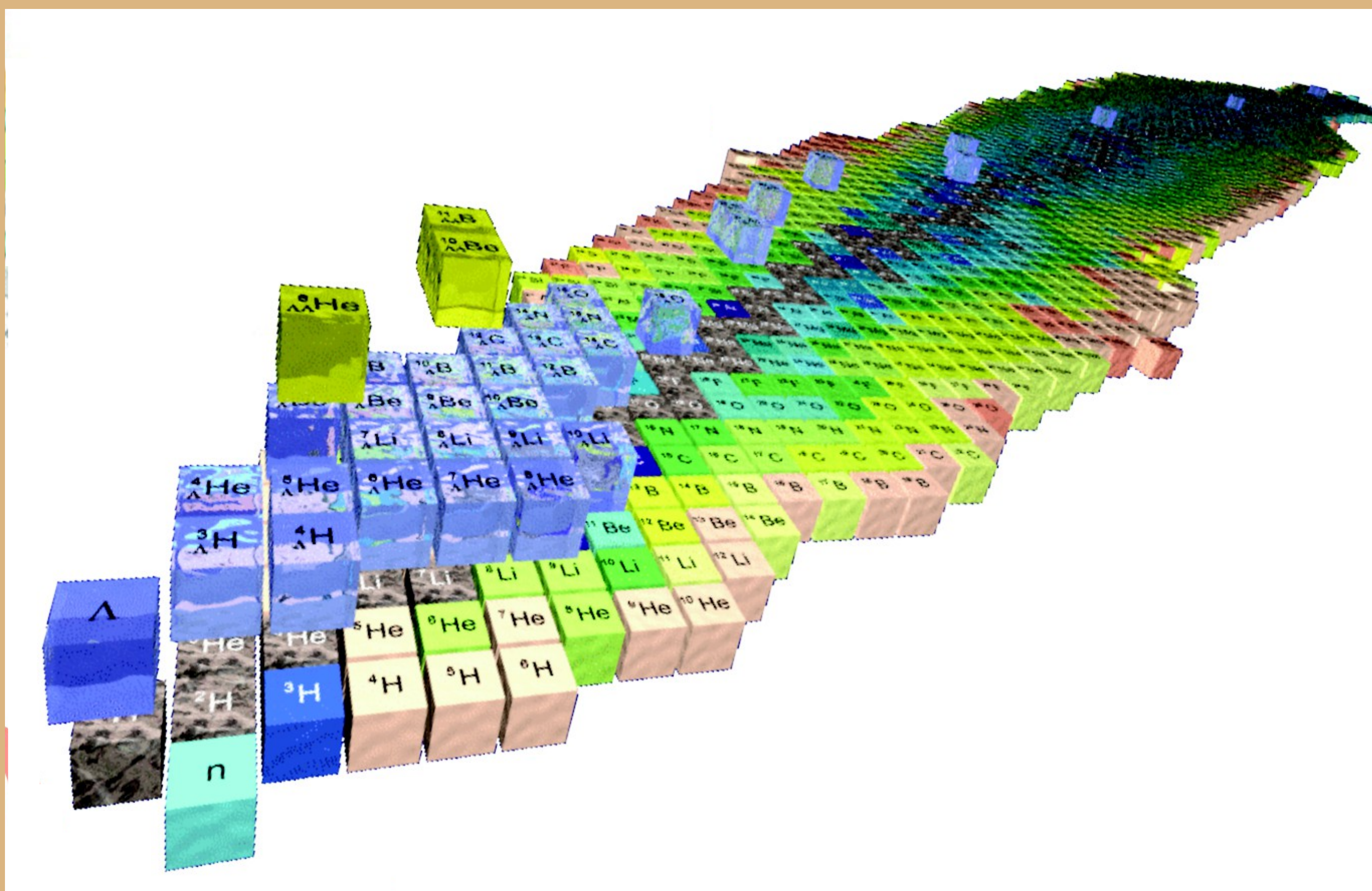
Credit: Bernhard Reischl

Results

- Neutron matter: Using NN forces alone
- Neutron matter: Using NN+3NF
- Neutron drops
- Neutron star crusts

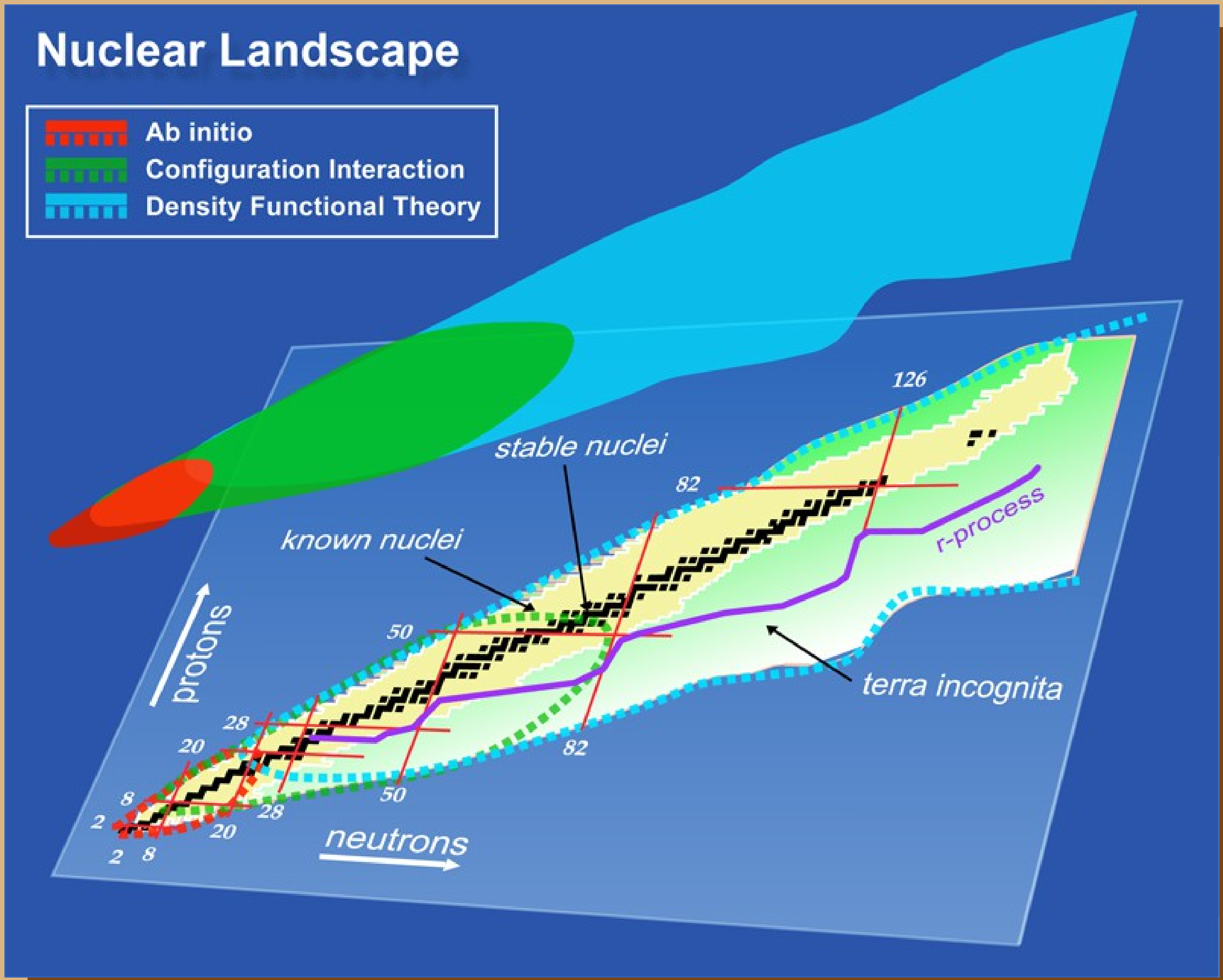
Many-nucleon problem: nuclei

Chart of nuclides



- Nuclear physics is developed and tested on earth
- Using complicated many-body methods we can try to “build nuclei from scratch”
- We then extrapolate that knowledge to more exotic systems

Many-nucleon problem: methods



- No universal method exists (yet?)
- A lot to be learned if the degrees of freedom are actual particles and there are no free parameters
- Regions of overlap between different methods are crucial
- Is it possible to work at the level of nucleons & pions but still connect to the underlying level?

Neutron-rich input

Quantum Monte Carlo:

stochastically solve the many-body Schrödinger equation in a fully non-perturbative manner

Energy-density functionals:

de facto include many-body correlations while being applicable throughout the nuclear chart

Rudiments of Diffusion Monte Carlo:

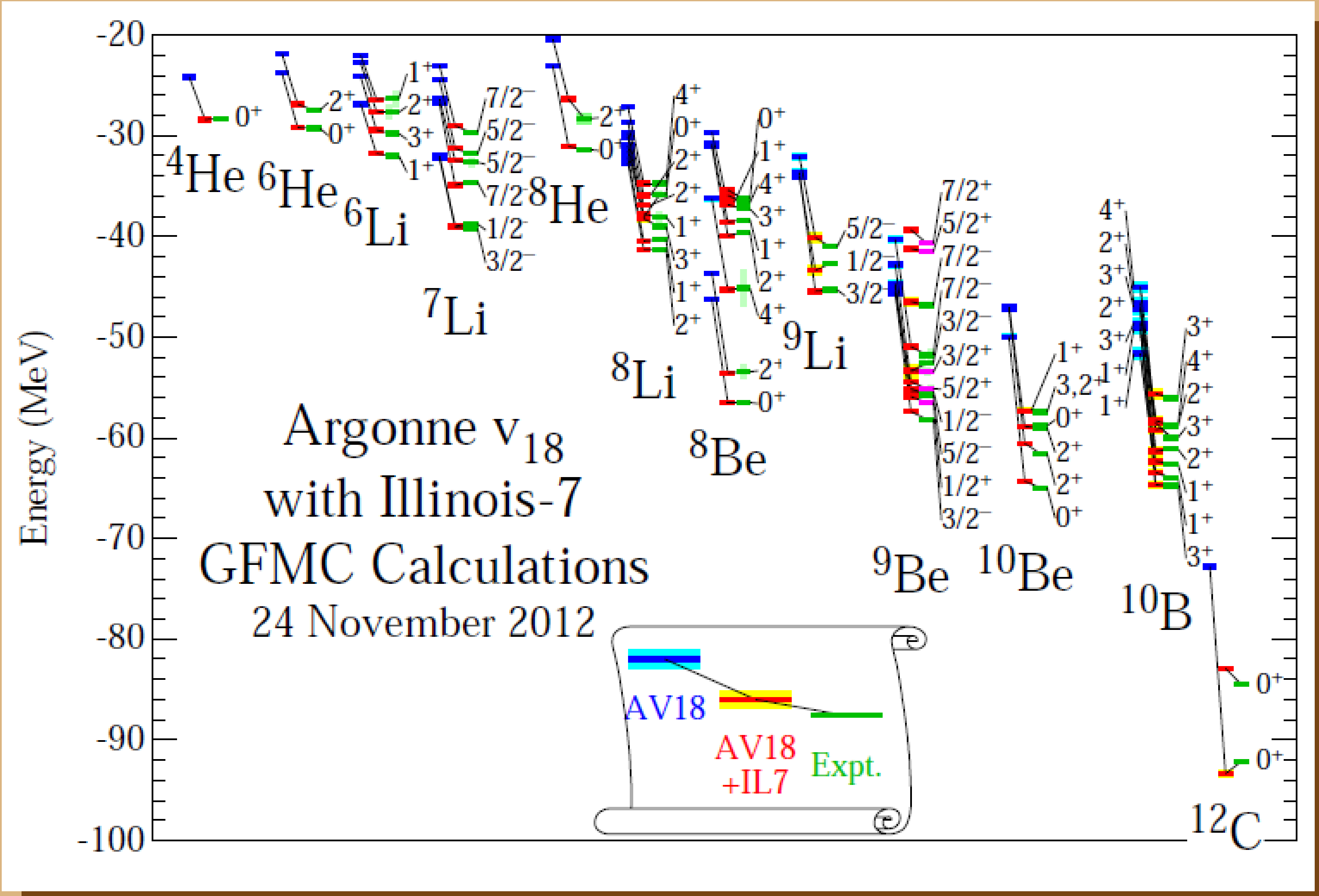
$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H}-E_T)\tau}\Psi_V$$
$$\to \alpha_0 e^{-(E_0-E_T)\tau}\Psi_0$$

Rudiments of Skyrme EDFs:

$$\mathcal{E}_{\text{Skyrme}} = \frac{\hbar^2}{2m}\tau + \frac{s_0}{4}\rho^2 + \frac{s_3}{24}\rho^{\alpha+2} + \frac{s_1+3s_2}{8}\rho\tau + 3\frac{s_1-s_2}{16}(\nabla\rho)^2$$

Nuclear GFMC preview

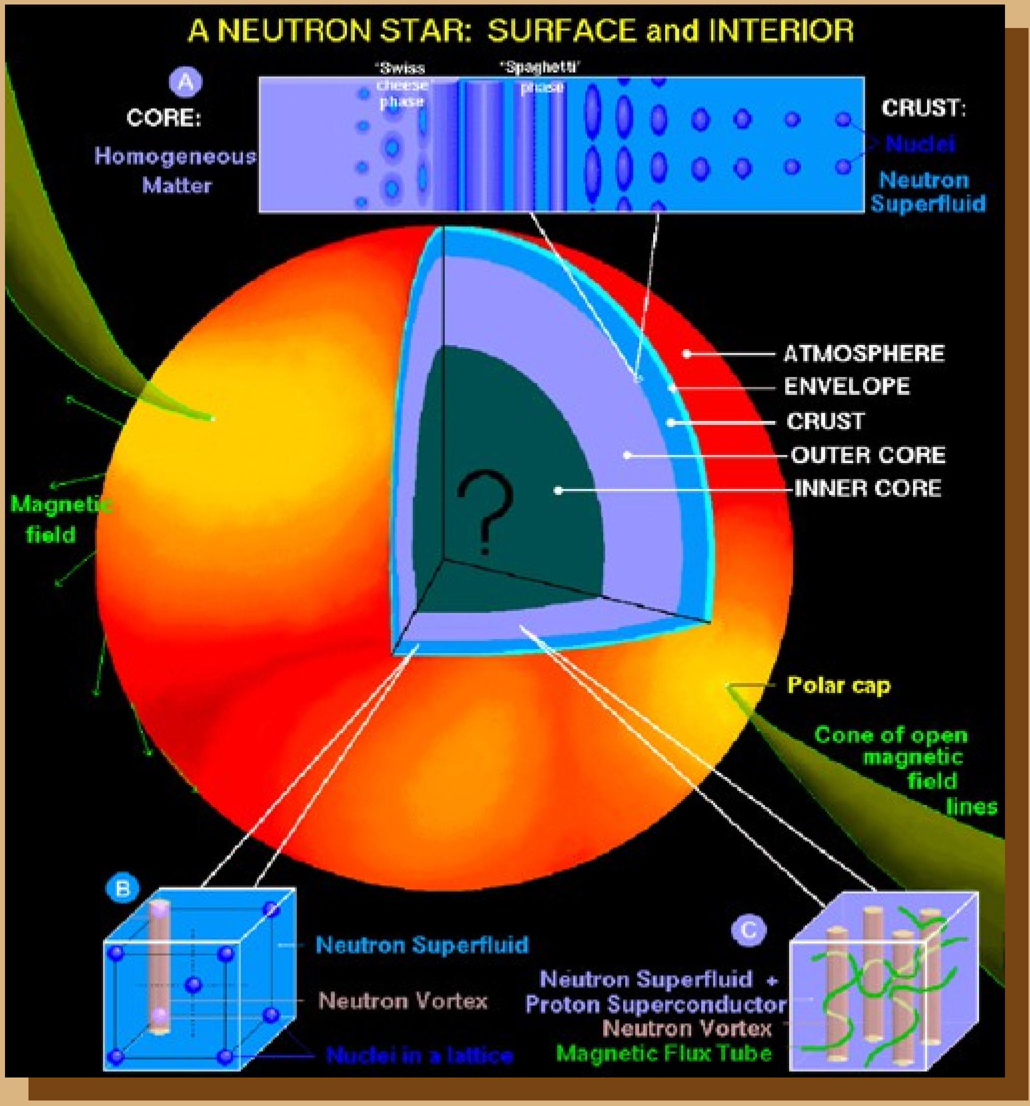
Joel Lynn's talk: nuclear Green's Function Monte Carlo is very accurate



Credit: Steve Pieper

Neutron stars

Ultra-dense matter laboratories



Credit: Dany Page

- Ultra-dense: 1.4 solar masses (or more) within a radius of 10 kilometres
- Terrestrial-like (outer layers) down to exotic (core) behaviour
- Observationally probed, but also (indirectly) experimentally accessible
- We wish to describe neutron-star matter from first principles

Neutron stars: gravity

Static spherically symmetric metric

$$g_{\mu\nu} = \begin{pmatrix} A(r) & 0 & 0 & 0 \\ 0 & r^2 & 0 & 0 \\ 0 & 0 & r^2 \sin^2\theta & 0 \\ 0 & 0 & 0 & -B(r) \end{pmatrix}$$

Einstein field equations

$$R_{\mu\nu} = \frac{8\pi G}{c^4}\left(T_{\mu\nu} - \frac{1}{2} T g_{\mu\nu}\right)$$

Ricci tensor

Energy-momentum tensor

Inside the source (for isotropic fluid with no shear forces):
Tolman-Oppenheimer-Volkoff (TOV) equation(s)

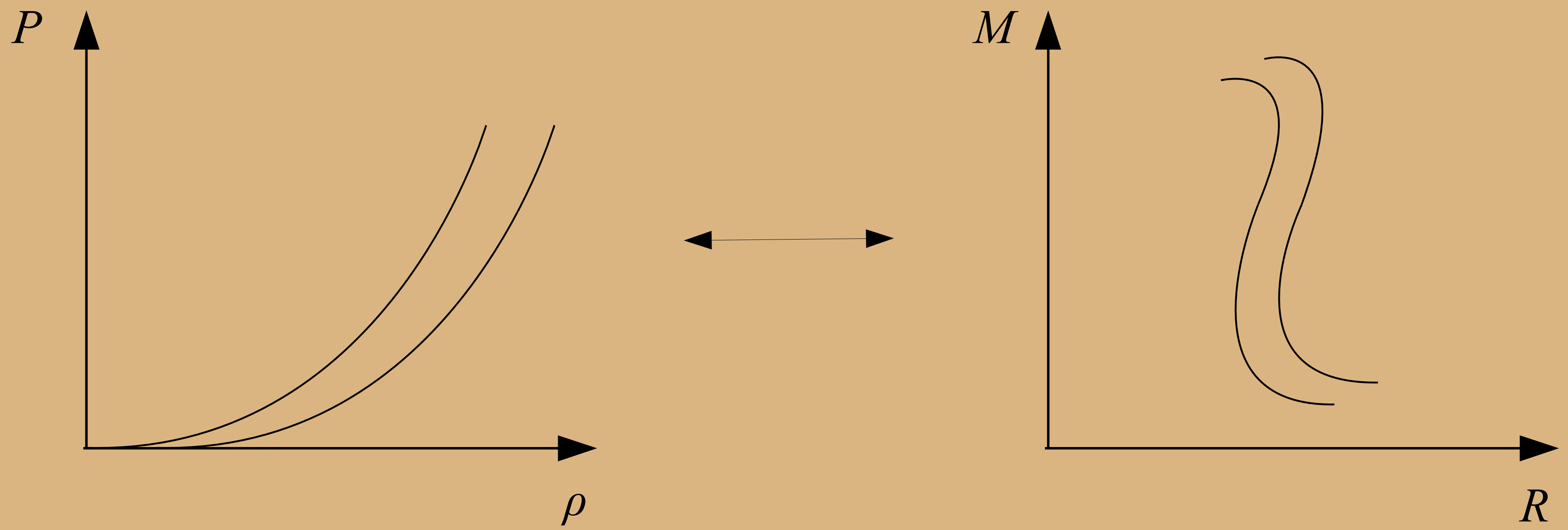
$$\frac{dP}{dr} = -\frac{GM(r)\rho(r)}{r^2}\left[\frac{1 + P(r)/\rho(r)c^2}{1 - 2GM(r)/c^2 r}\right]\left[1 + \frac{4\pi P(r) r^3}{M(r)c^2}\right]$$

Uncertainty estimates

TOV equations
(or Hartle-Thorne, etc)

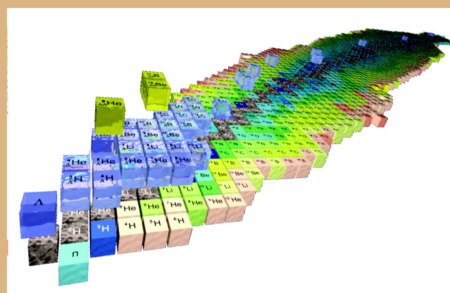
Pressure vs density

Mass vs radius



Modern goal: systematic theoretical error bars

Outline



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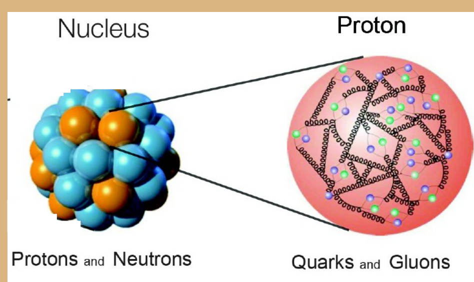
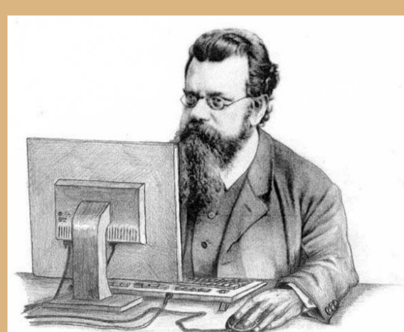


Nuclear forces

- Chiral Effective Field Theory
- Local chiral EFT



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Results

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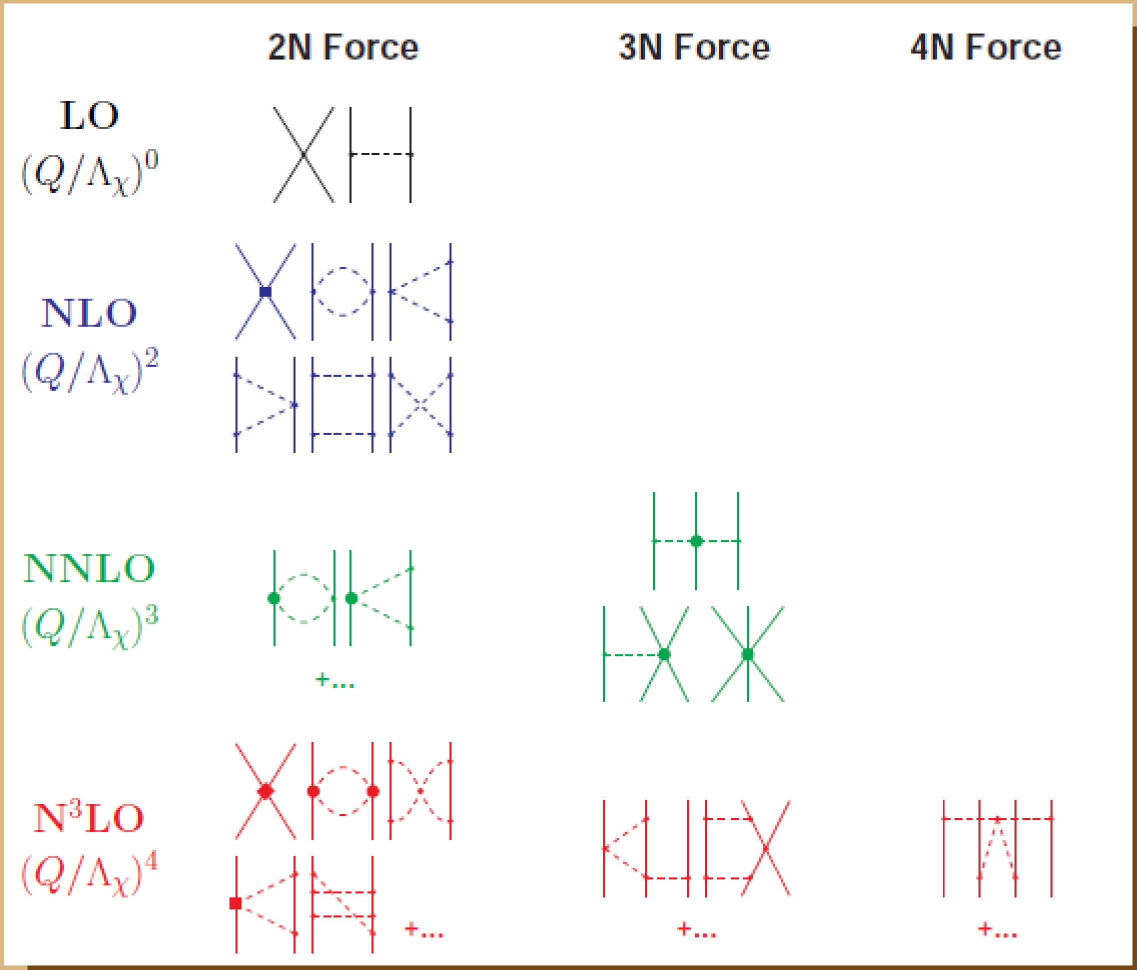
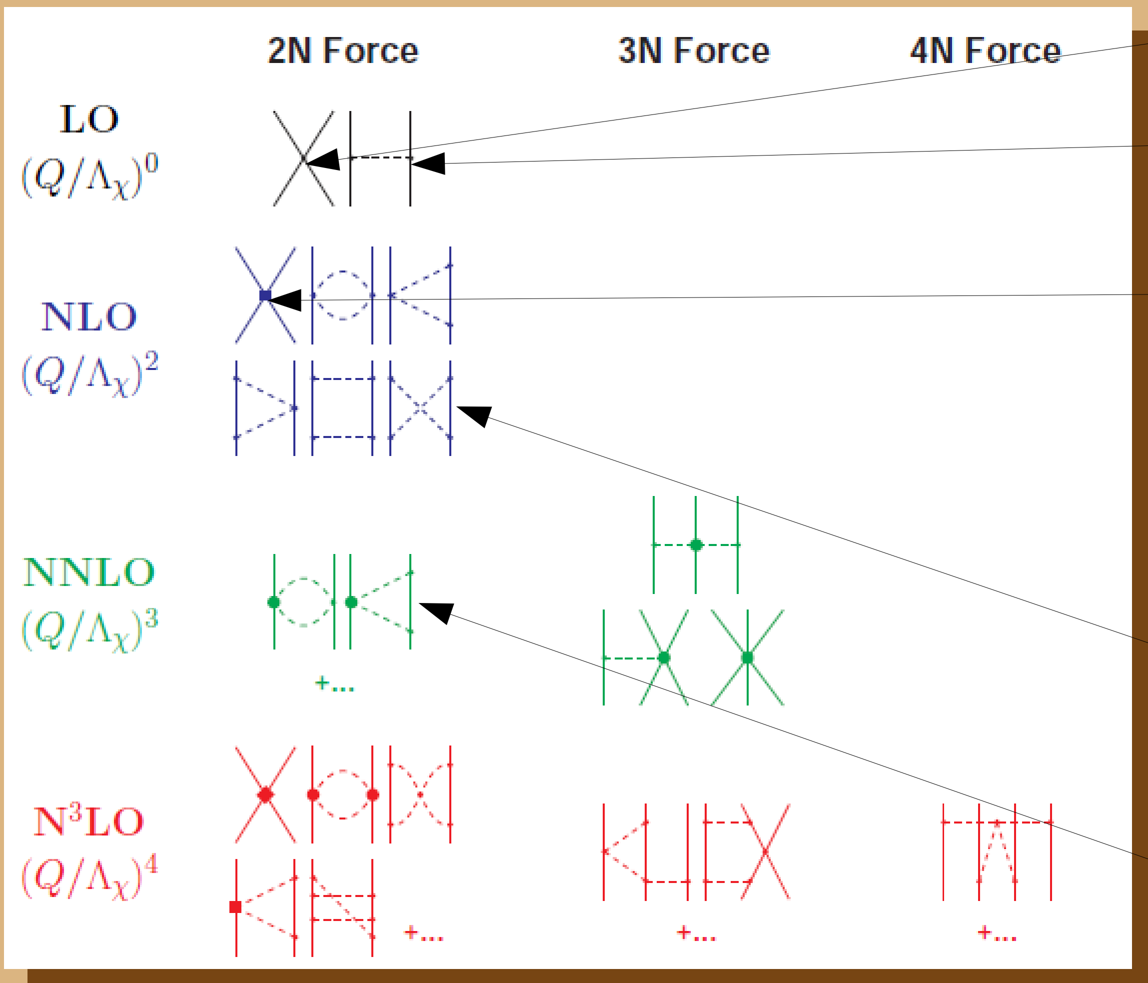
Nuclear Hamiltonian: chiral EFT



- Attempts to connect with underlying theory (QCD)
- Systematic low-momentum expansion
- Consistent many-body forces
- Low-energy constants from experiment or lattice QCD
- Until recently non-local in coordinate space, so unused in continuum QMC
- Power counting's relation to renormalization still an open question

Weinberg, van Kolck, Kaplan, Savage, Wise, Machleidt, Epelbaum, ...

Nuclear Hamiltonian: chiral EFT



$$V_{\rm ct}^{(0)} = C_S + C_T\ \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

$$V_{1\pi}^{(0)} = -\left(\frac{g_A}{2f_\pi}\right)^2\ \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \frac{(\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q})}{q^2 + m_\pi^2}$$

$$\begin{aligned} V_{\rm ct}^{(2)} &= C_1\ q^2 + C_2\ k^2 \\ &+ \left(C_3\ q^2 + C_4\ k^2\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\ &+ i\frac{C_5}{2}(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{q} \times \mathbf{k}) \\ &+ C_6(\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\ &+ C_7(\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) \end{aligned}$$

Long-studied
two-pion exchange

Contains couplings
from πN scattering

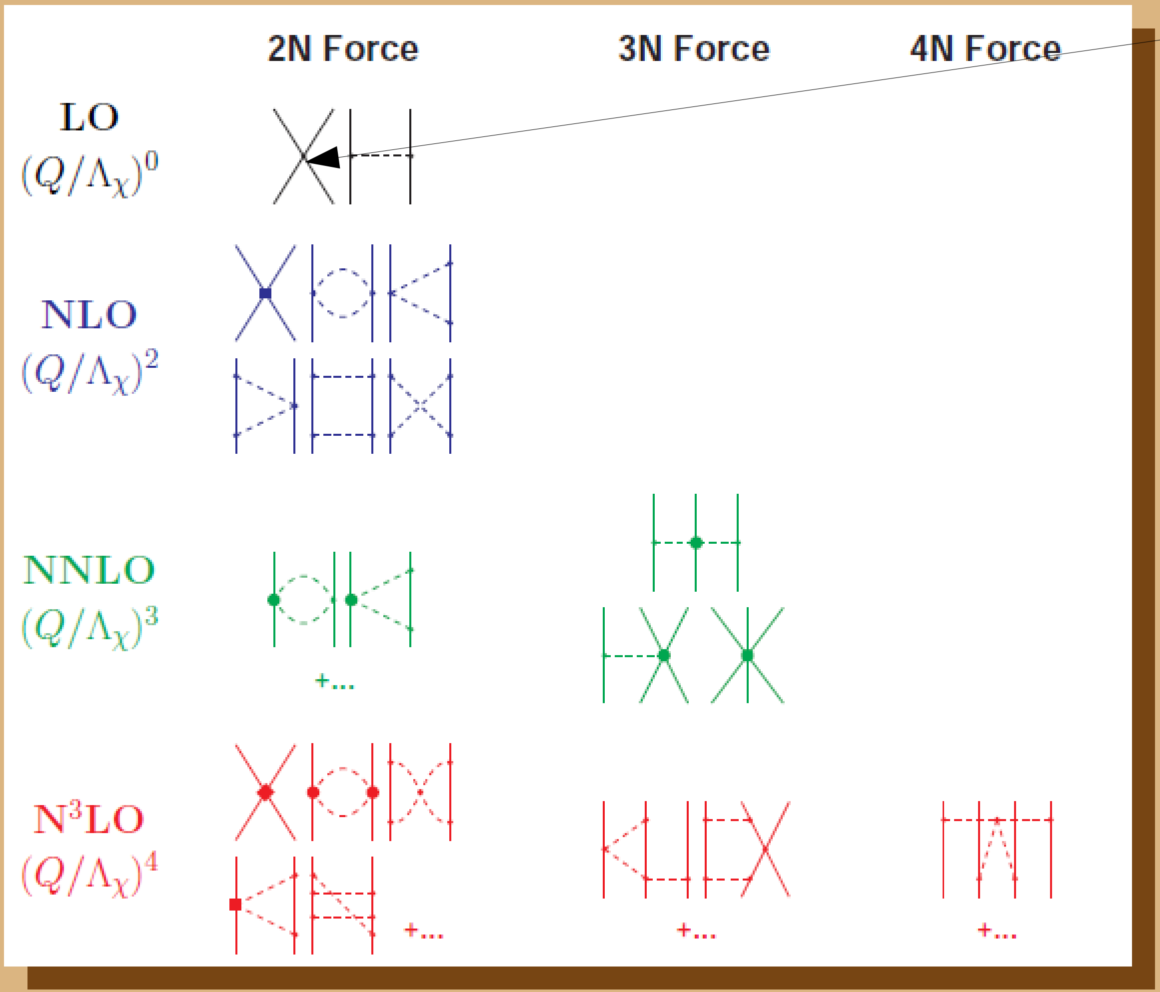
$\mathbf{k}$ means non-local

$\mathbf{q}$ means local

$$\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2 \qquad \mathbf{k} = (\mathbf{p}' + \mathbf{p})/2$$

$$\mathbf{p}' = (\mathbf{p}_1' - \mathbf{p}_2')/2 \qquad \mathbf{q} = \mathbf{p}' - \mathbf{p}$$

Nuclear Hamiltonian: chiral EFT



$$V_{\rm ct}^{(0)} = C_S + C_T \, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

Merely the standard choice.

Actually 4 terms in full set consistent with the symmetries of QCD

$$V_{\rm ct}^{(0)} = C_1 + C_2 \, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + C_3 \, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + C_4 \, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

Pick 2 and antisymmetrize

A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. Lett. **111**, 032501 (2013).

A. Gezerlis, I. Tews, E. Epelbaum, M. Freunek, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, Phys. Rev. C **90**, 054323 (2014).

Local chiral EFT

Use the analogous freedom for NLO contacts

Write down a local energy-independent NN potential

- Pick 7 different contacts at NLO, just make sure that when antisymmetrized they lead to a set obeying the required symmetry principles

$$
\begin{aligned}
V_{\mathrm{ct}}^{(2)} &= C_1\, q^2 + C_2\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
&+ \left(C_3\, q^2 + C_4\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\
&+ i\, \frac{C_5}{2}\, (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{q} \times \mathbf{k} \\
&+ C_6\, (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\
&+ C_7\, (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q})\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2
\end{aligned}
$$

cf.

$$
\begin{aligned}
V_{\mathrm{ct}}^{(2)} &= C_1\; q^2 + C_2\; k^2 \\
&+ \left(C_3\; q^2 + C_4\; k^2\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\
&+ i \frac{C_5}{2} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{q} \times \mathbf{k}) \\
&+ C_6 (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\
&+ C_7 (\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k})
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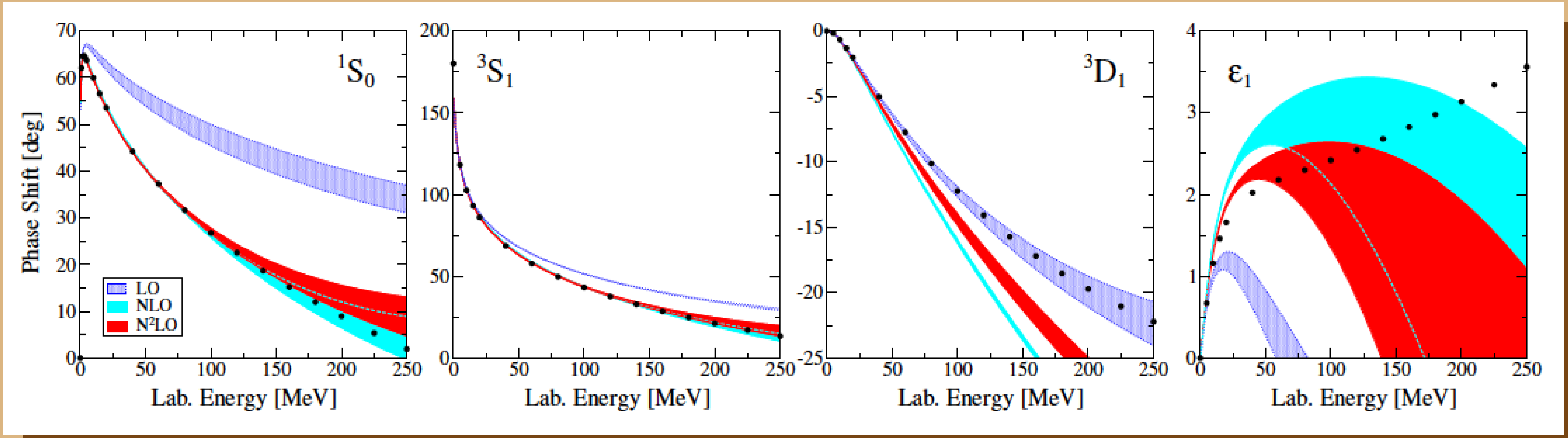
Phase shifts



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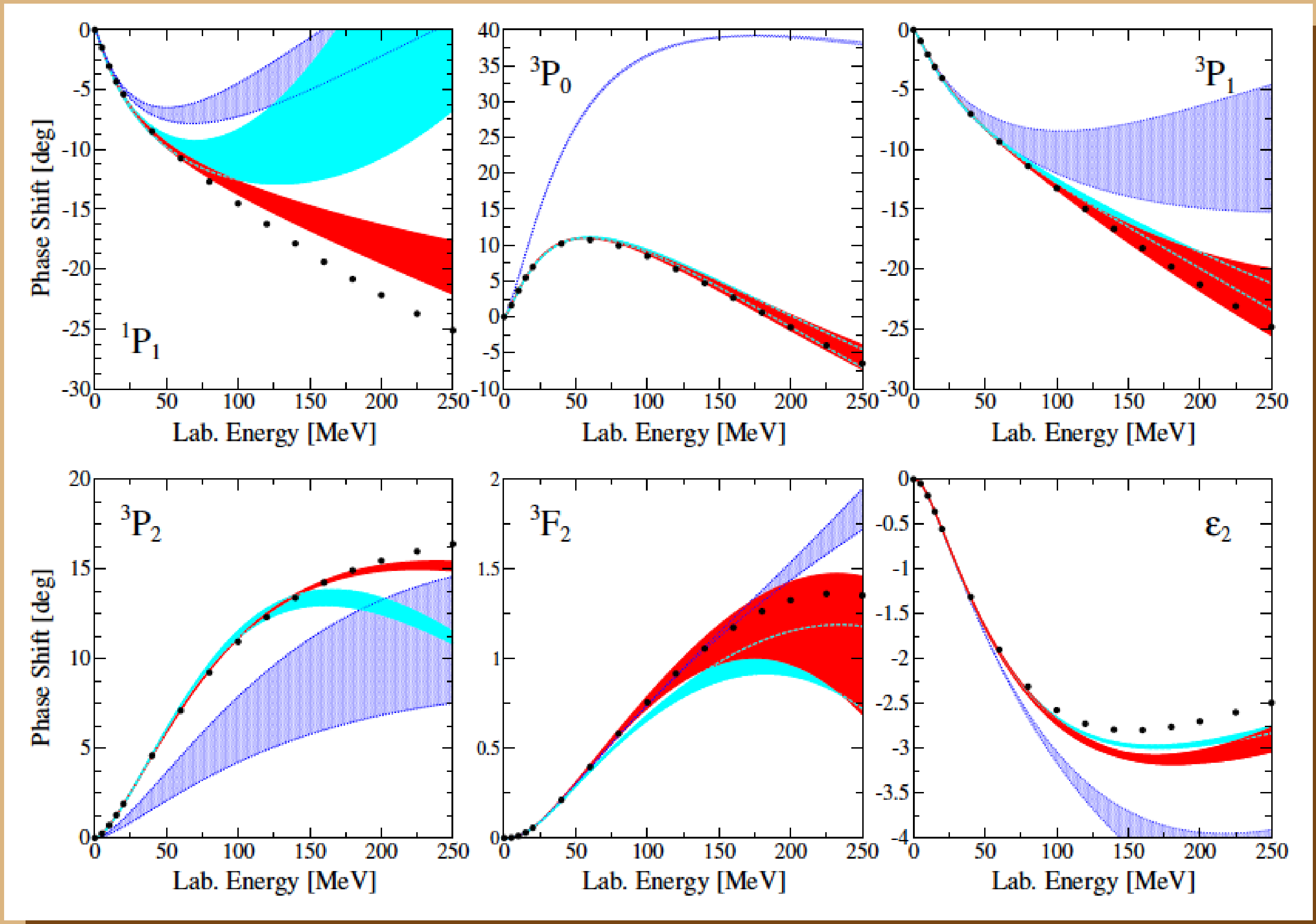

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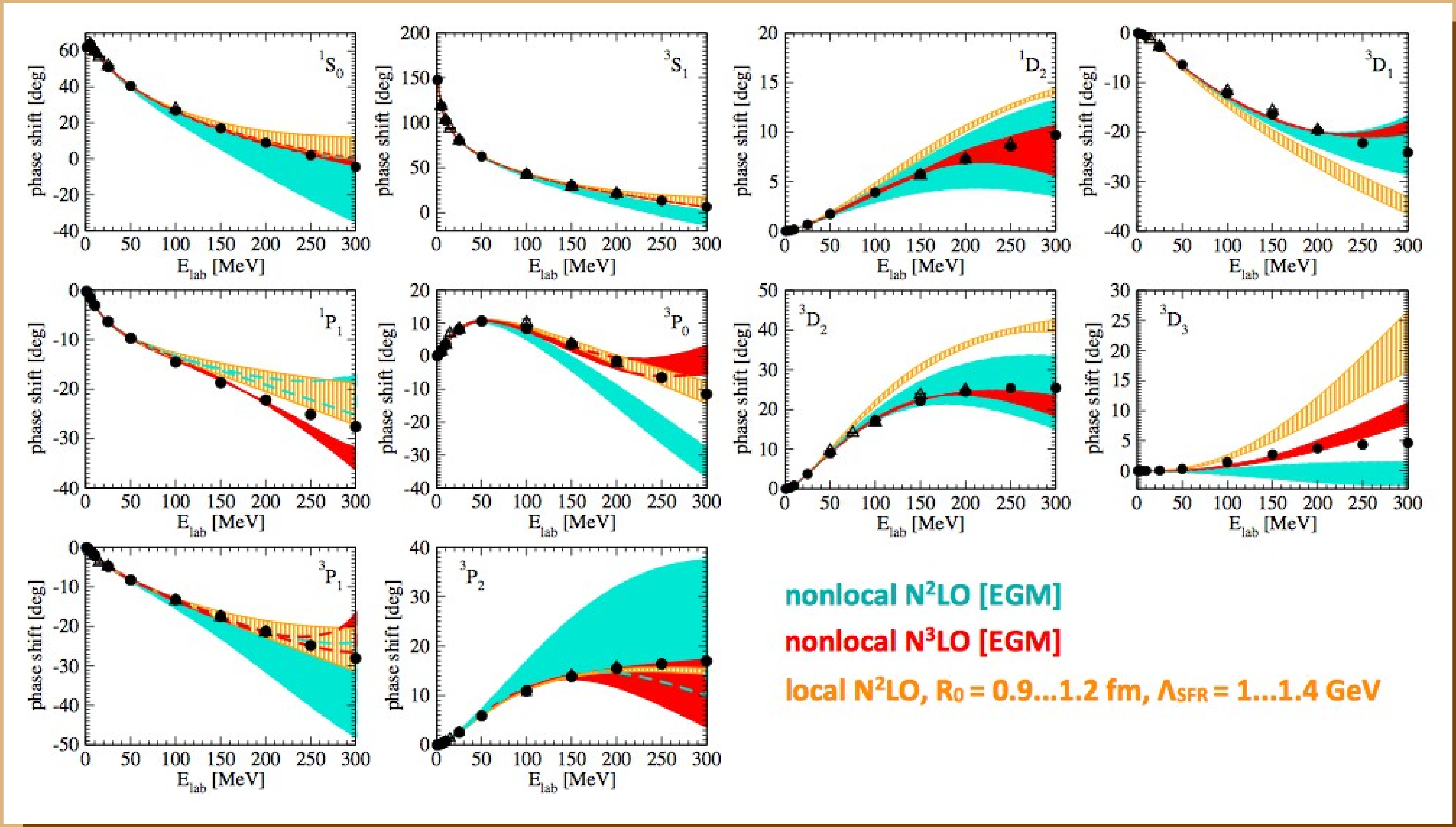
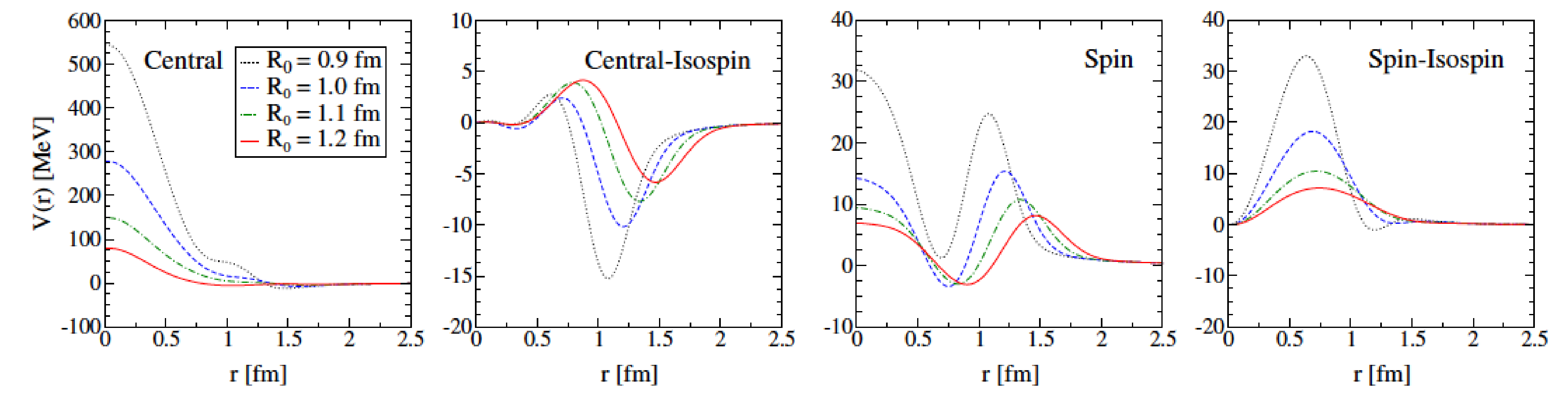
Compare to non-local EGM

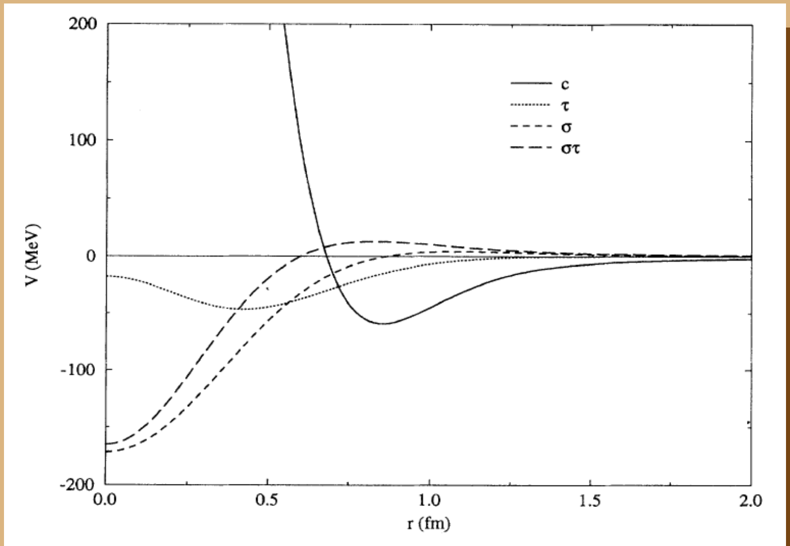


Credit: Hermann Krebs

Since it's local, let's plot it (N^2LO)



Compare with AV18



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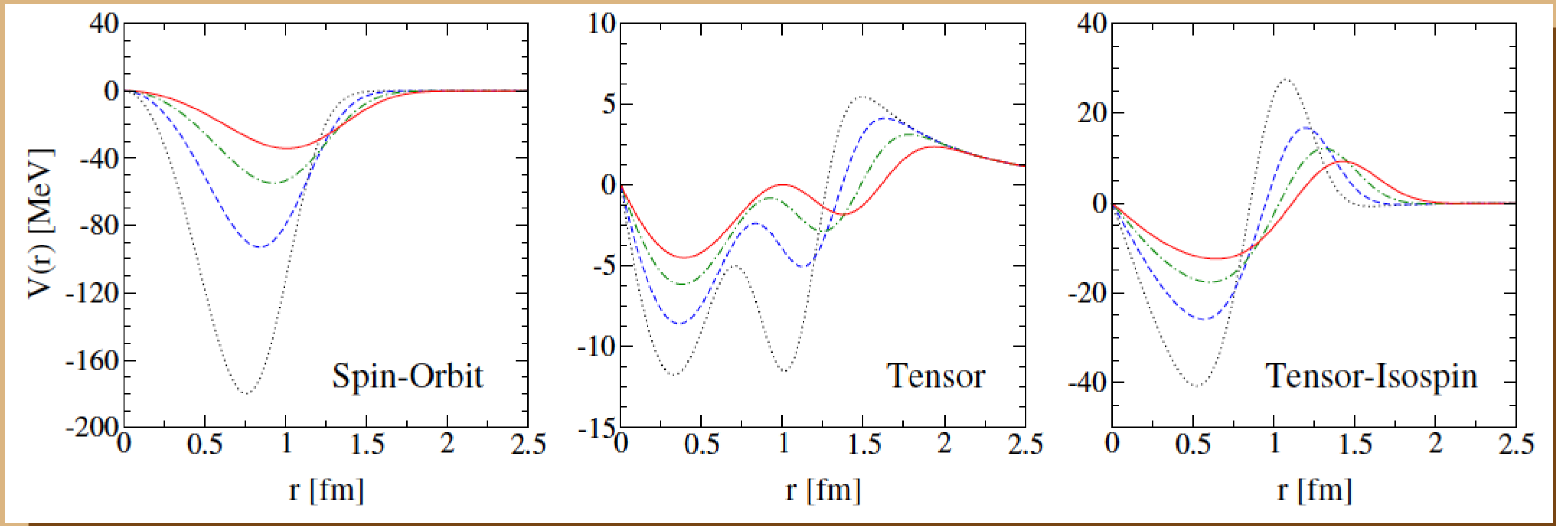

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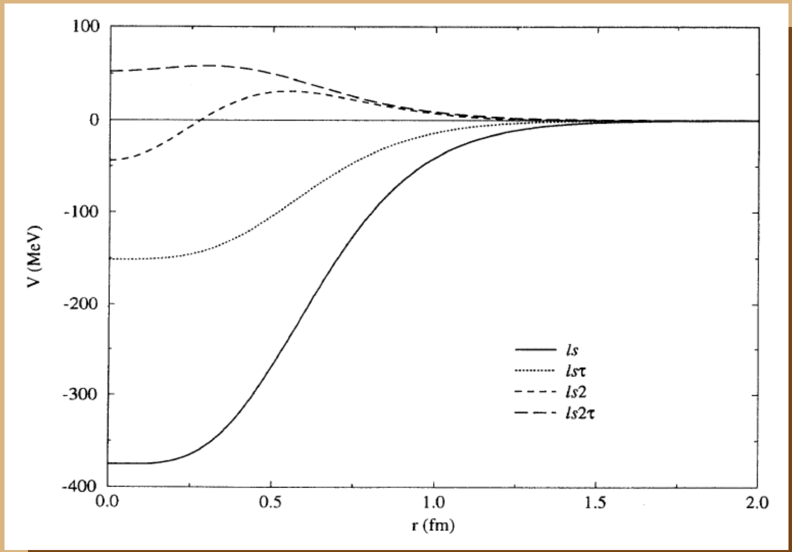

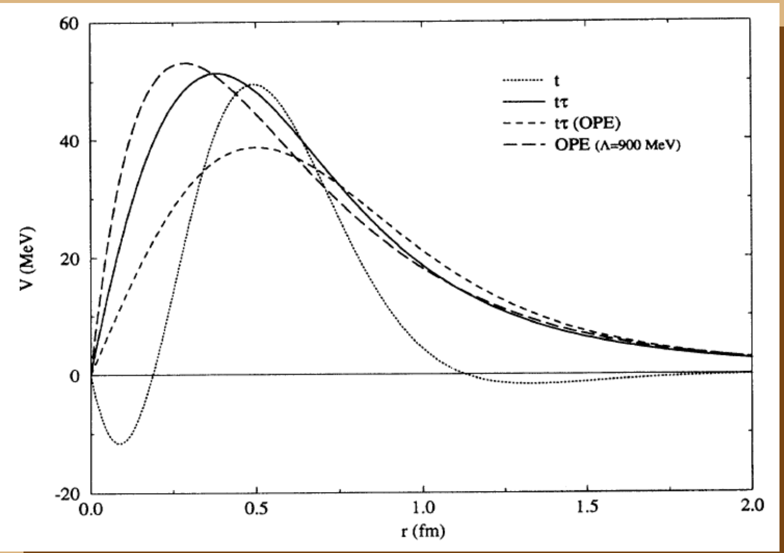

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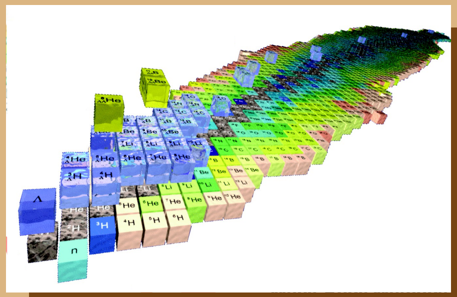

Many neutrons

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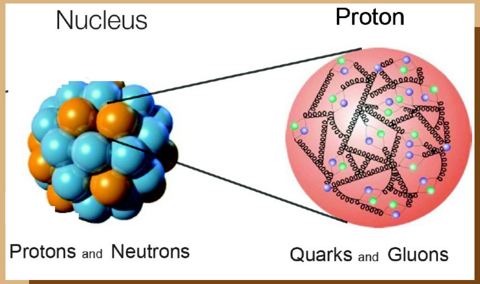
- Neutron stars



Nuclear forces

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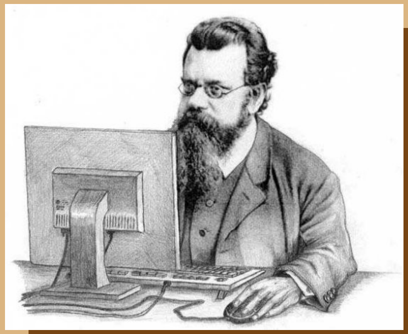

Credit: Bernhard Reischl

Results

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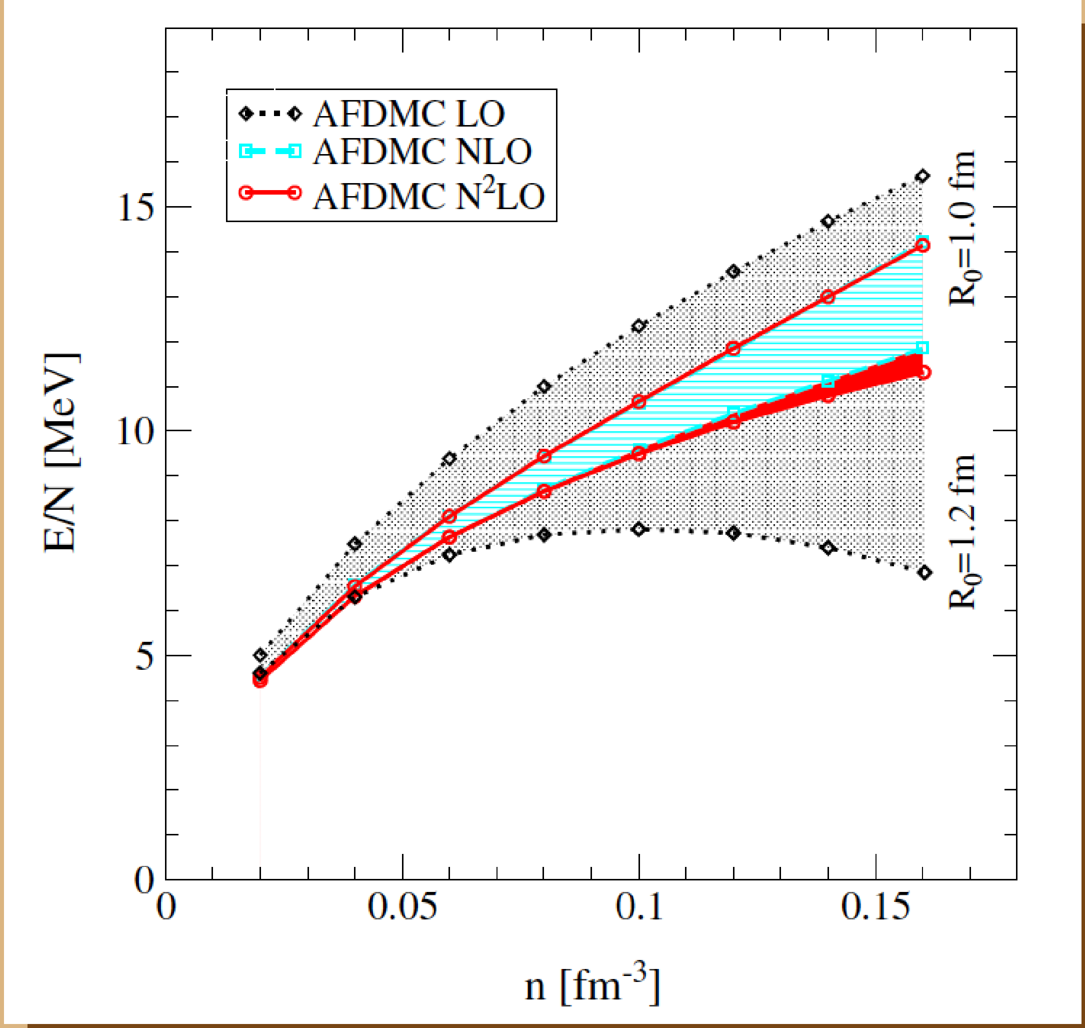
Chiral EFT in QMC



- 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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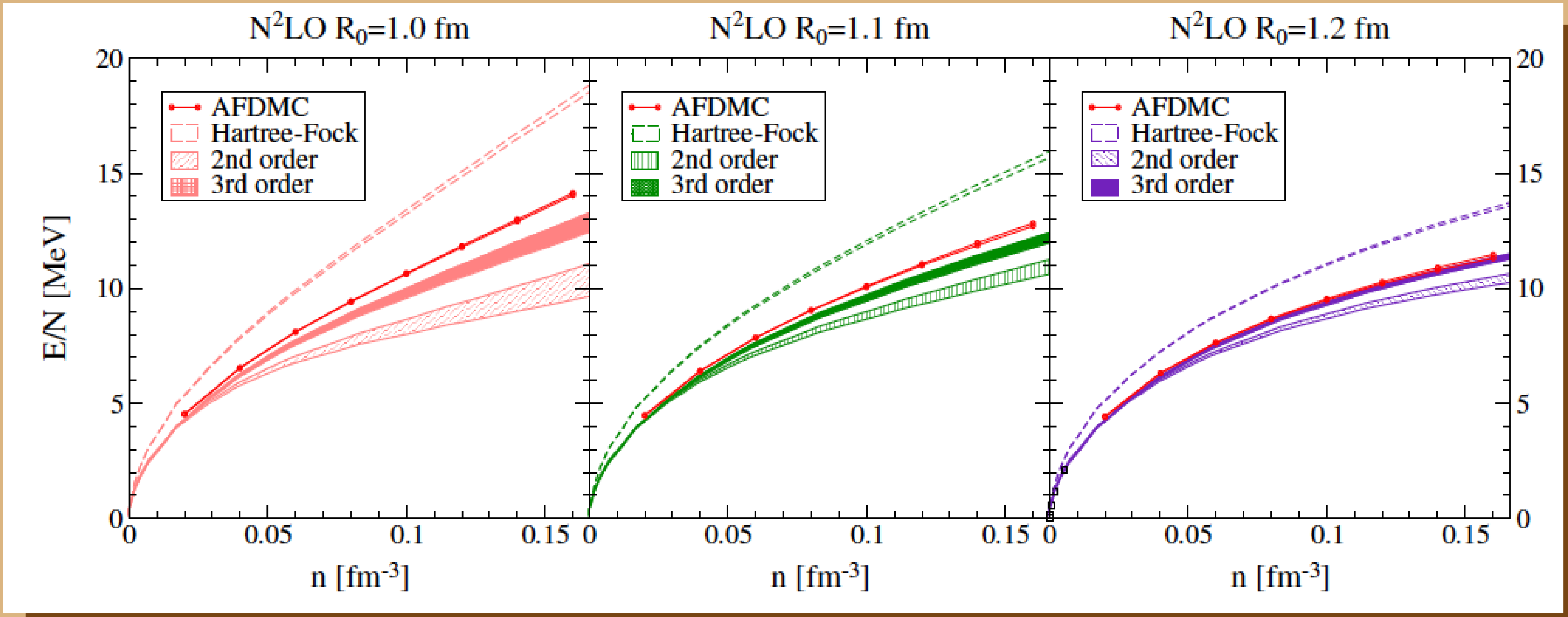
QMC vs MBPT



- MBPT bands come from diff. single-particle spectra
- Soft potential in excellent agreement with AFDMC

NEUTRONS

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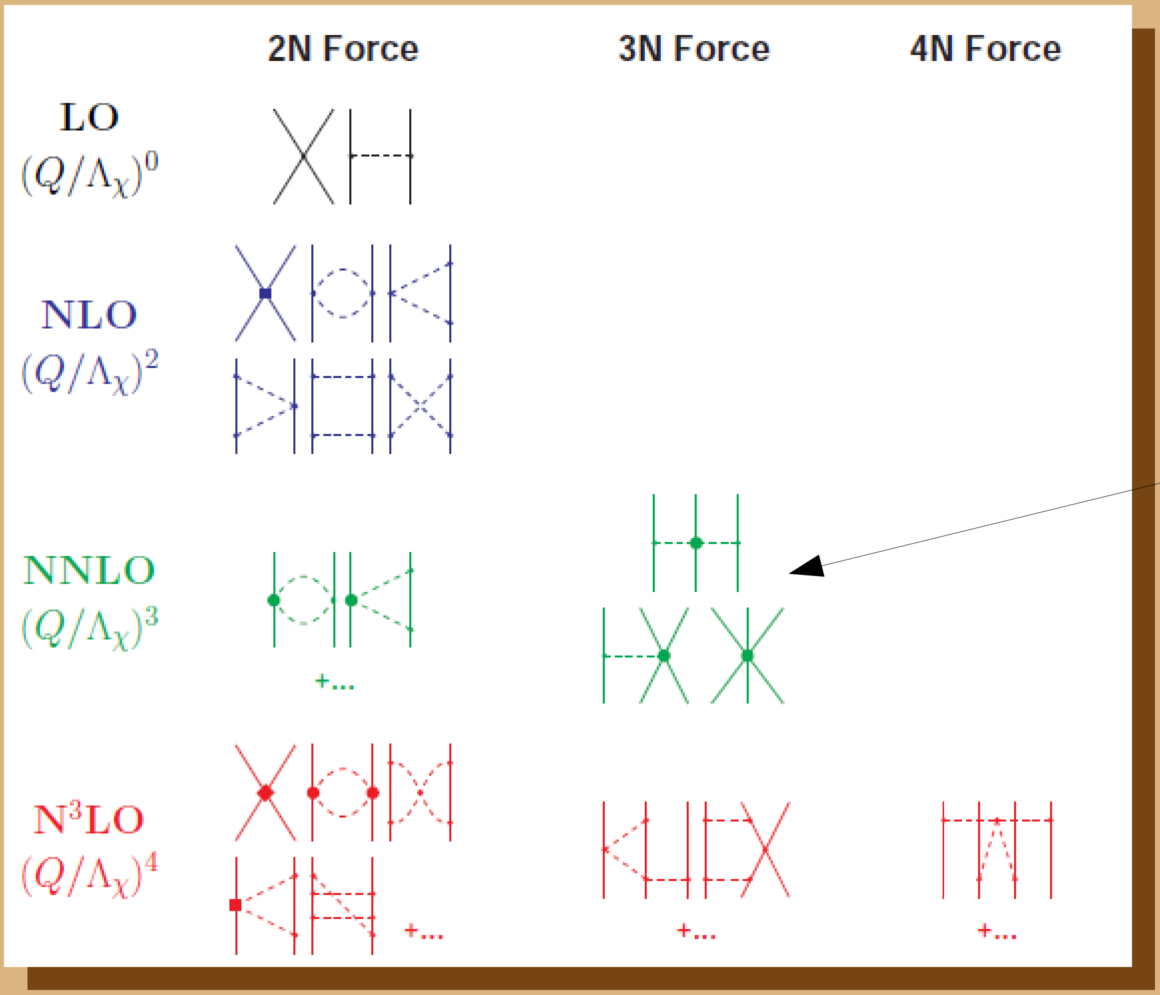
What about three-nucleon forces?

I. Tews, S. Gandolfi, A. Gezerlis, A. Schwenk, *in preparation*

Nuclear Hamiltonian: chiral EFT



N2LO 3NF

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

V_D and V_E are merely regulator effects in PNM

3NF TPE in PNM

Momentum space

$$V_{\rm TPE}^{\rm PNM} = \frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2 \frac{(\boldsymbol{\sigma}_i\cdot\mathbf{q}_i)(\boldsymbol{\sigma}_k\cdot\mathbf{q}_k)}{(q_i^2+m_\pi^2)(q_k^2+m_\pi^2)}\left[-\frac{4c_1 m_\pi^2}{f_\pi^2}+\frac{2c_3}{f_\pi^2}\mathbf{q}_i\cdot\mathbf{q}_k\right]$$

Coordinate space

$$\begin{aligned} V_{\rm TPE}^{\rm PNM} = &-\frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2\left(\frac{m_\pi}{4\pi}\right)^2\left(-\frac{4c_1 m_\pi^2}{f_\pi^2}\right)\boldsymbol{\sigma}_i\cdot\hat{\mathbf{r}}_{ij}\boldsymbol{\sigma}_k\cdot\hat{\mathbf{r}}_{kj}U(r_{ij})Y(r_{ij})U(r_{kj})Y(r_{kj}) \\ &+\frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2\left(\frac{1}{4\pi}\right)^2\left(\frac{2c_3}{f_\pi^2}\right)\left[\frac{m_\pi^4}{9}X_{ij}(\mathbf{r}_{ij})X_{kj}(\mathbf{r}_{kj})-\frac{4\pi m_\pi^2}{9}X_{ik}(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj})\right. \\ &\left.-\frac{4\pi m_\pi^2}{9}X_{ik}(\mathbf{r}_{kj})\delta(\mathbf{r}_{ij})+\frac{(4\pi)^2}{9}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_k\delta(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj})\right] \end{aligned}$$

3NF TPE in PNM

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&+\frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2\left(\frac{1}{4\pi}\right)^2\left(\frac{2c_3}{f_\pi^2}\right)\left[\frac{m_\pi^4}{9}X_{ij}(\mathbf{r}_{ij})X_{kj}(\mathbf{r}_{kj})-\frac{4\pi m_\pi^2}{9}X_{ik}(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj})\right.\\
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Long-range (LR)

3NF TPE in PNM

Momentum space

$$V_{\rm TPE}^{\rm PNM} = \frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2 \frac{(\boldsymbol{\sigma}_i\cdot\mathbf{q}_i)(\boldsymbol{\sigma}_k\cdot\mathbf{q}_k)}{(q_i^2+m_\pi^2)(q_k^2+m_\pi^2)}\left[-\frac{4c_1m_\pi^2}{f_\pi^2}+\frac{2c_3}{f_\pi^2}\mathbf{q}_i\cdot\mathbf{q}_k\right]$$

Coordinate space

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V_{\rm TPE}^{\rm PNM} = &-\frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2\left(\frac{m_\pi}{4\pi}\right)^2\left(-\frac{4c_1m_\pi^2}{f_\pi^2}\right)\boldsymbol{\sigma}_i\cdot\hat{\mathbf{r}}_{ij}\boldsymbol{\sigma}_k\cdot\hat{\mathbf{r}}_{kj}U(r_{ij})Y(r_{ij})U(r_{kj})Y(r_{kj})\\
&+\frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2\left(\frac{1}{4\pi}\right)^2\left(\frac{2c_3}{f_\pi^2}\right)\left[\frac{m_\pi^4}{9}X_{ij}(\mathbf{r}_{ij})X_{kj}(\mathbf{r}_{kj})-\frac{4\pi m_\pi^2}{9}X_{ik}(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj})\right.\\
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\end{aligned}$$

Intermediate-range (IR)

3NF TPE in PNM

Momentum space

$$V_{\mathrm{TPE}}^{\mathrm{PNM}} = \frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2 \frac{(\boldsymbol{\sigma}_i\cdot\mathbf{q}_i)(\boldsymbol{\sigma}_k\cdot\mathbf{q}_k)}{(q_i^2+m_\pi^2)(q_k^2+m_\pi^2)}\left[-\frac{4c_1 m_\pi^2}{f_\pi^2}+\frac{2c_3}{f_\pi^2}\mathbf{q}_i\cdot\mathbf{q}_k\right]$$

Coordinate space

Short-range (SR)

$$\begin{aligned}V_{\mathrm{TPE}}^{\mathrm{PNM}} = &-\frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2\left(\frac{m_\pi}{4\pi}\right)^2\left(-\frac{4c_1 m_\pi^2}{f_\pi^2}\right)\boldsymbol{\sigma}_i\cdot\hat{\mathbf{r}}_{ij}\boldsymbol{\sigma}_k\cdot\hat{\mathbf{r}}_{kj}U(r_{ij})Y(r_{ij})U(r_{kj})Y(r_{kj})\\ &+\frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2\left(\frac{1}{4\pi}\right)^2\left(\frac{2c_3}{f_\pi^2}\right)\left[\frac{m_\pi^4}{9}X_{ij}(\mathbf{r}_{ij})X_{kj}(\mathbf{r}_{kj})-\frac{4\pi m_\pi^2}{9}X_{ik}(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj})\right.\\ &\left.-\frac{4\pi m_\pi^2}{9}X_{ik}(\mathbf{r}_{kj})\delta(\mathbf{r}_{ij})+\frac{(4\pi)^2}{9}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_k\delta(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj})\right]\end{aligned}$$

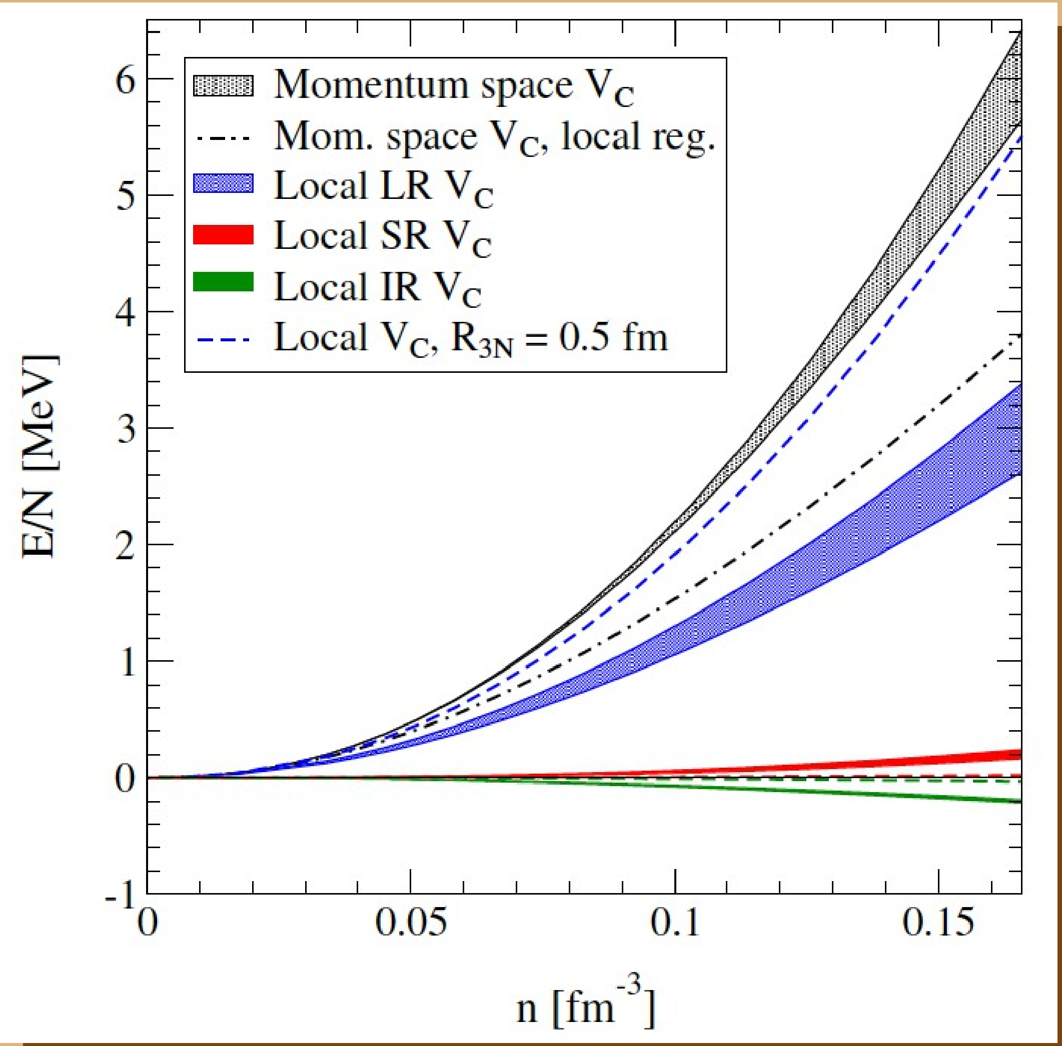
Regularizing

Attempt to be consistent with NN regularization

$$\delta(\mathbf{r}) \;\to\; \delta_{R_{3\mathrm{N}}}(\mathbf{r}) = \frac{1}{\pi\Gamma(3/4)\,R_{3\mathrm{N}}^3}\, e^{-(r/R_{3\mathrm{N}})^4}$$

$$Y(r) \;\to\; Y(r)\left(1 - e^{-(r/R_{3\mathrm{N}})^4}\right)$$

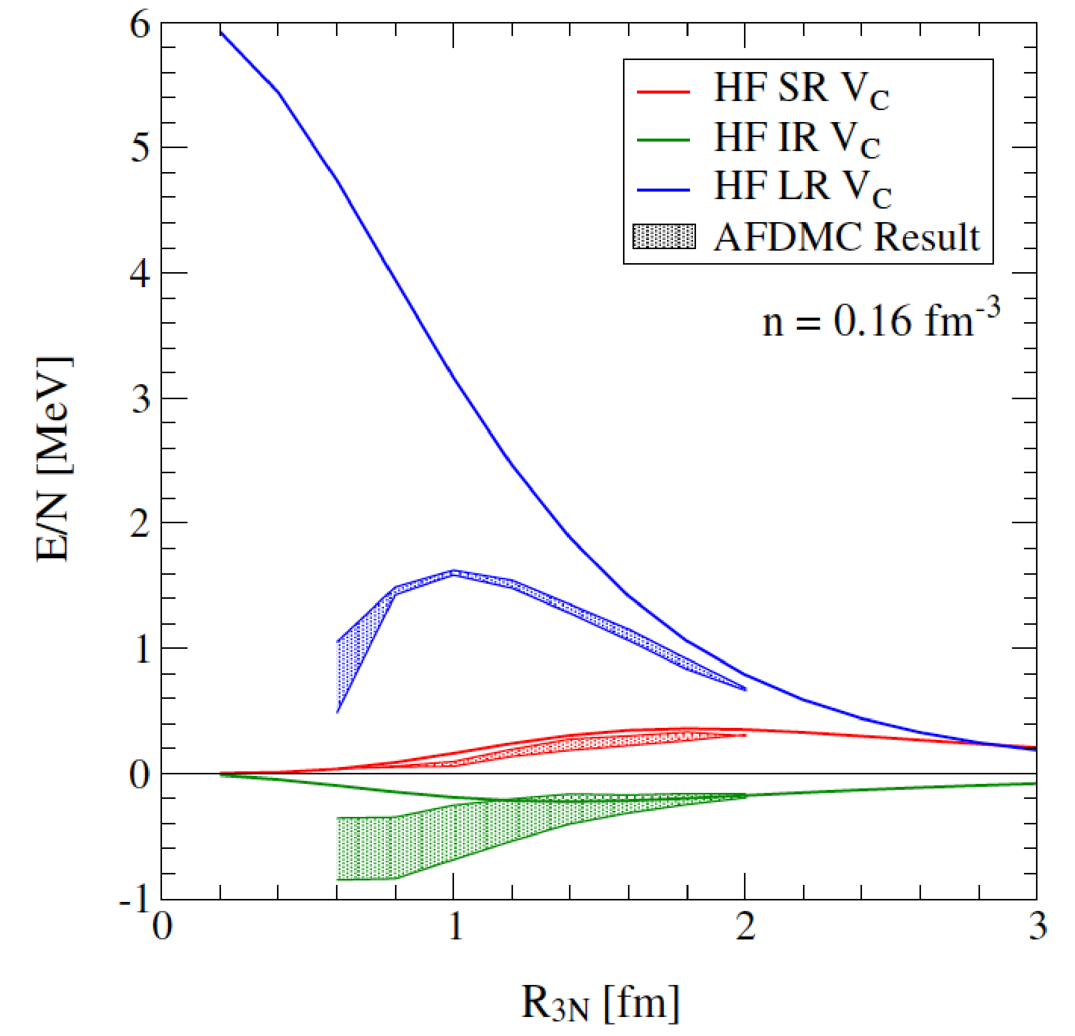
3NF contributions: Hartree-Fock



- Local 3NFs (Navratil + ours) lead to ~2.5 MeV lower energy at saturation density
- Our new local 3NF results agree with Navratil local 3NF result for very short coordinate-space cutoff

NEUTRONS

3NF contributions



- Shown are both HF (lines) and AFDMC (bands) for 3NF contrib
- HF shows IR & SR vanishing at low R_{3N}
- AFDMC at low R_{3N} shows collapse of LR and IR

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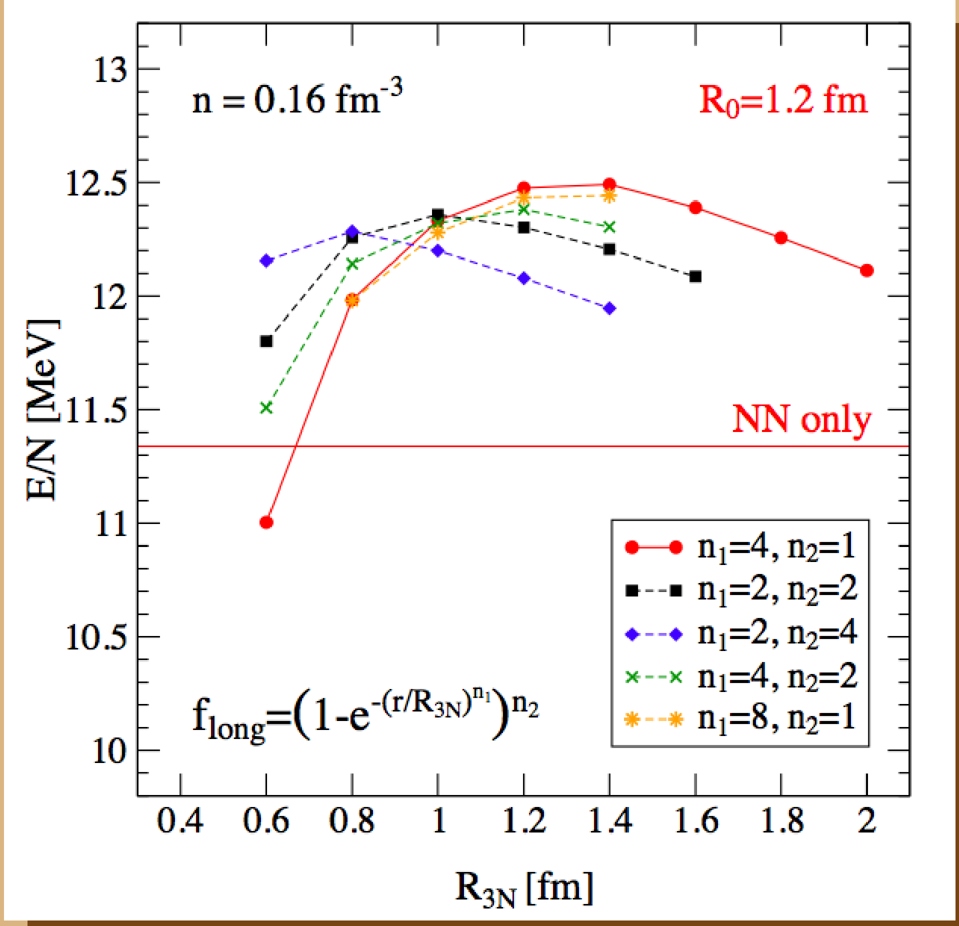
3NF cutoff choice



- Too large cutoff chops off too much
- Too small cutoff leads to collapse
- Plateau appears at intermediate values of the cutoff
- Result does not appear to depend on specific form of the regulator

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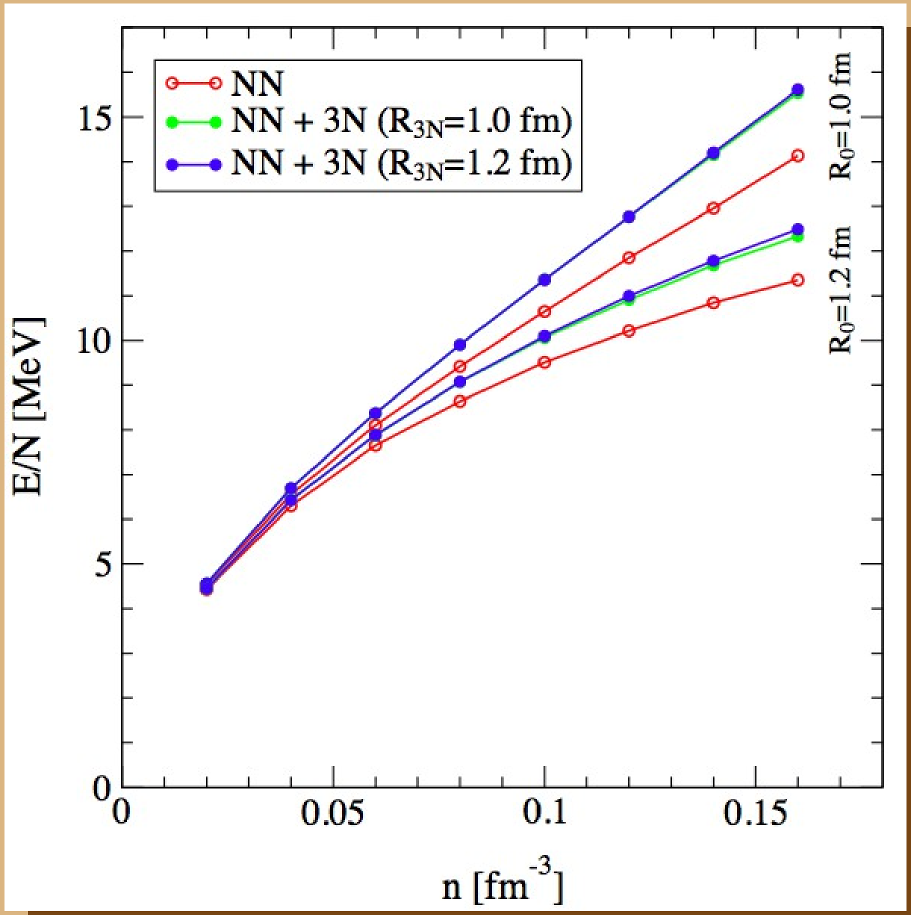
Overall error bands



- 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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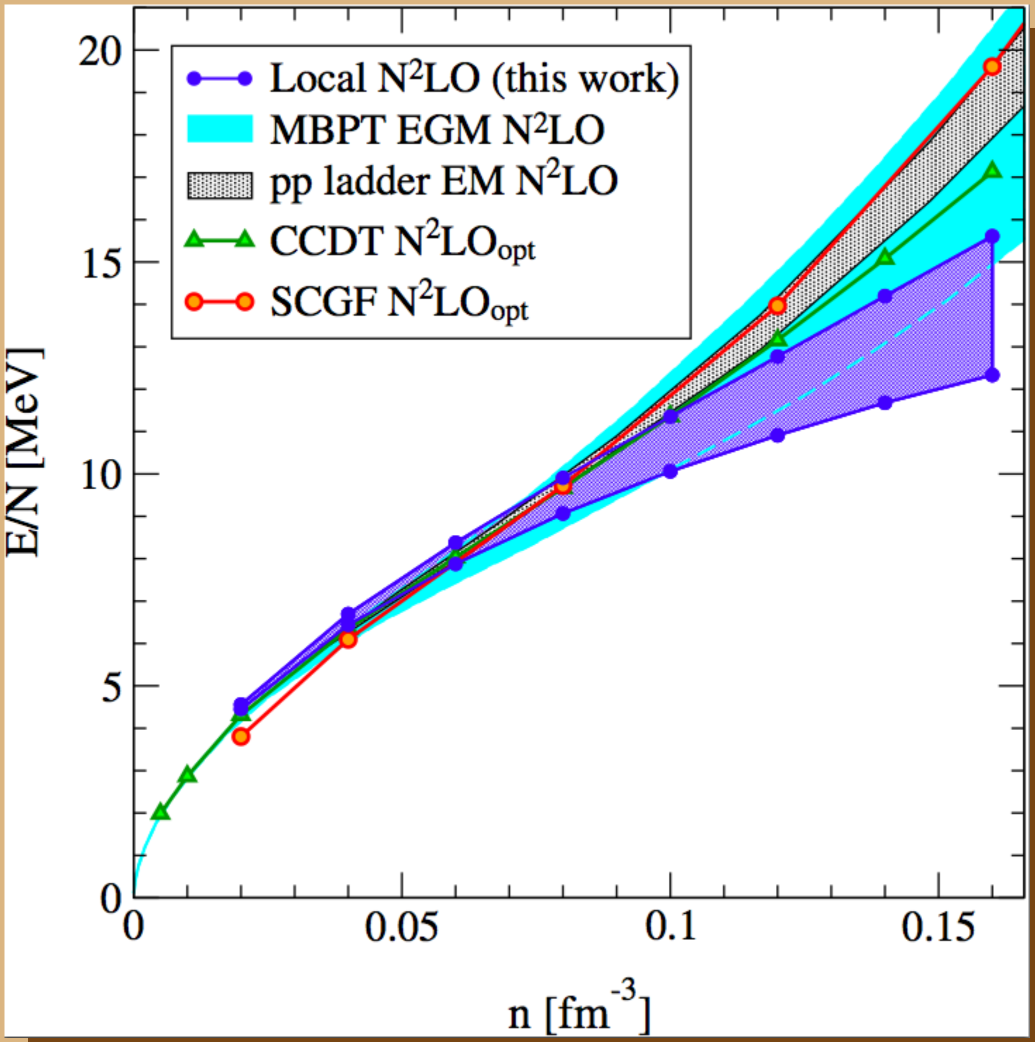
Compare with other calculations at N2LO



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

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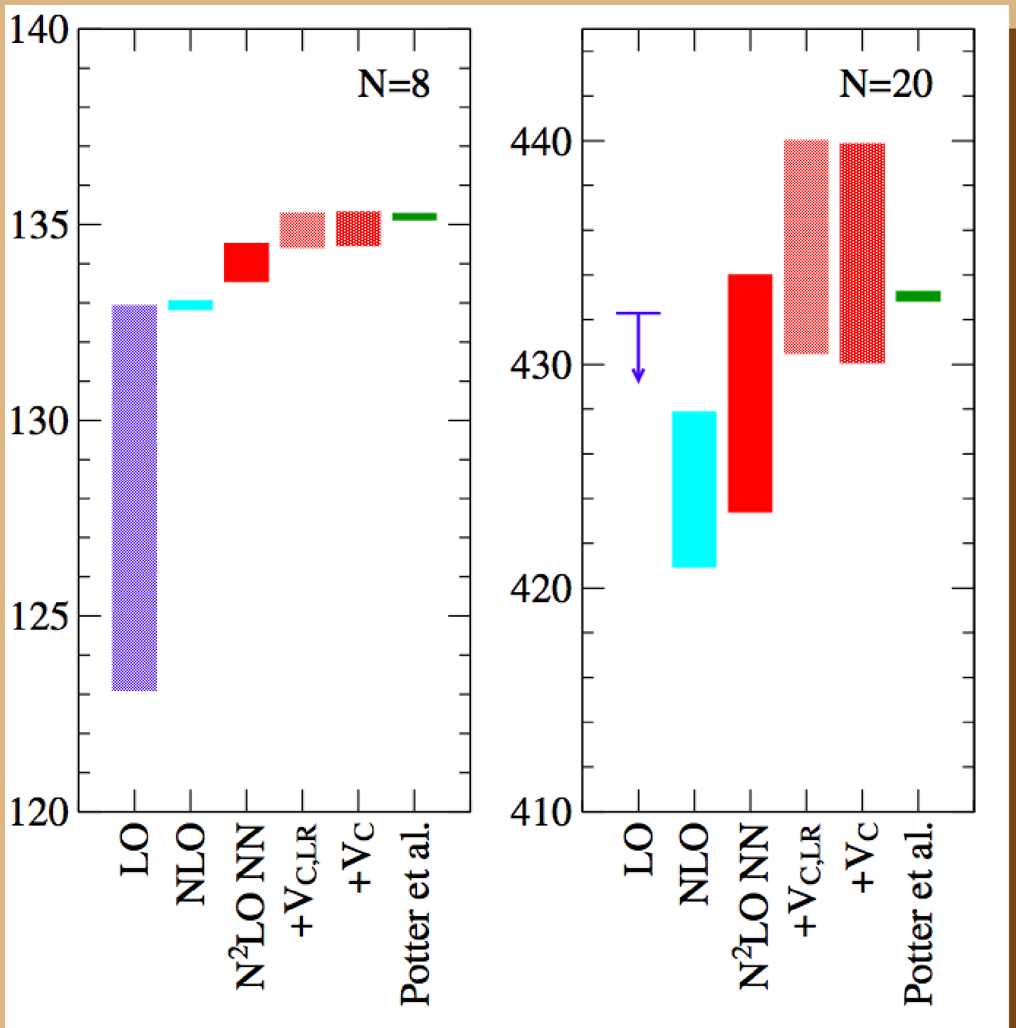
Now turn to neutron drops

I. Tews, S. Gandolfi, A. Gezerlis, A. Schwenk, *in preparation*

Neutron drops with NN+3NF chiral forces



- 10 MeV harmonic oscillator trap
- Order-by-order systematics studied
- Soft LO potential leads to very low energies, especially in larger systems
- Reasonable agreement with ΛCCSD calculations

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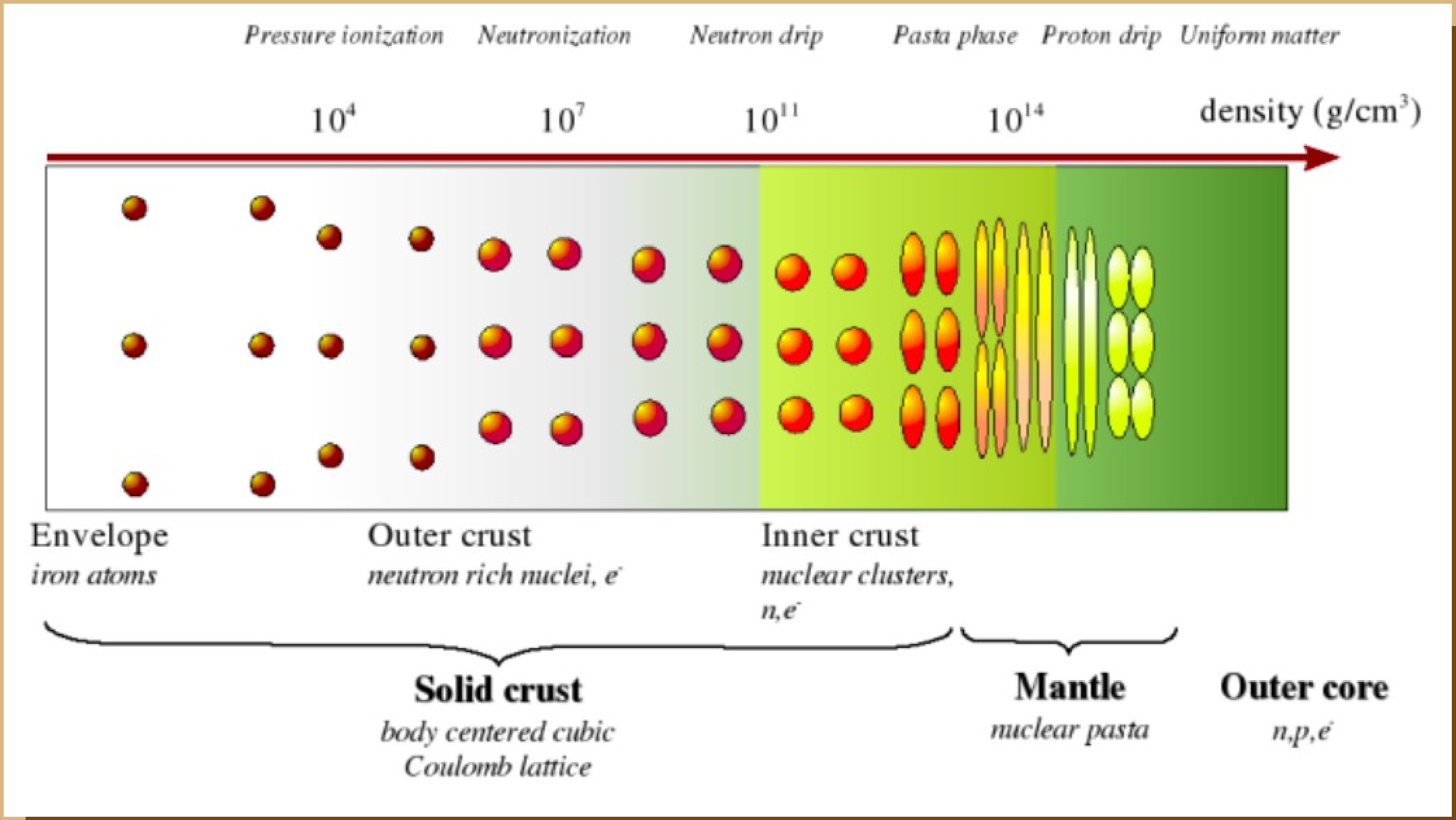
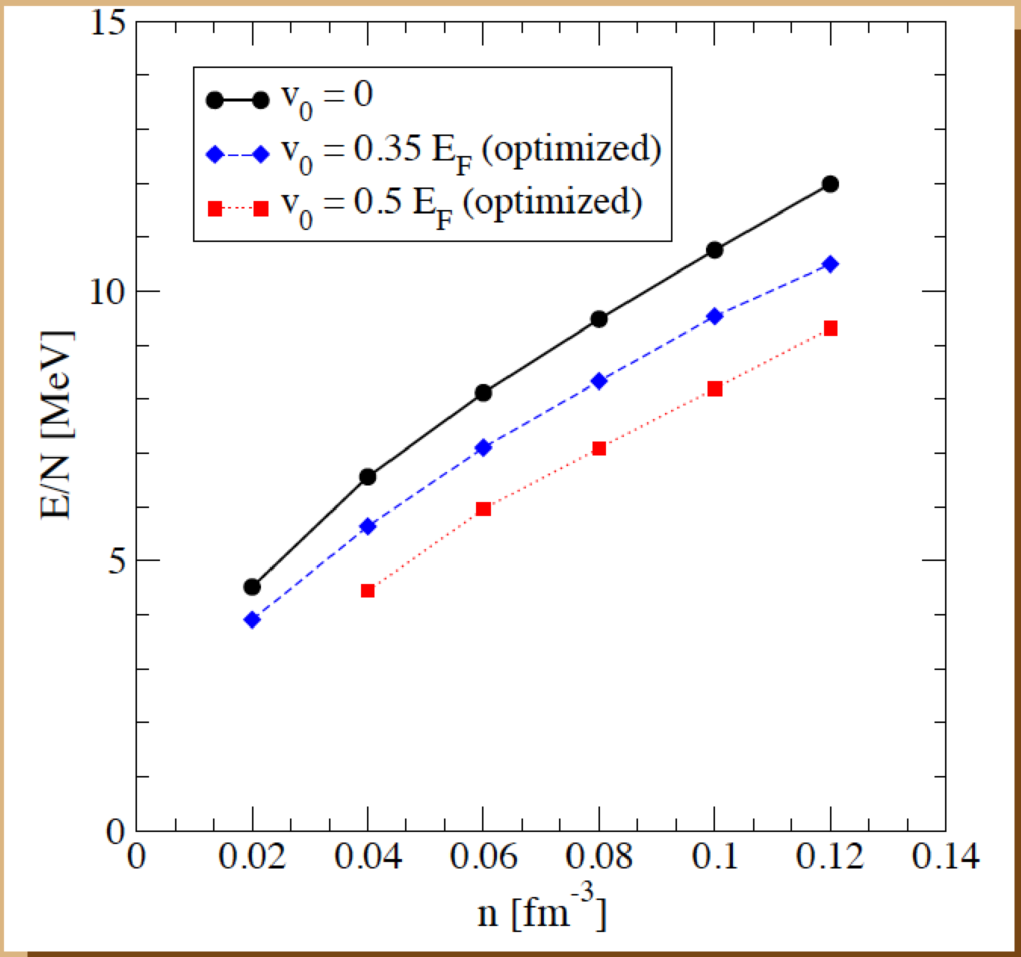
Remember that neutron-star crusts also involve a lattice of nuclei

M. Buraczynski and A. Gezerlis, *in preparation*

Neutron star crusts more than PNM



Static response of neutron matter



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

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Conclusions

- Local chiral N2LO 3NF forces derived and being used in the many-body context
- Local 3NF contributions much smaller than non-local ones
- Effects of the regulator intriguing and being further explored
- Static response also being investigated

Acknowledgments

Funding

NSERC
CRSNG

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Collaborators

- **Matt Buraczynski** (Guelph)
- Evgeny Epelbaum (Bochum)
- Stefano Gandolfi (LANL)
- Achim Schwenk (Darmstadt)
- **Ingo Tews** (Darmstadt)