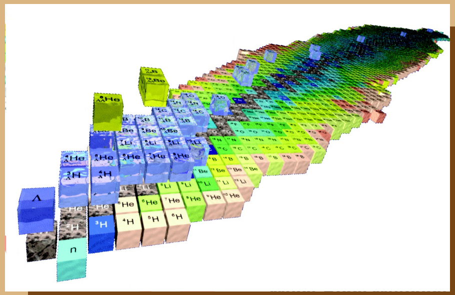
Quantum Monte Carlo for neutron-rich systems

Alexandros Gezerlis

UNIVERSITY of GUELPH

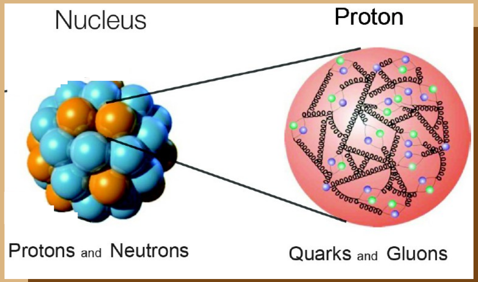
TRIUMF Nuclear Theory Workshop
Vancouver, BC
February 20, 2015

Outline



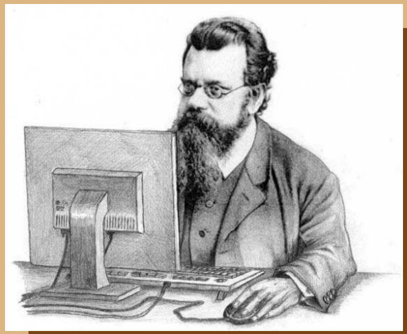
Many nucleons

- Neutron stars
- Quantum Monte Carlo



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

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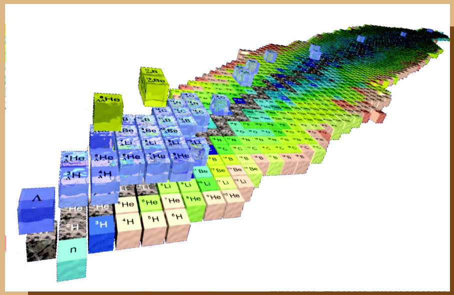

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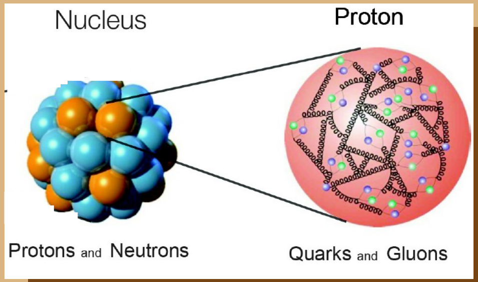

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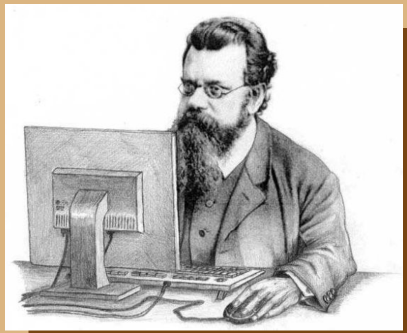

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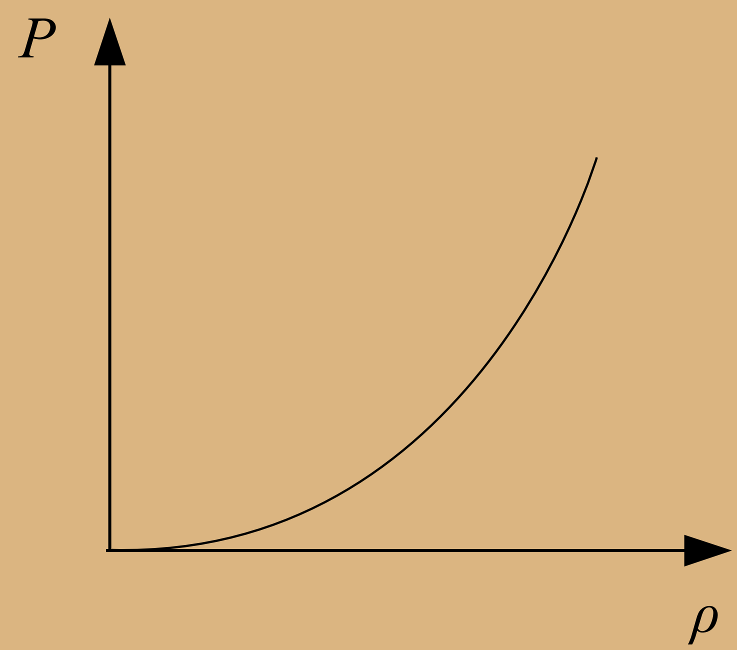
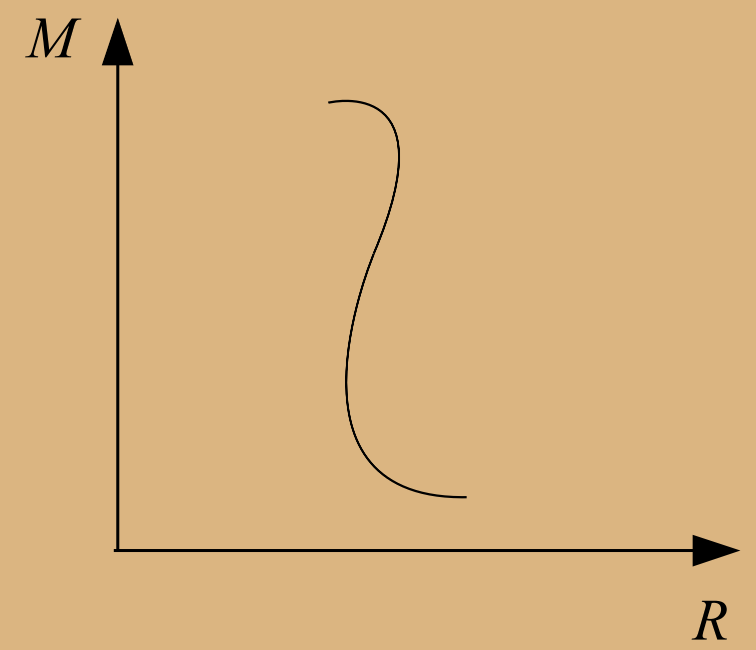
Neutron stars: micro-macro

TOV equations
(or Hartle-Thorne, etc)

Pressure vs density



Mass vs radius

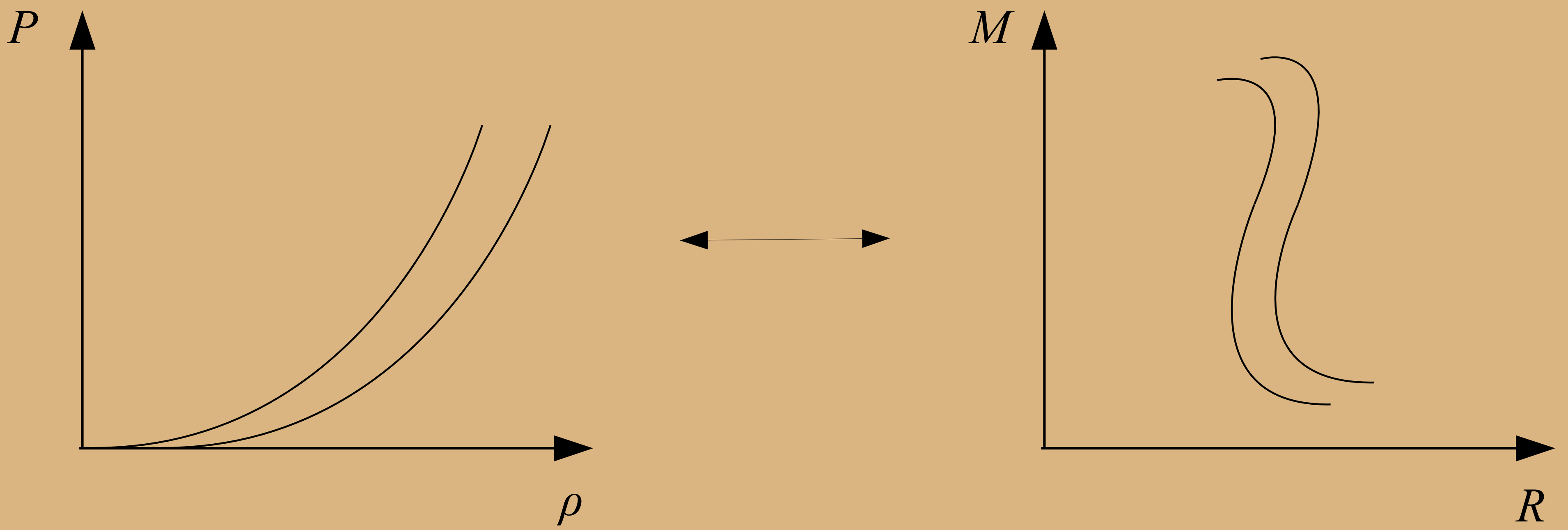


Uncertainty estimates

TOV equations
(or Hartle-Thorne, etc)

Pressure vs density

Mass vs radius



Modern goal: systematic theoretical error bars

Many-body problem: QMC

Quantum Monte Carlo: stochastically solve the many-body Schrödinger equation in a fully non-perturbative manner

Many-body problem: QMC

Quantum Monte Carlo: stochastically solve the many-body Schrödinger equation in a fully non-perturbative manner

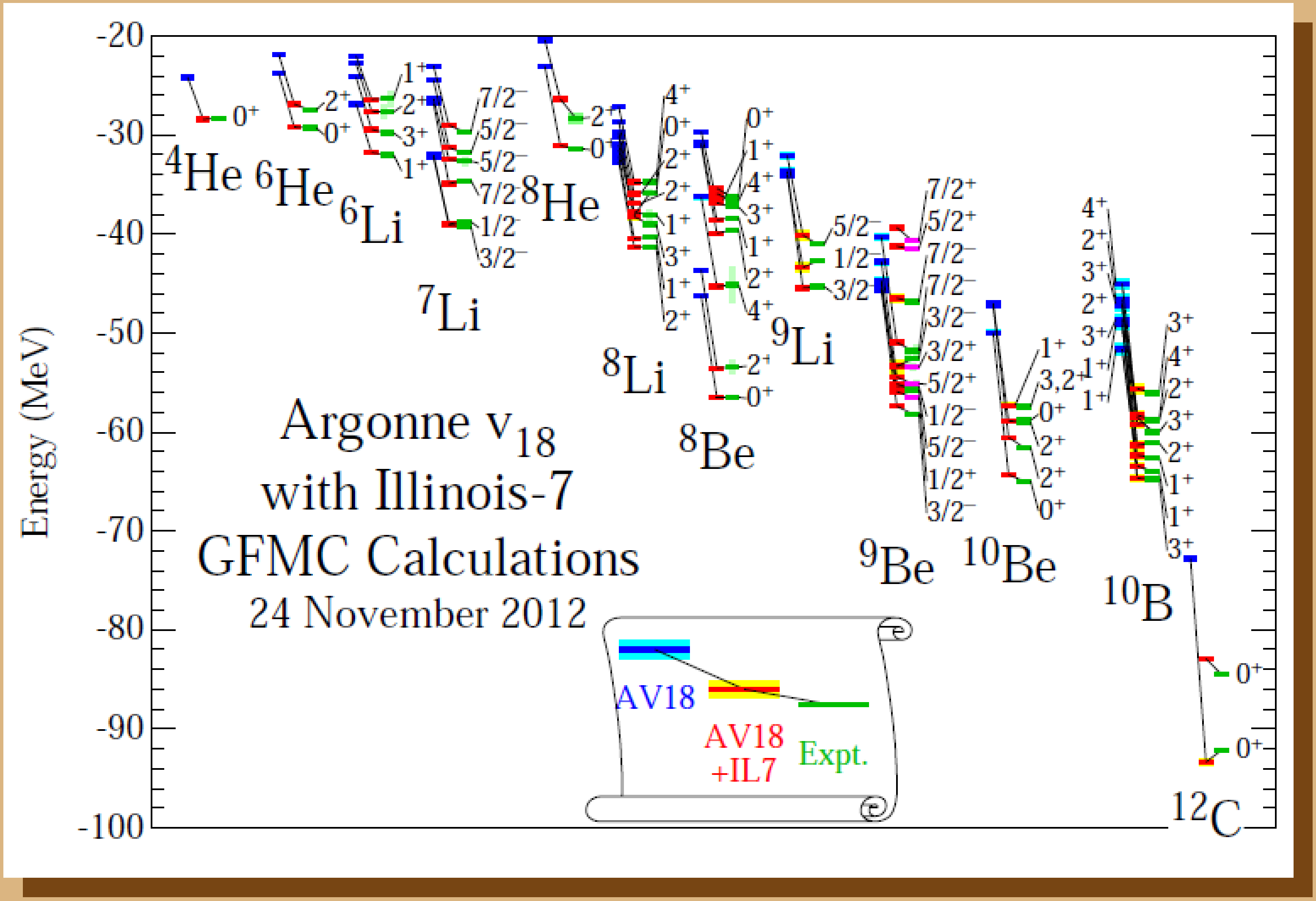
Rudiments of Diffusion Monte Carlo:

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

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

Argonne/Illinois + nuclear GFMC

B. Wiringa's talk: nuclear Green's Function Monte Carlo is very accurate



Credit: Steve Pieper

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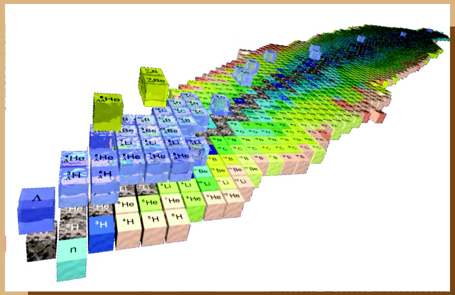

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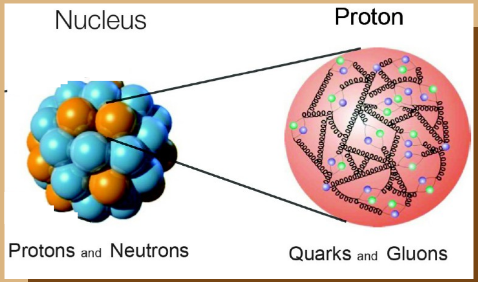

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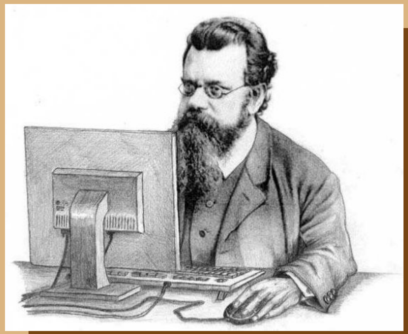

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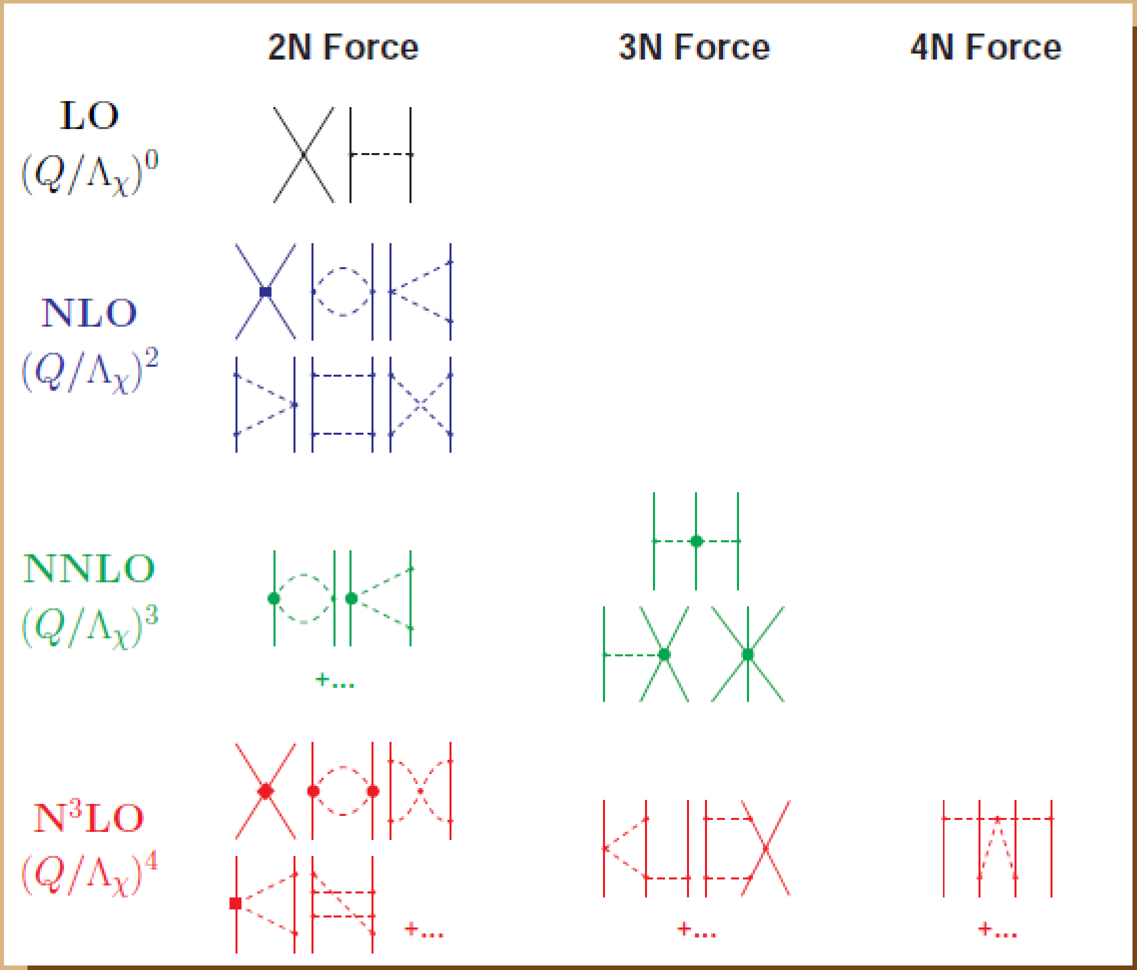
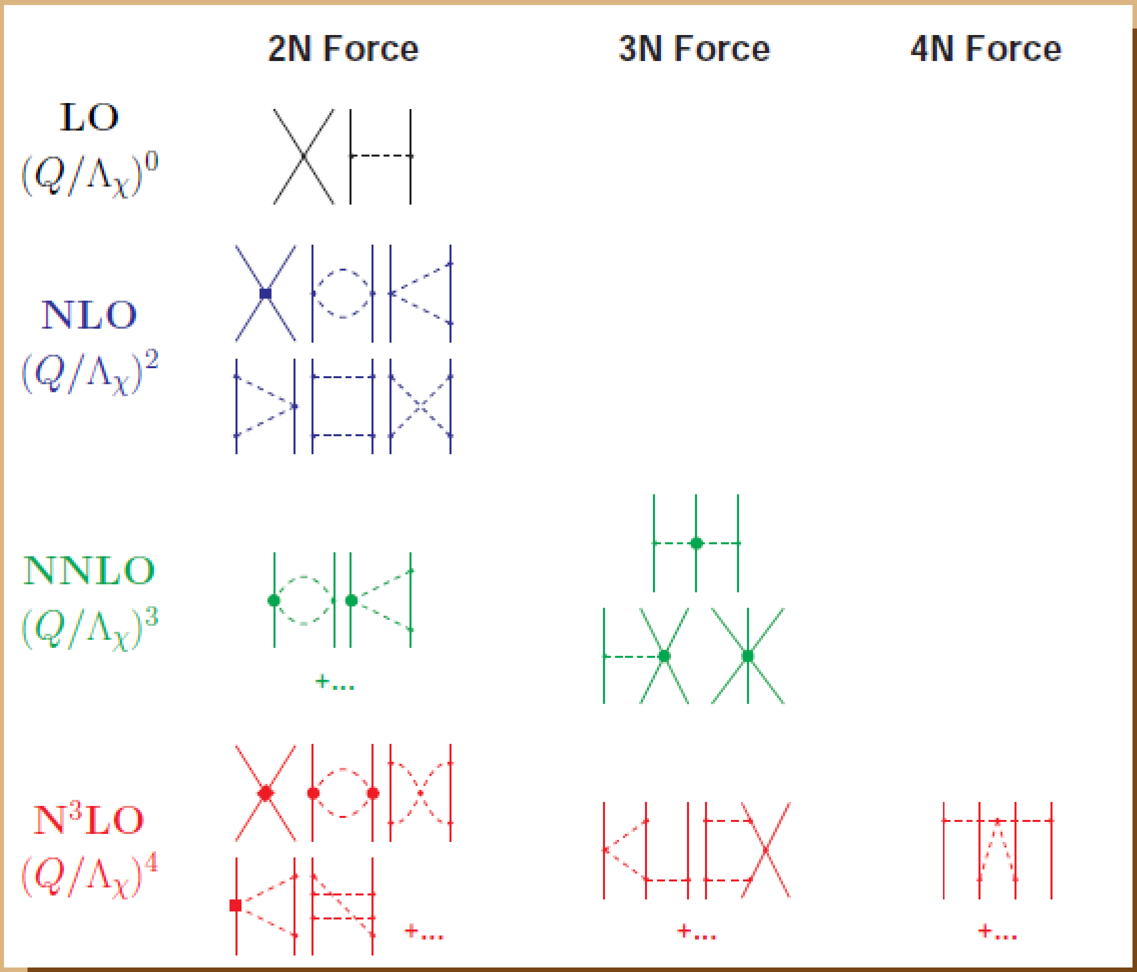
Nuclear Hamiltonian: chiral EFT



- 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



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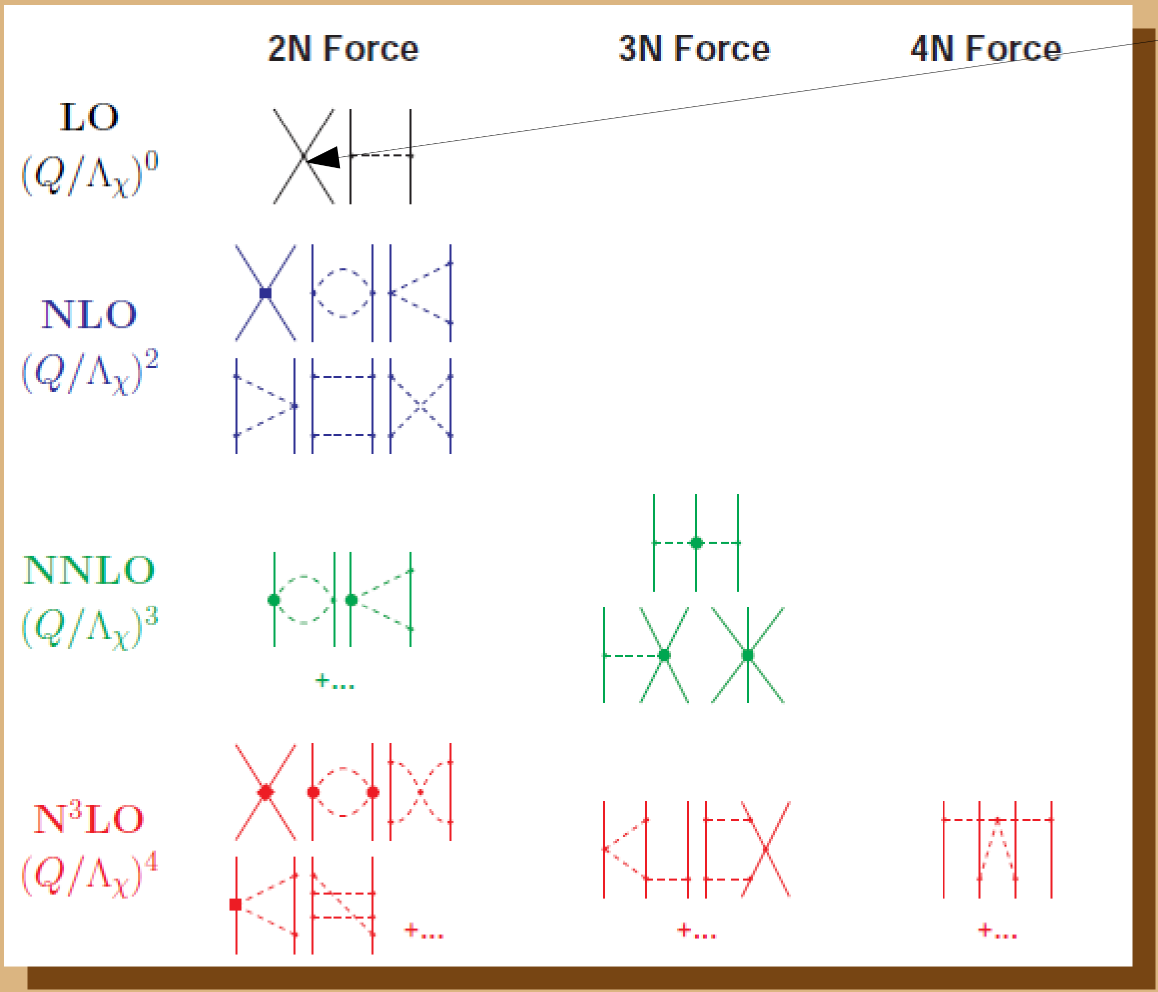

$$V_{\rm ct}^{(0)} = C_S + C_T\ \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

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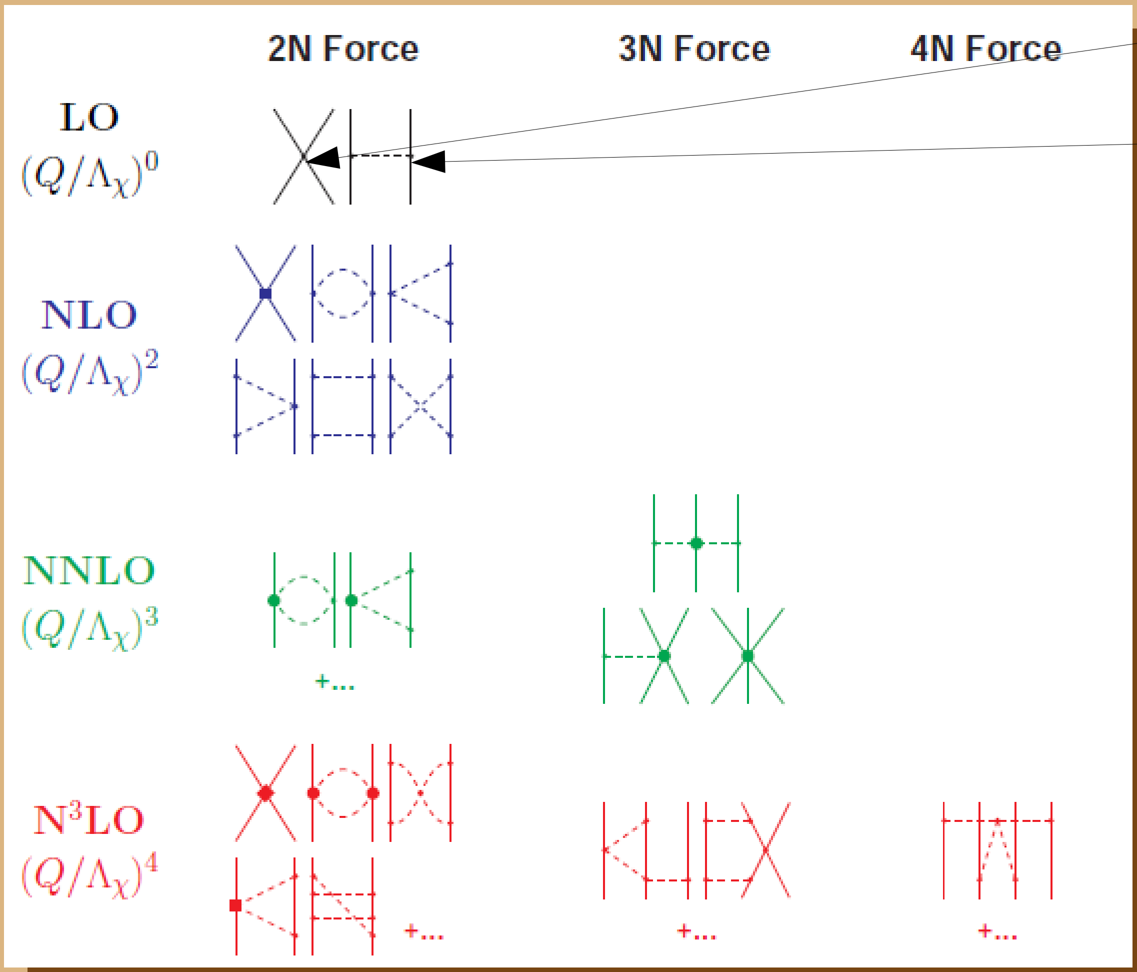

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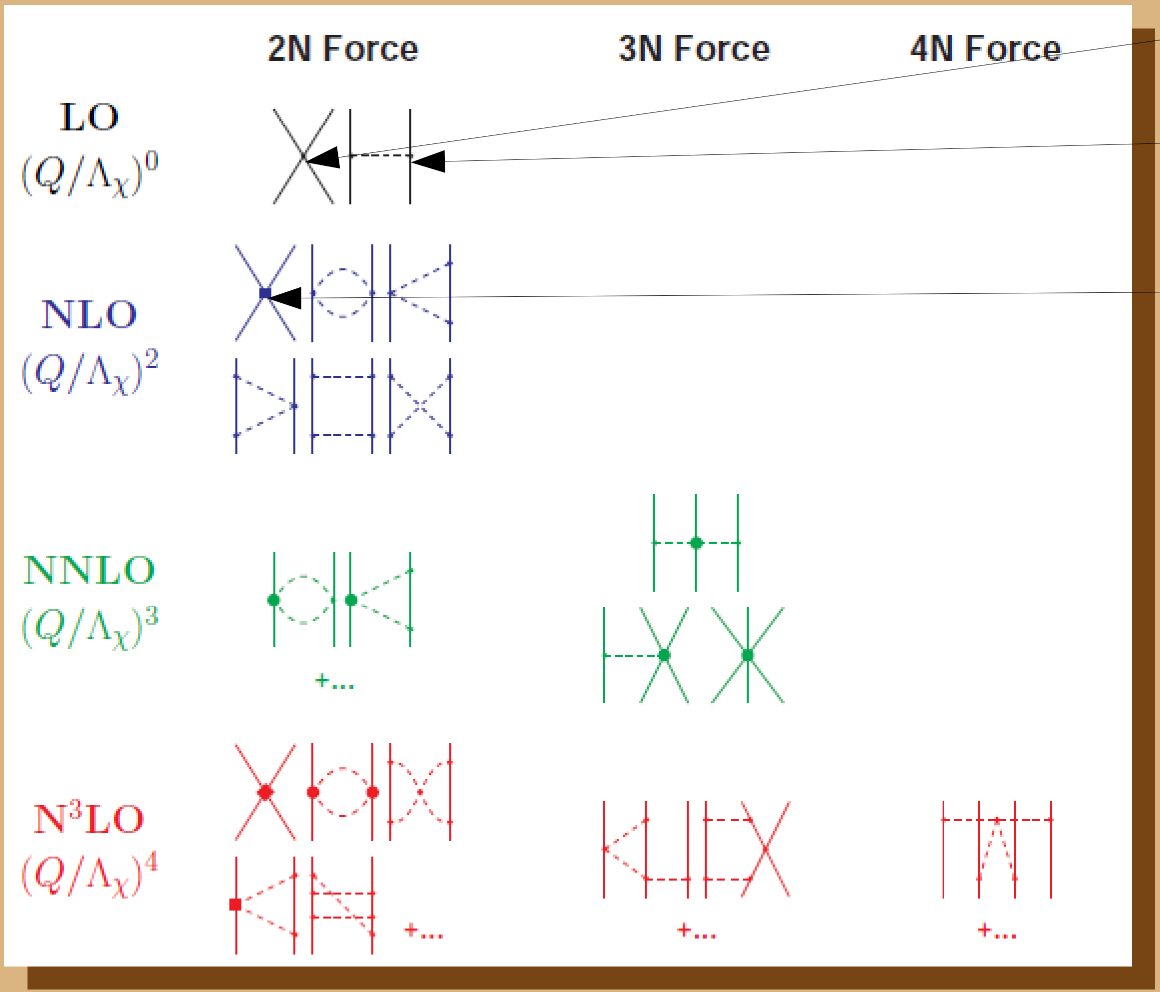

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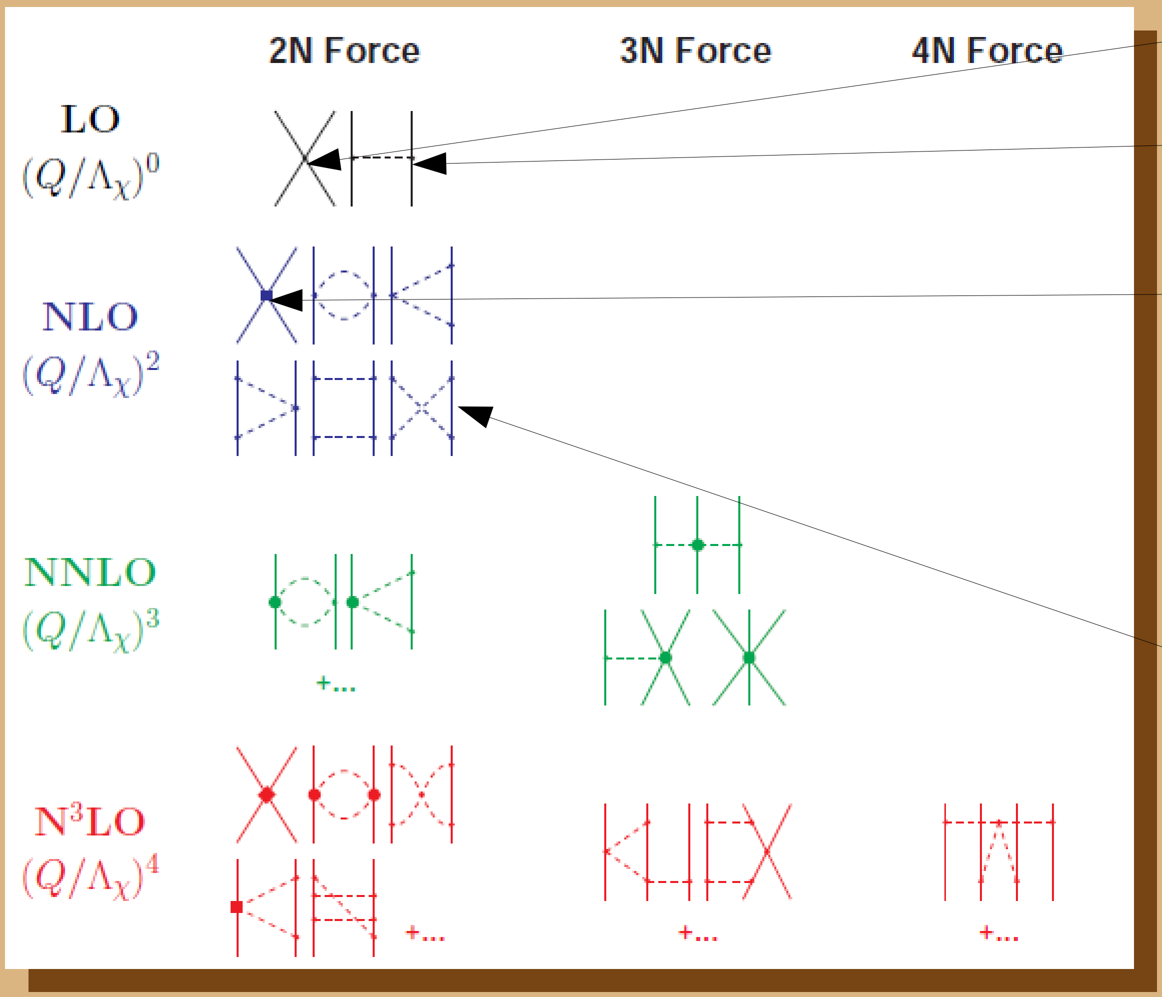

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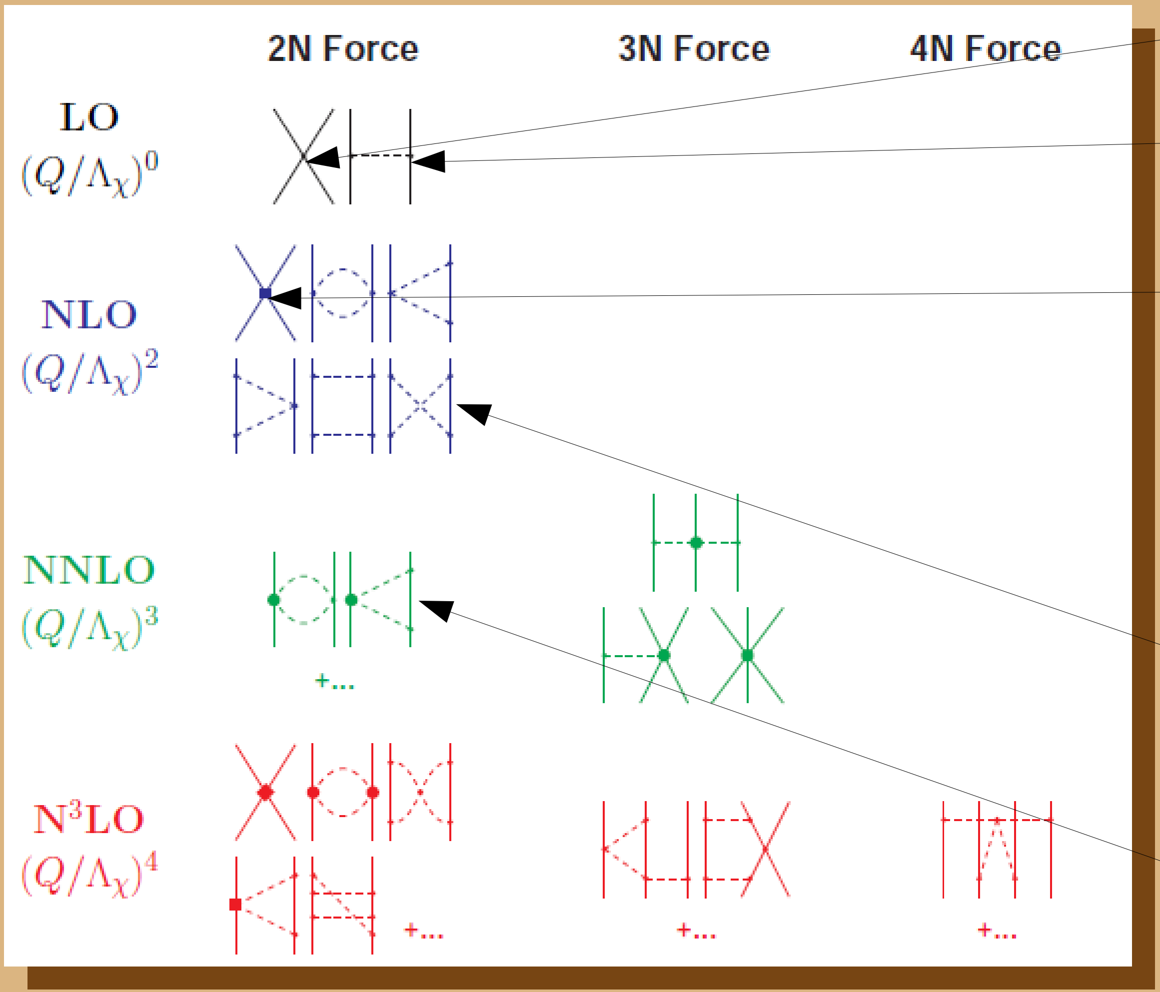
Long-studied
two-pion exchange

Nuclear Hamiltonian: chiral EFT



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Contains couplings
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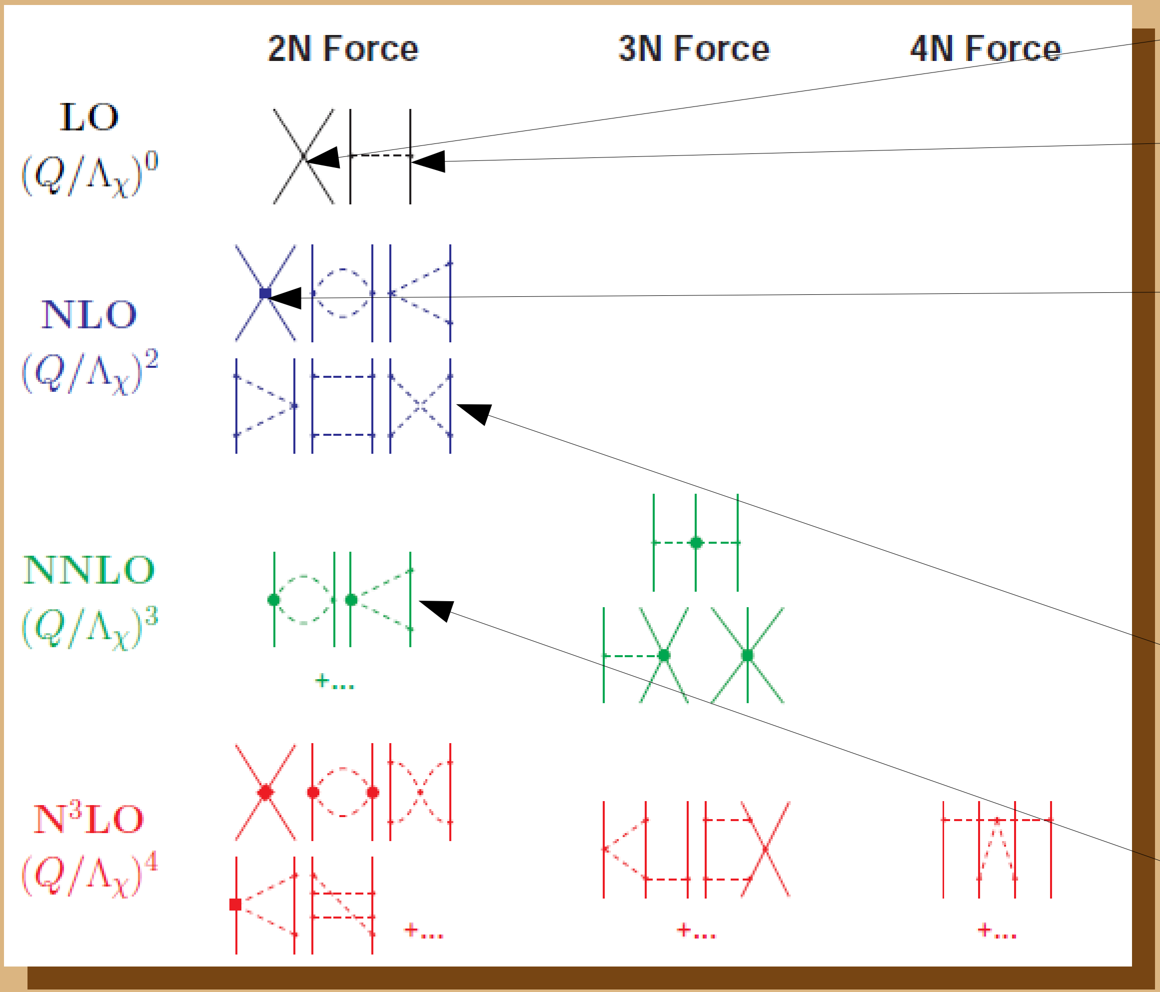

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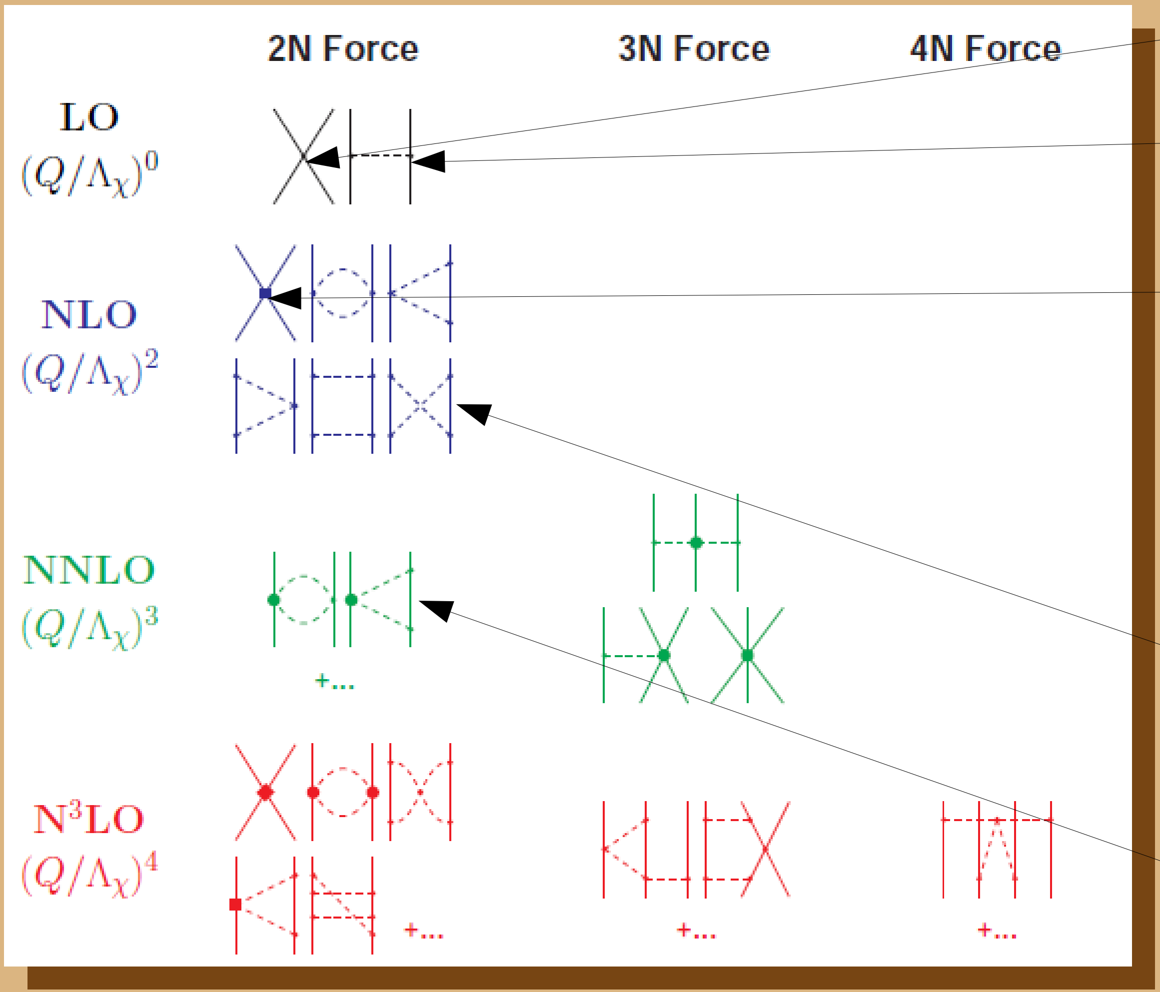
$$\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2 \qquad \mathbf{k} = (\mathbf{p}' + \mathbf{p})/2$$

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

Nuclear Hamiltonian: chiral EFT



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Contains couplings
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$\mathbf{k}$ means non-local

$\mathbf{q}$ means local

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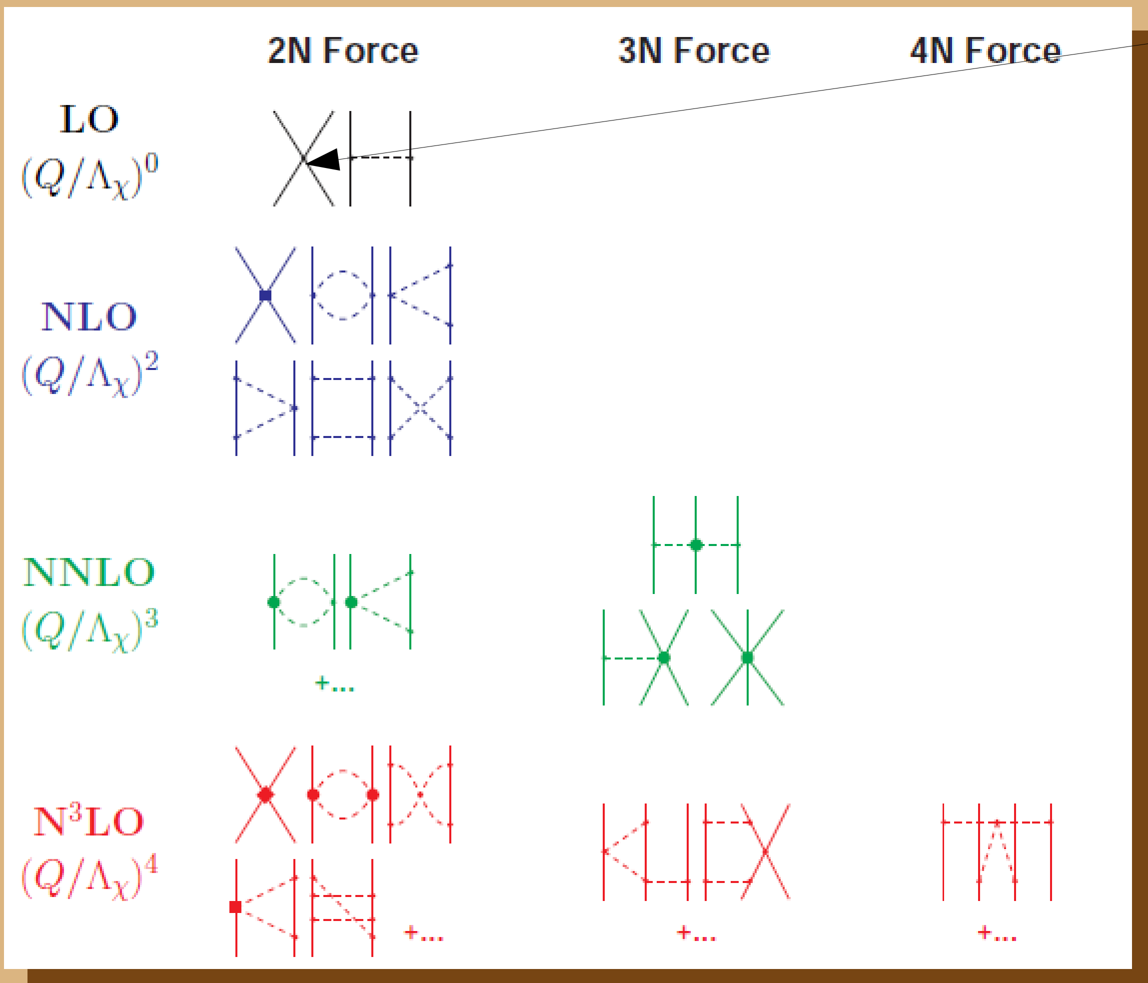
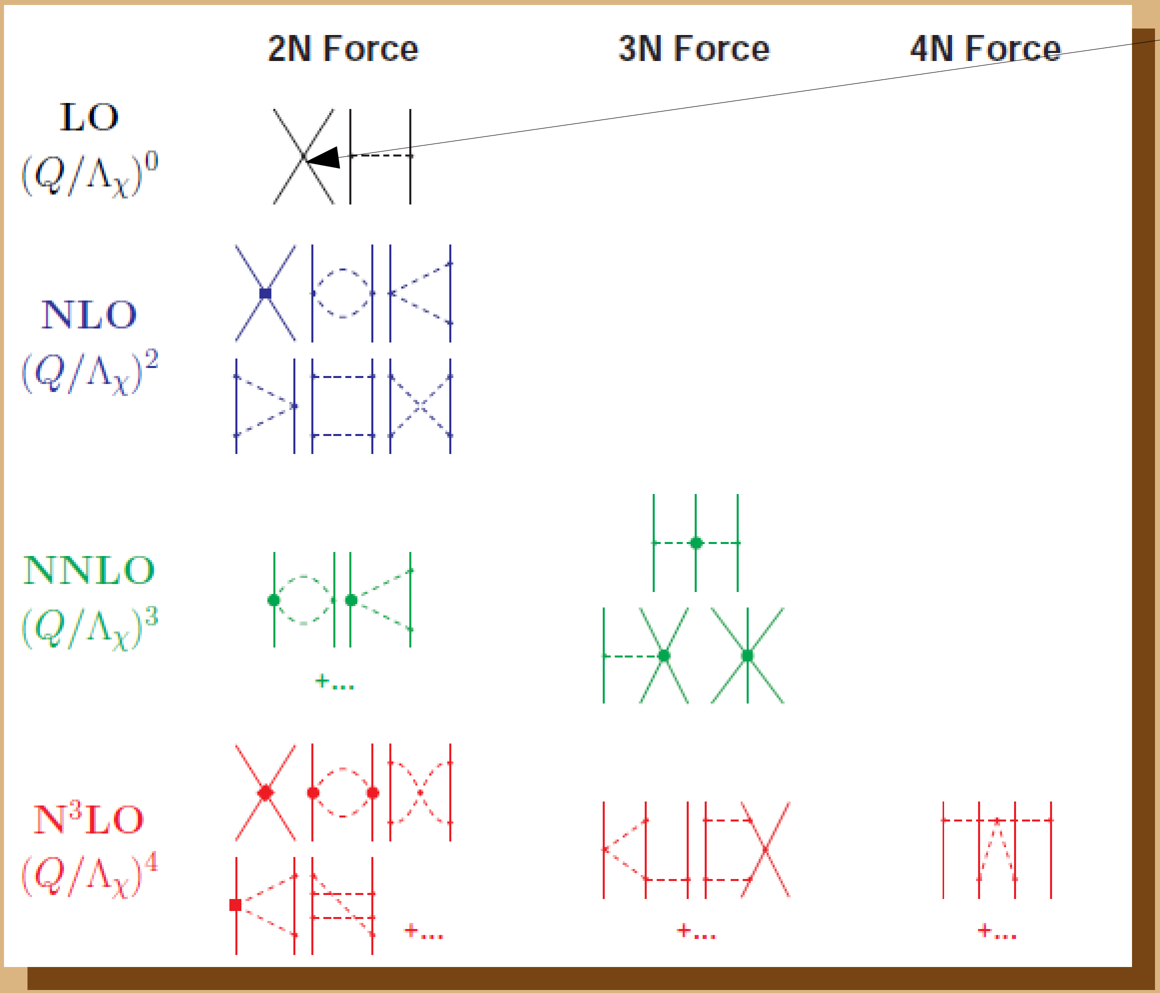
Nuclear Hamiltonian: chiral EFT



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

Merely the standard choice.

Nuclear Hamiltonian: chiral EFT



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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).
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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

$$
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$$

cf.

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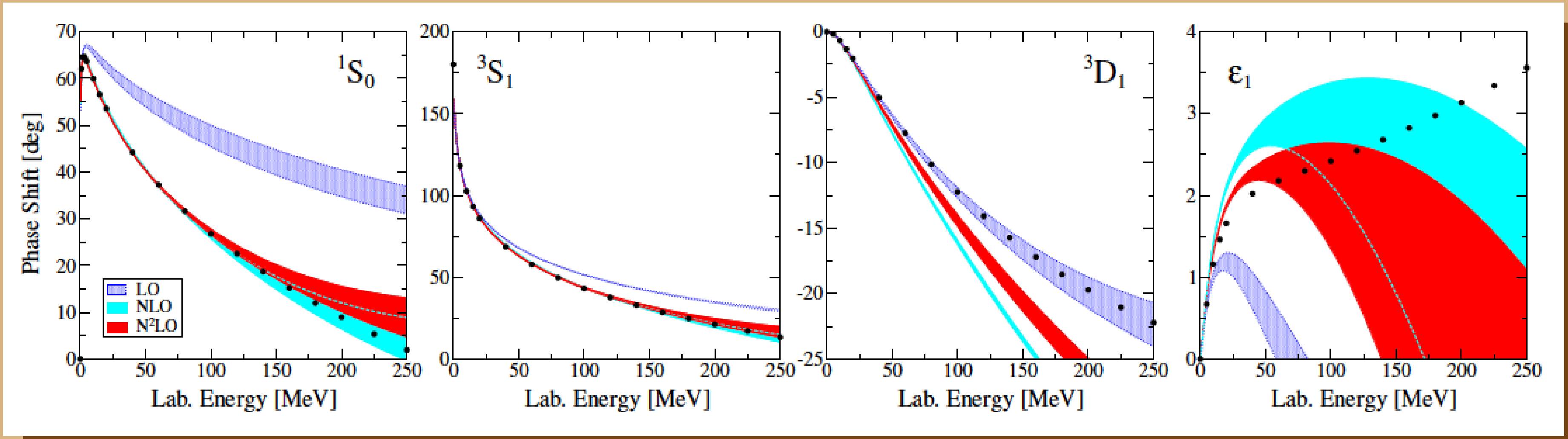
Phase shifts



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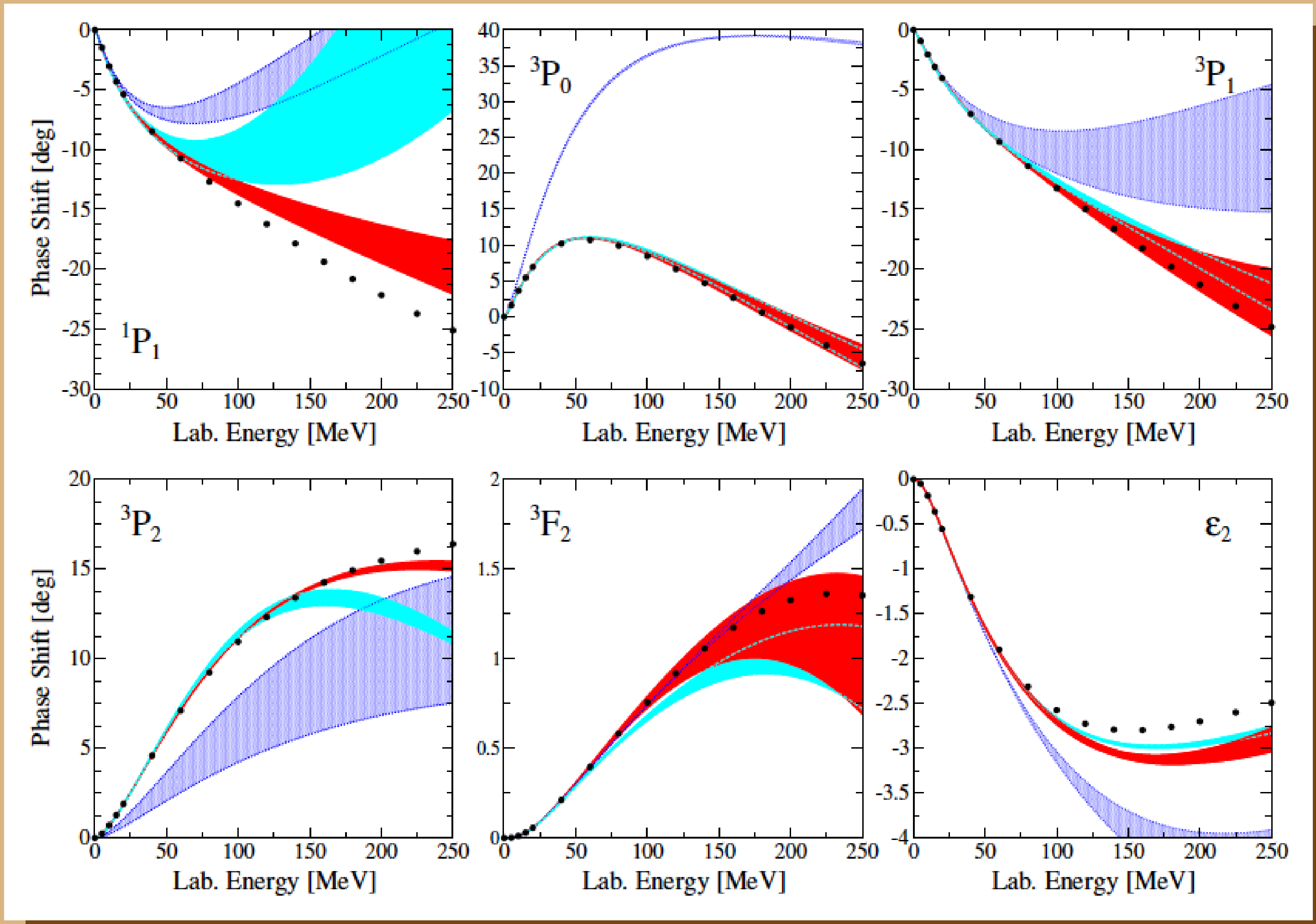

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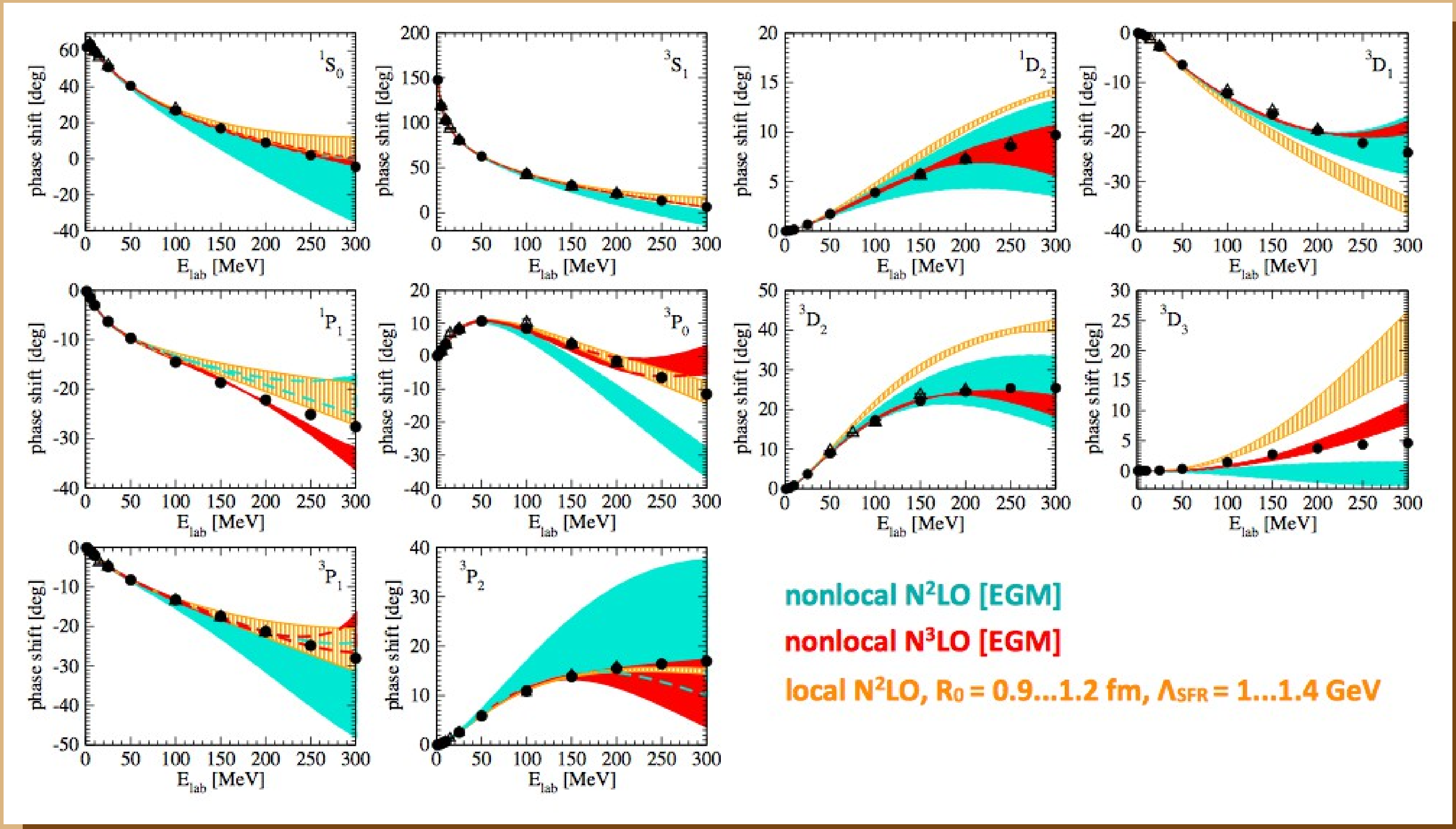
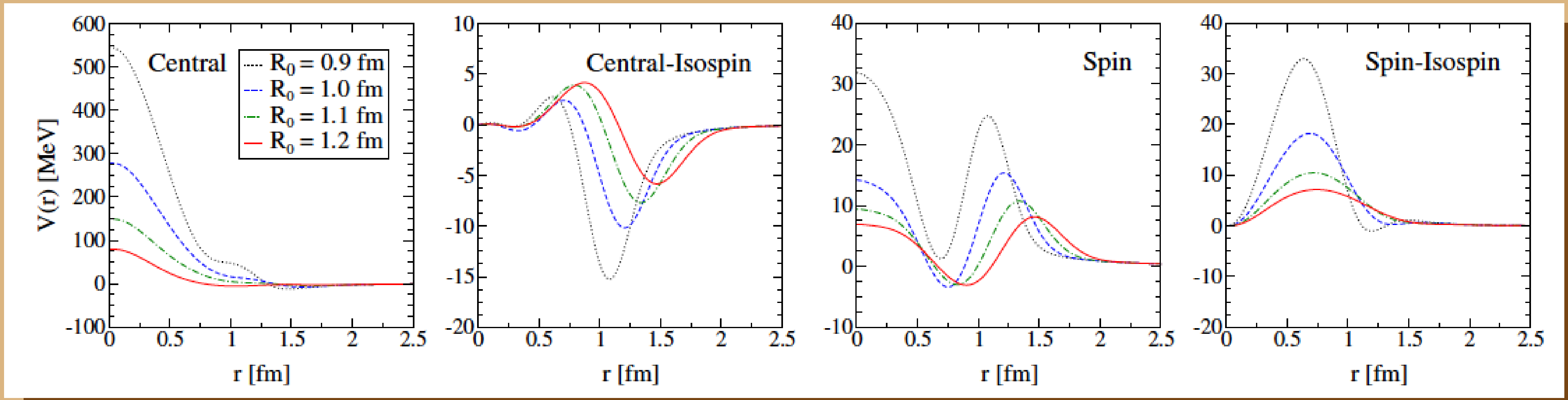
Compare to non-local EGM



Credit: Hermann Krebs

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



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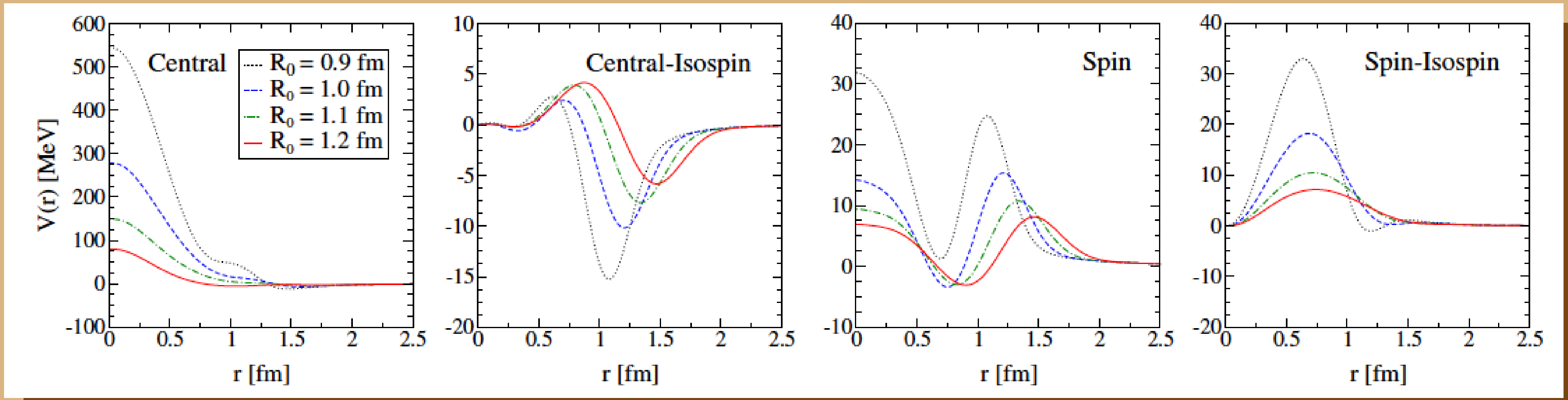
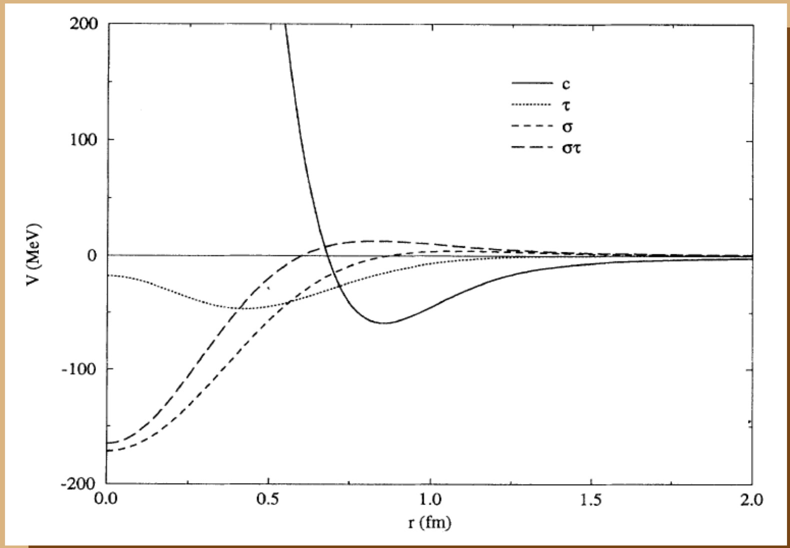


Compare with AV18



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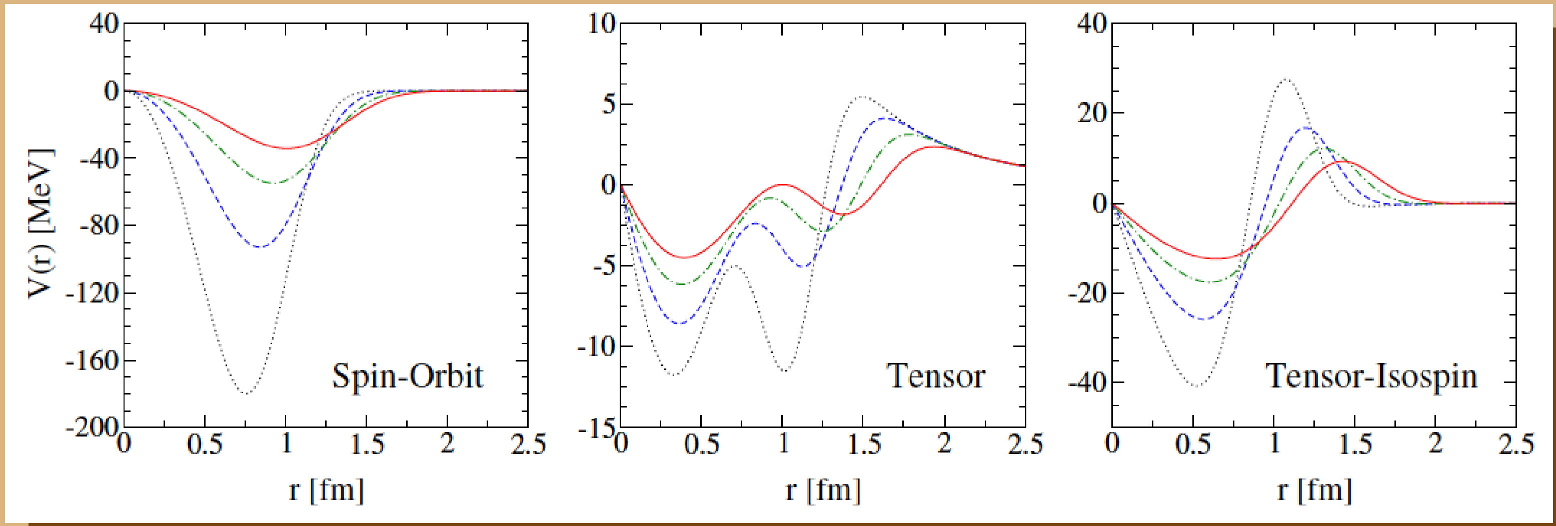

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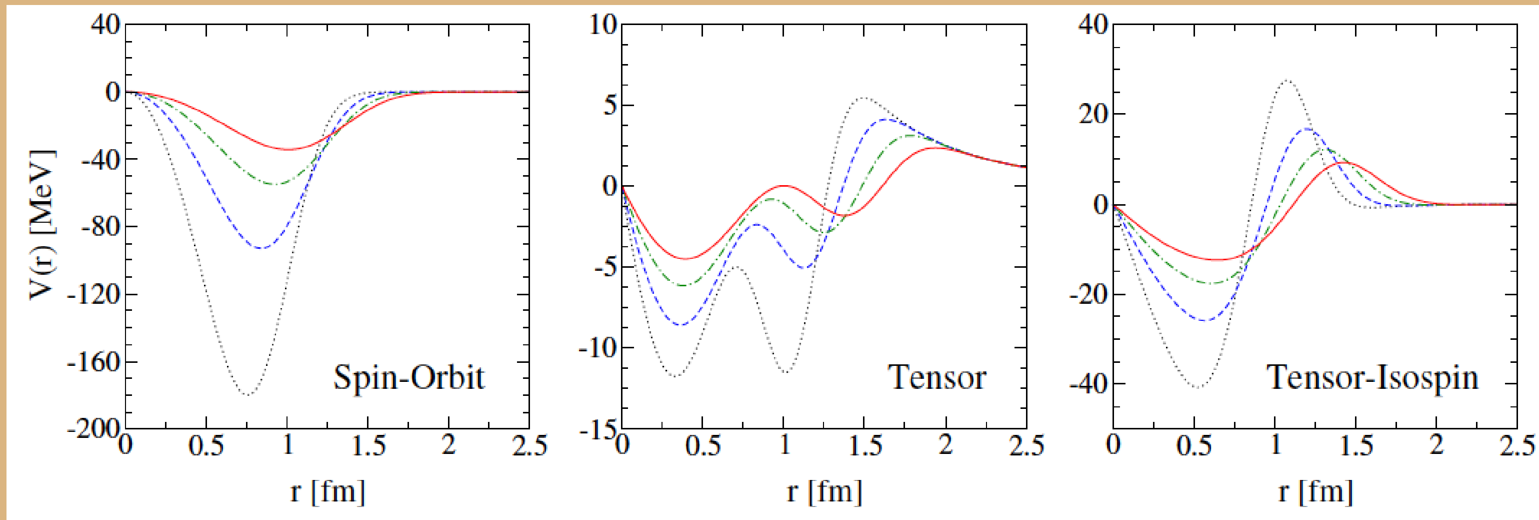

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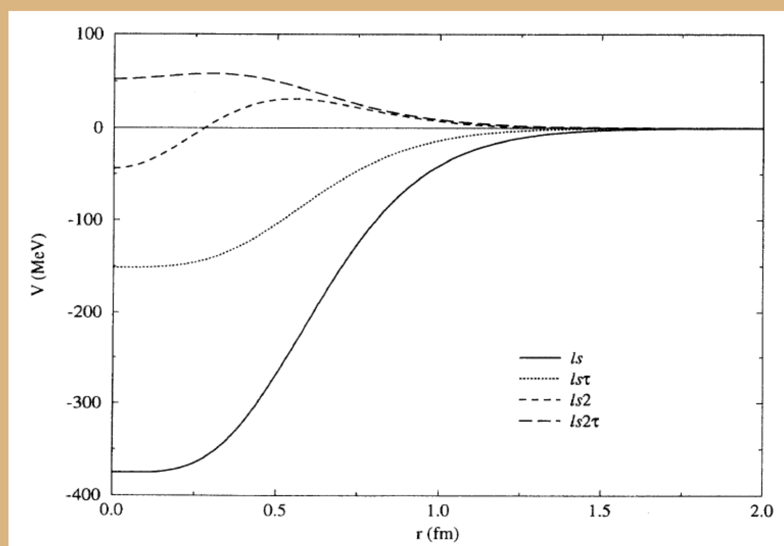

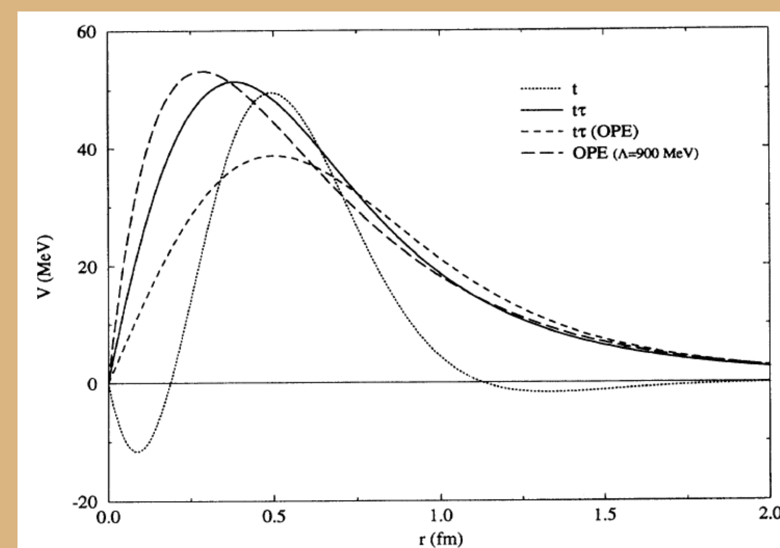

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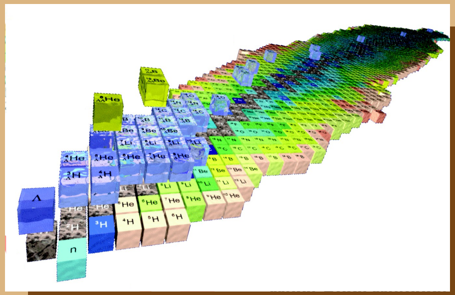

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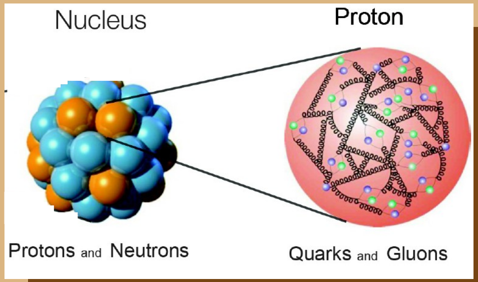

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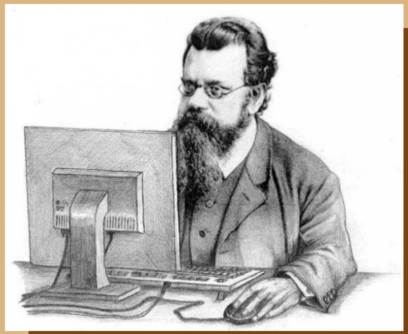

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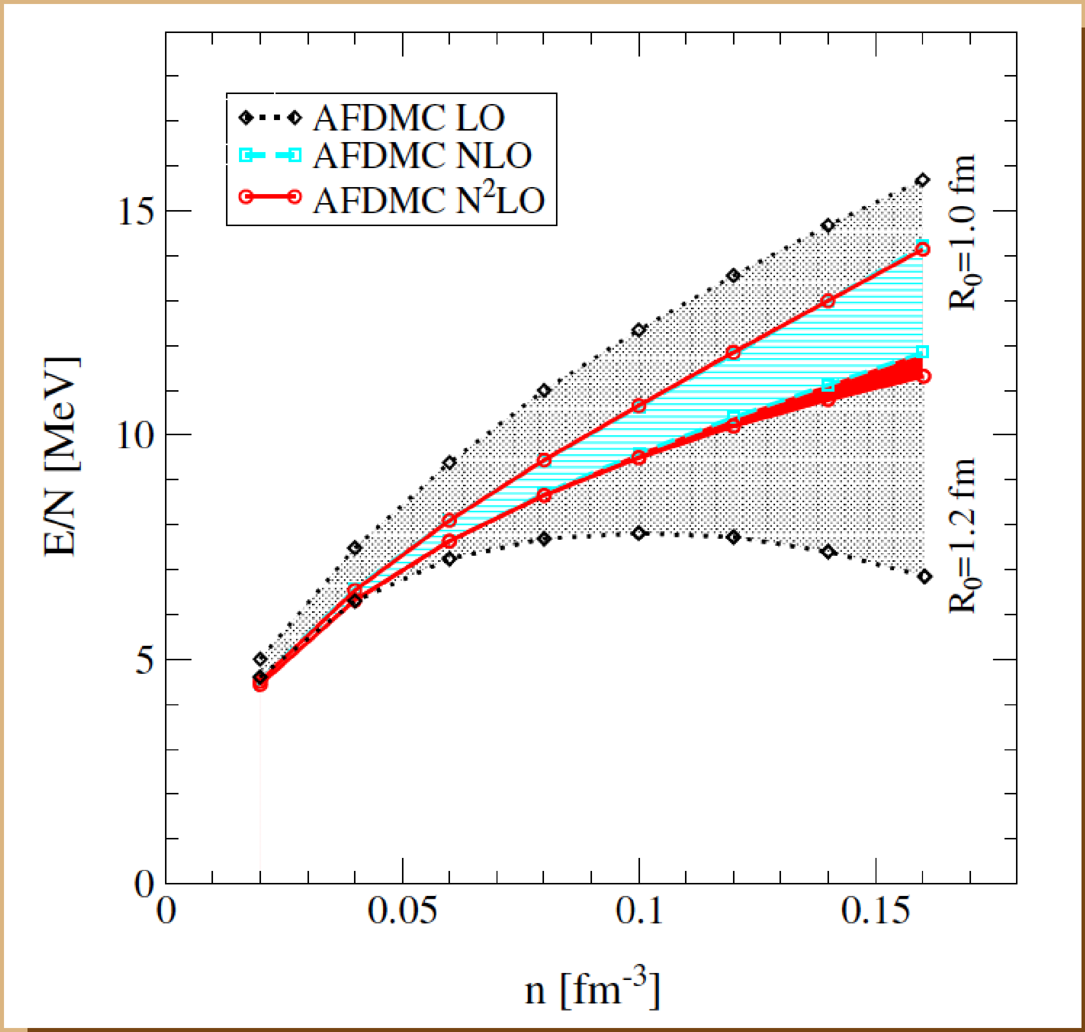
Chiral EFT in QMC

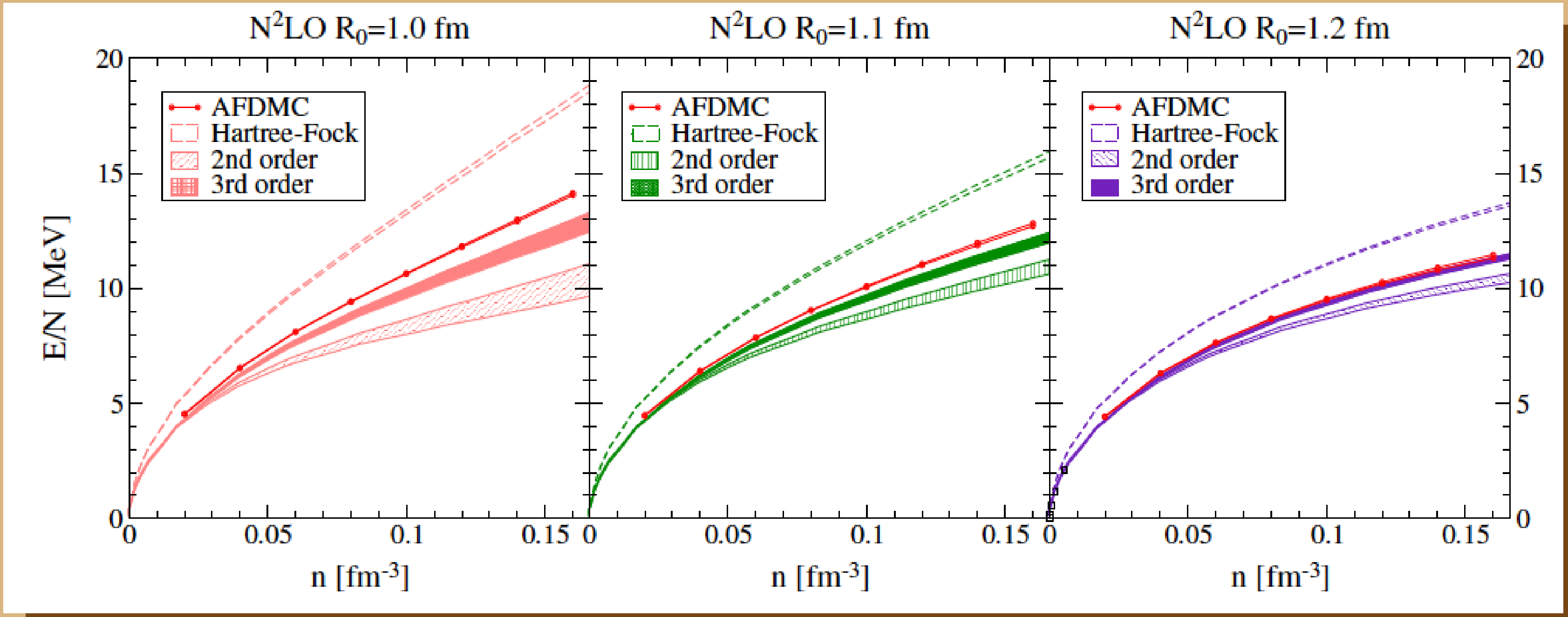


- Use Auxiliary-Field Diffusion Monte Carlo to handle the full interaction
- First ever non-perturbative systematic error bands
- Band sizes to be expected
- Many-body forces will emerge systematically

NEUTRONS

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

QMC vs MBPT



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

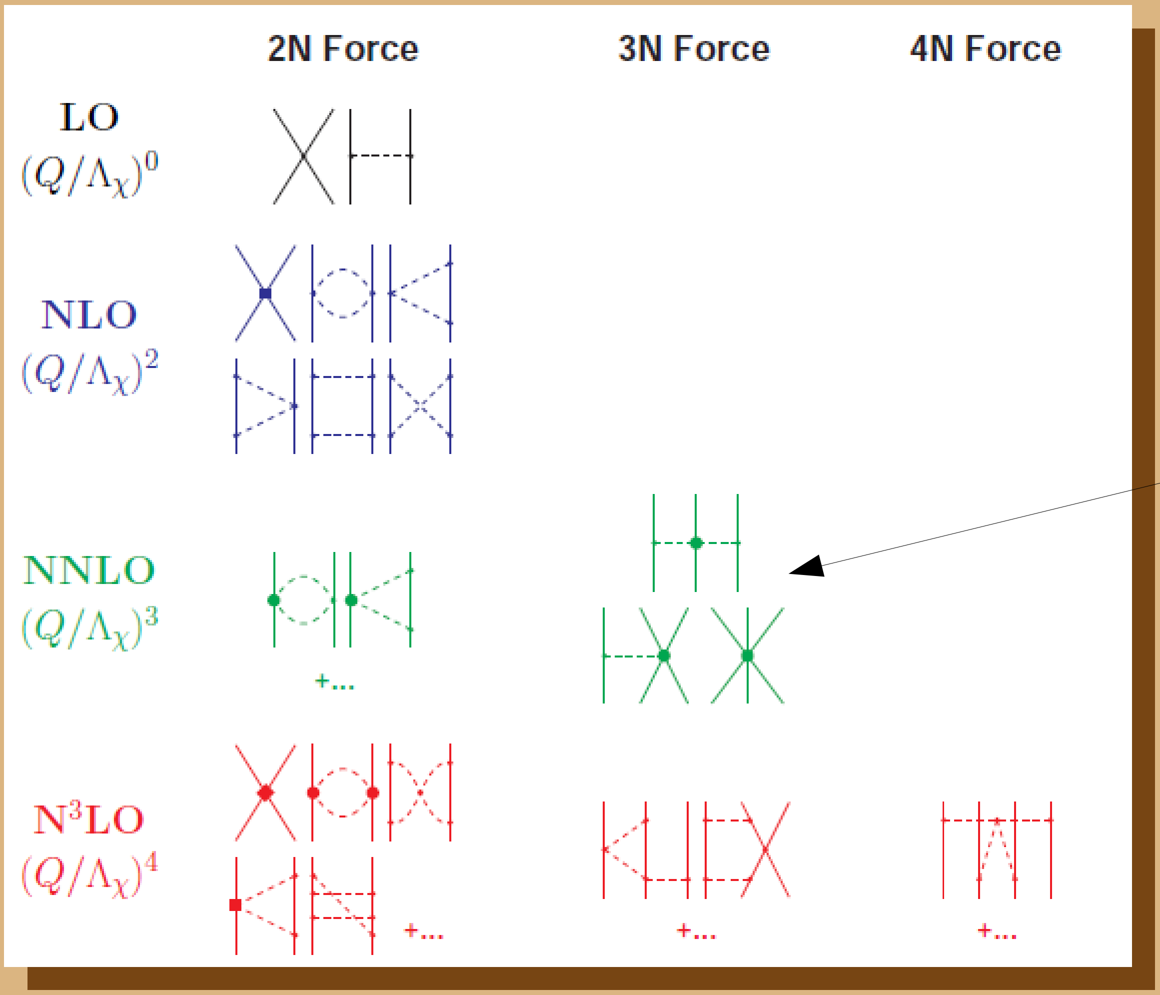
NEUTRONS

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

What about three-nucleon forces?

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

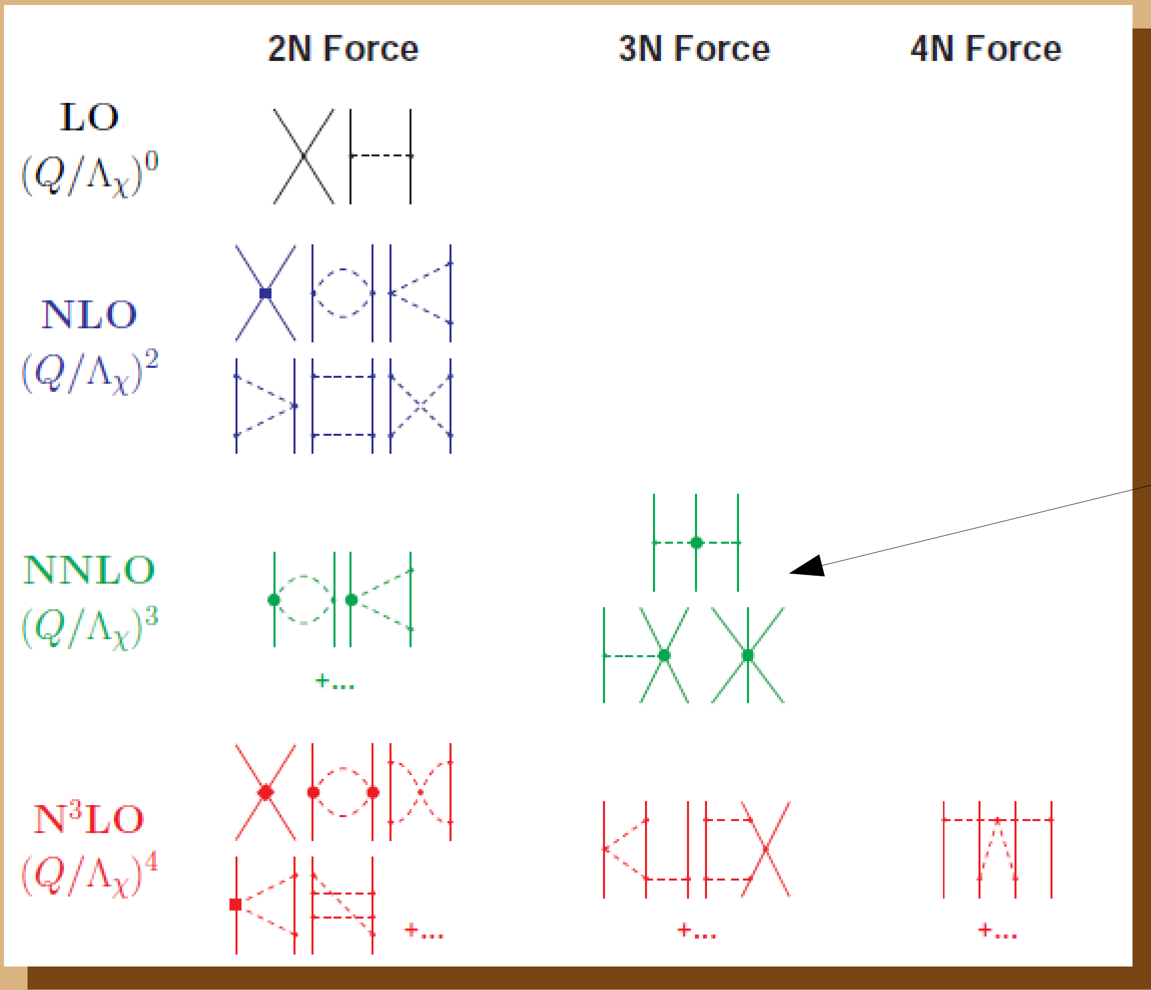
Nuclear Hamiltonian: chiral EFT



N2LO 3NF

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

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

3NF TPE in PNM

Momentum space

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

3NF TPE in PNM

Momentum space

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

Coordinate space

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

3NF TPE in PNM

Momentum space

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

Coordinate space

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

Long-range (LR)

3NF TPE in PNM

Momentum space

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

Coordinate space

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

Intermediate-range (IR)

3NF TPE in PNM

Momentum space

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

Coordinate space

Short-range (SR)

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

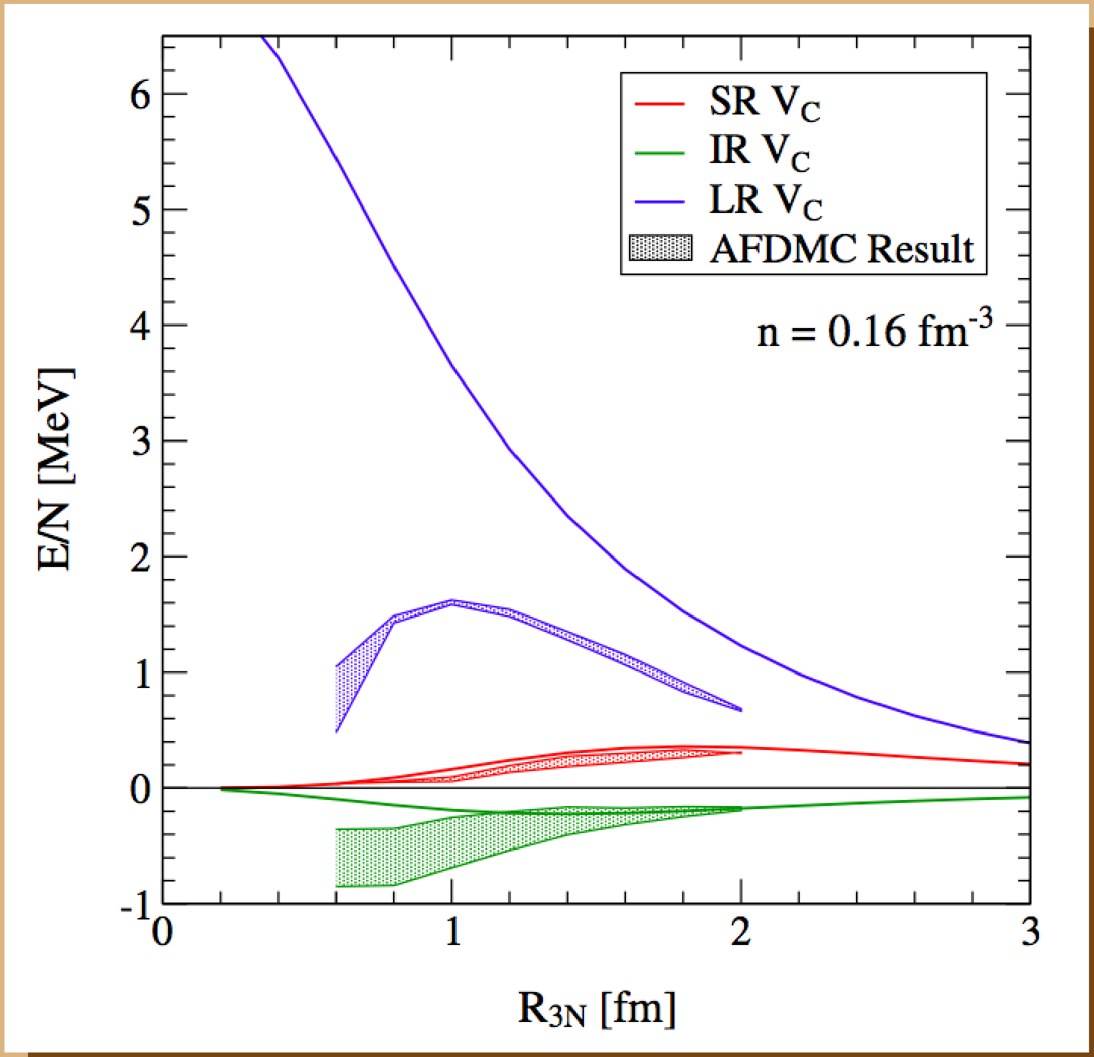
Regularizing

Attempt to be consistent with NN regularization

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

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

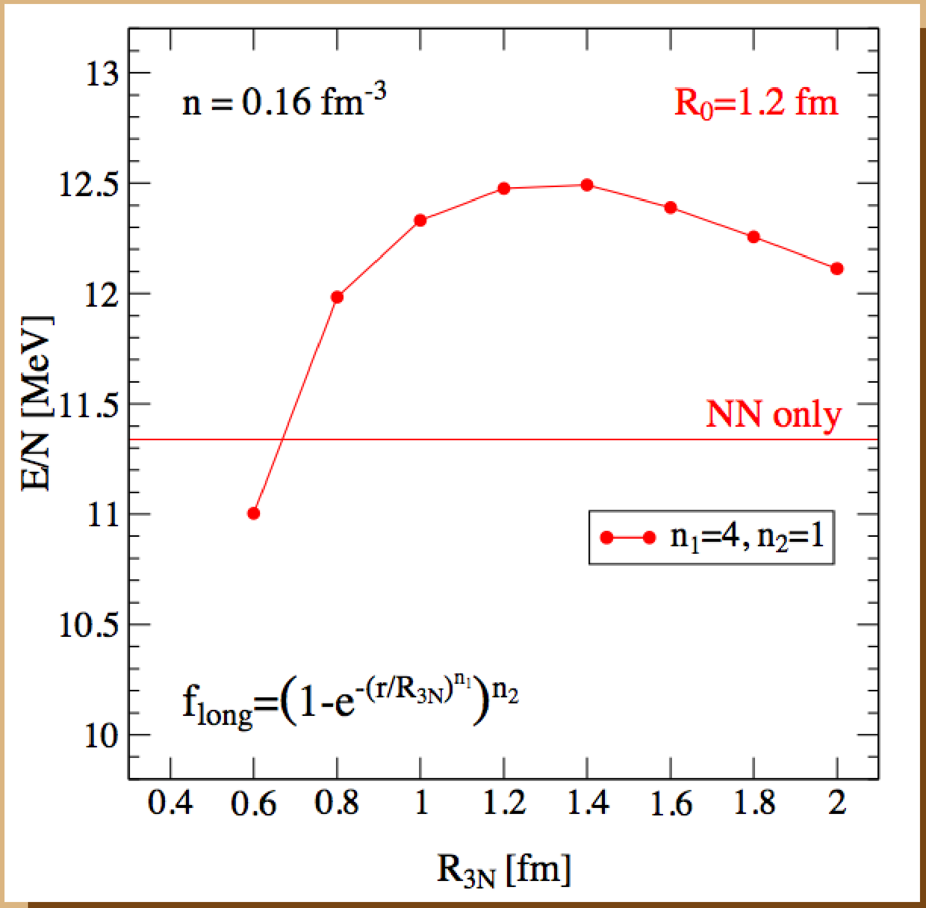
3NF contributions



- 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

NEUTRONS

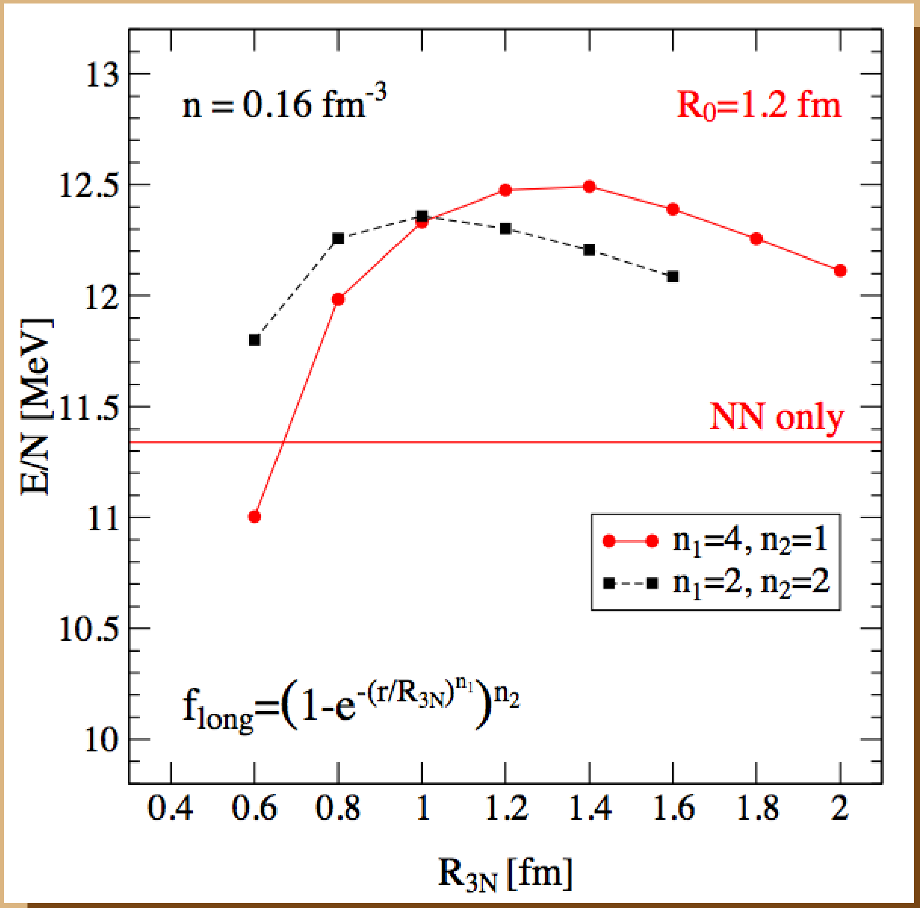
3NF cutoff choice



- Too large cutoff chops off too much
- Too small cutoff leads to collapse
- Plateau appears at intermediate values of the cutoff

NEUTRONS

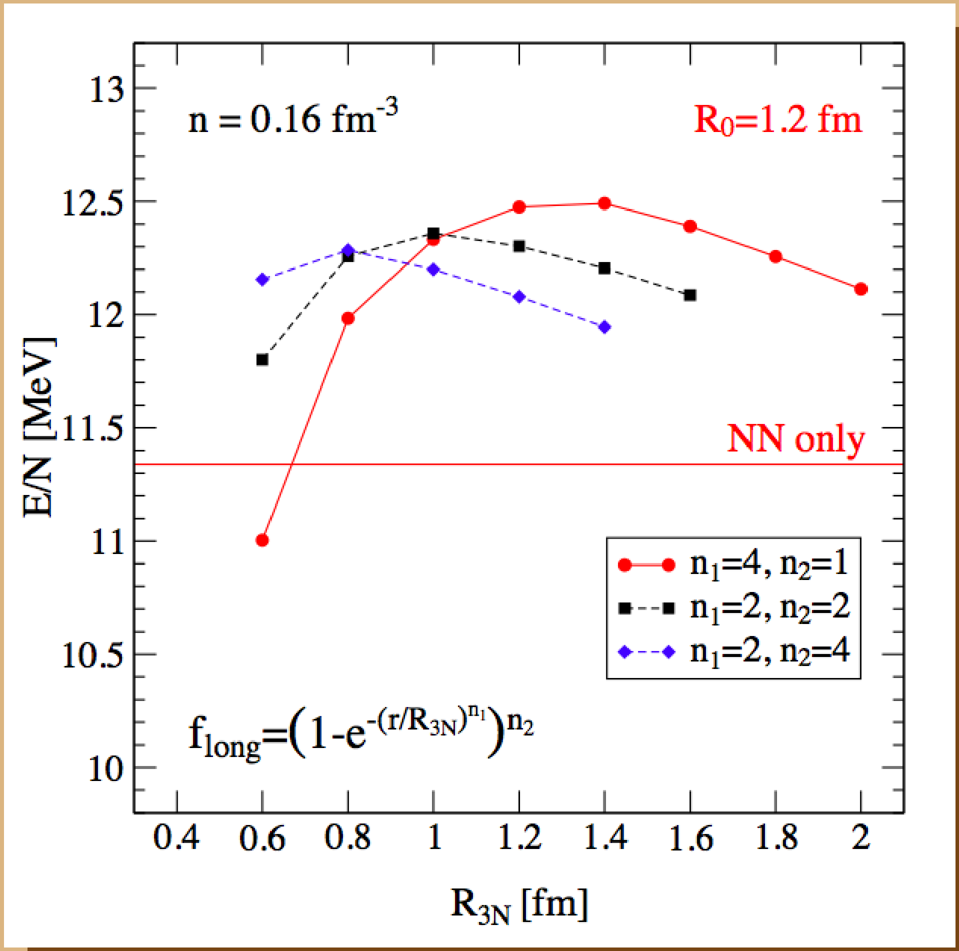
3NF cutoff choice



- 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

NEUTRONS

3NF cutoff choice



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NEUTRONS

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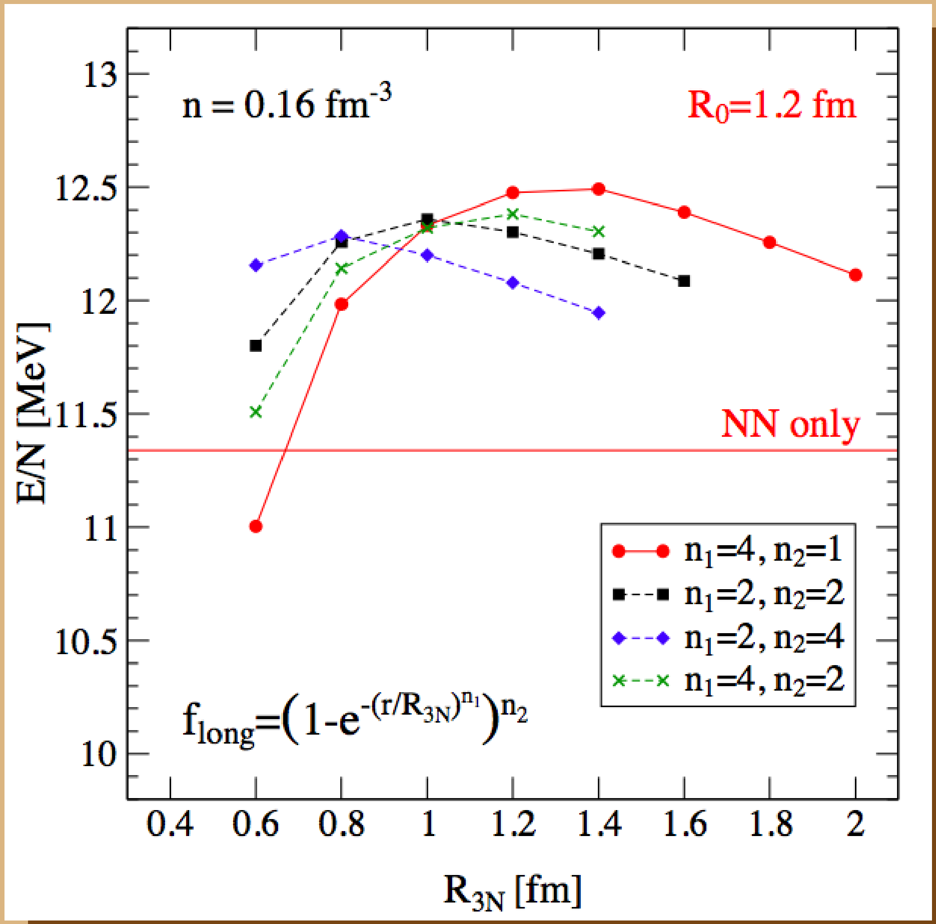

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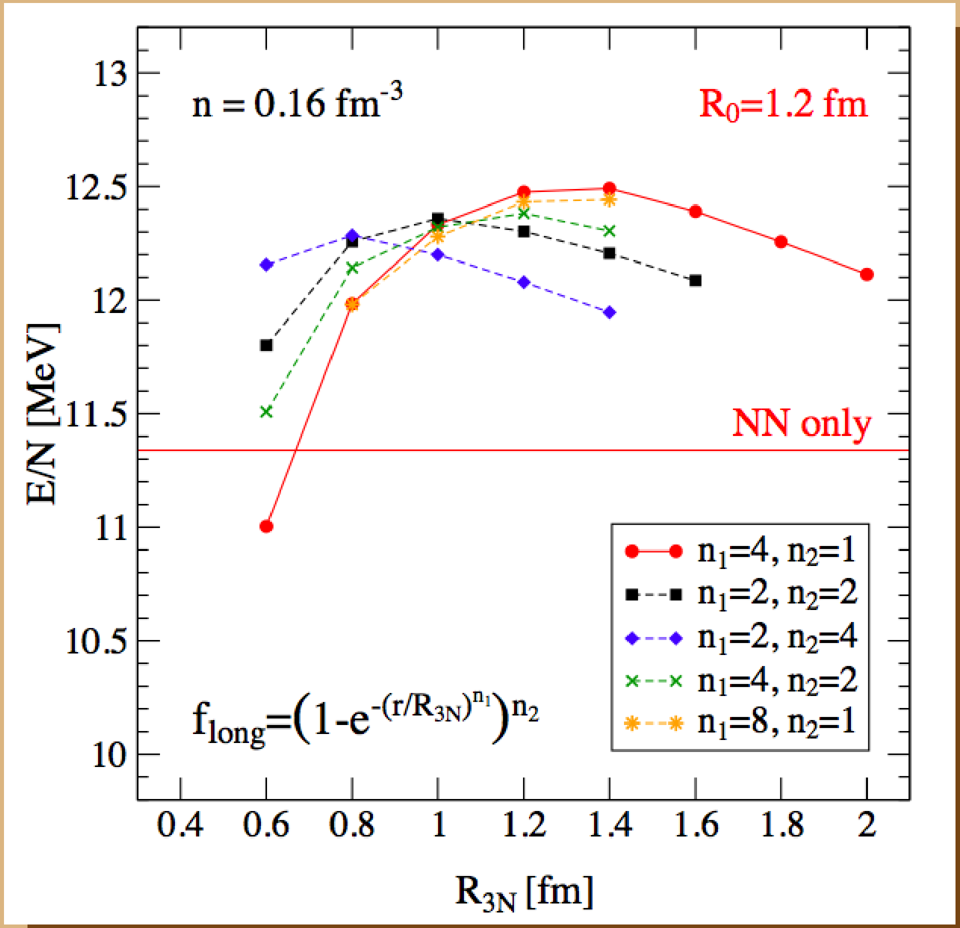
NEUTRONS

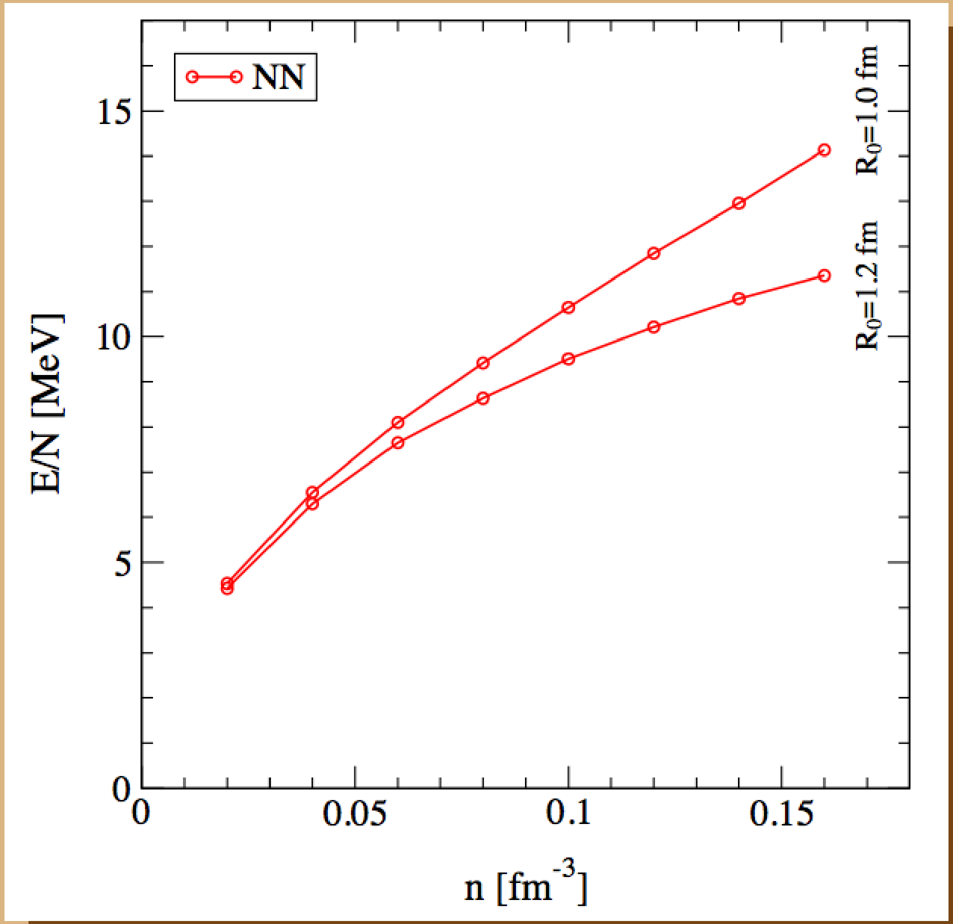
3NF cutoff choice



- 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

NEUTRONS

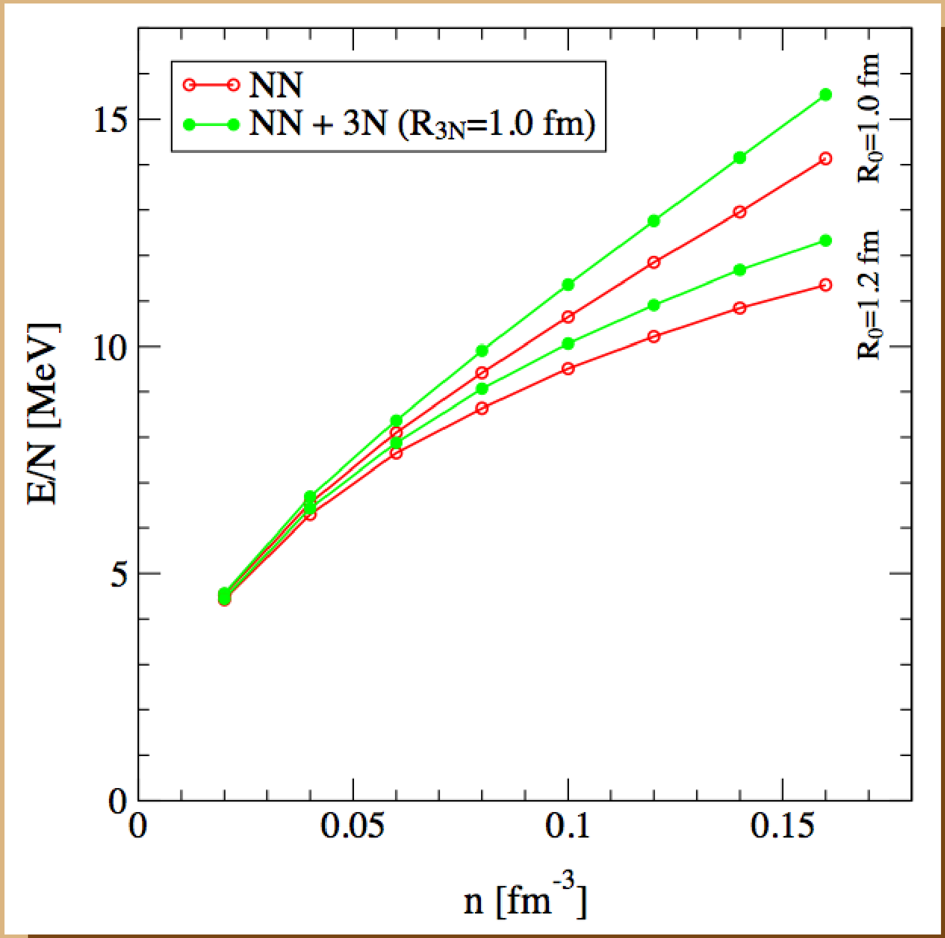
Overall error bands



- NN error band already published

NEUTRONS

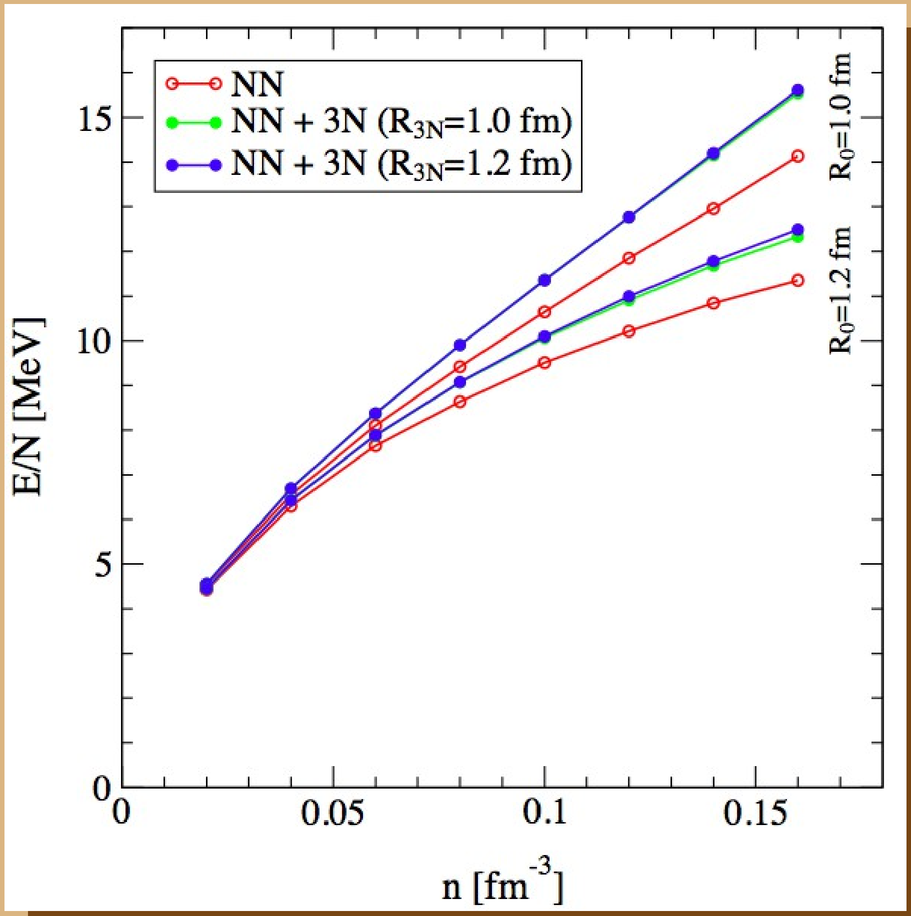
Overall error bands



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

NEUTRONS

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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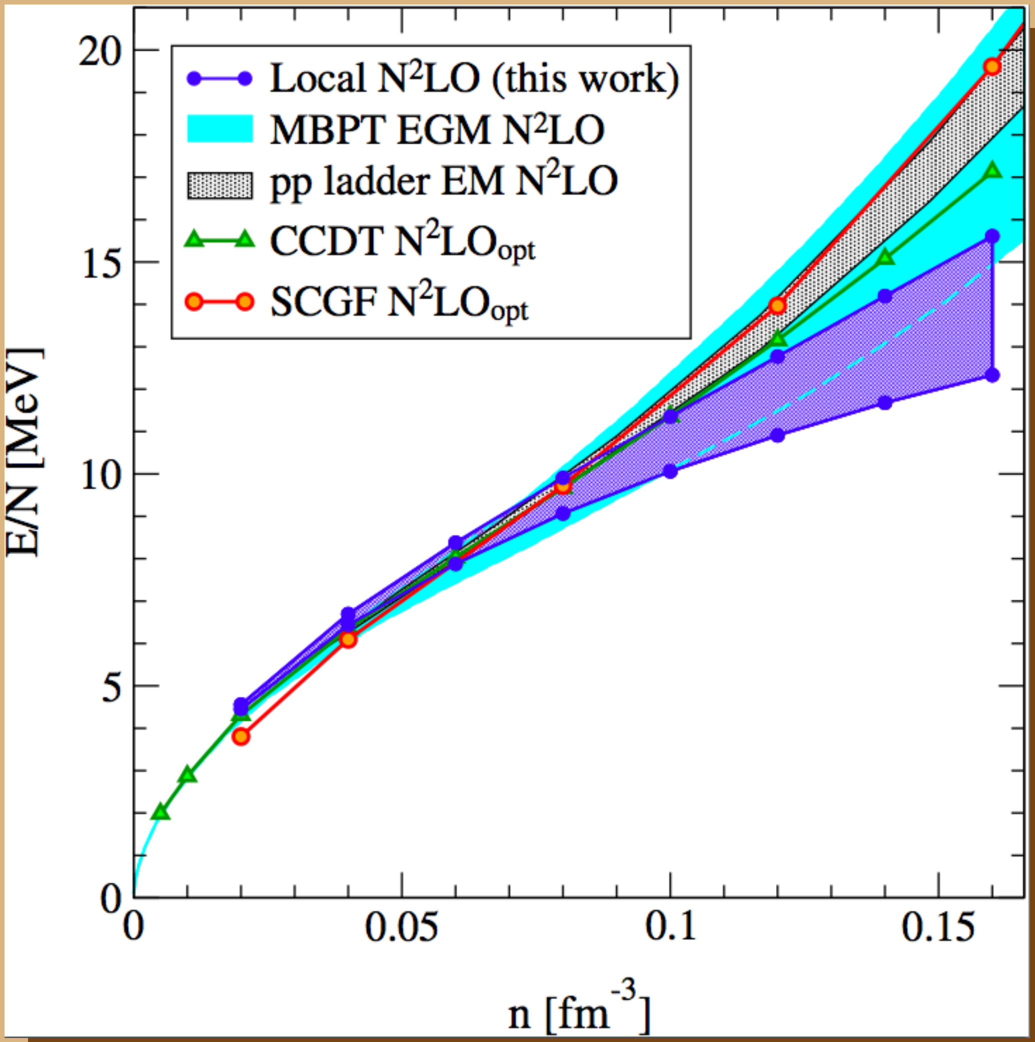
Compare with other calculations at N2LO



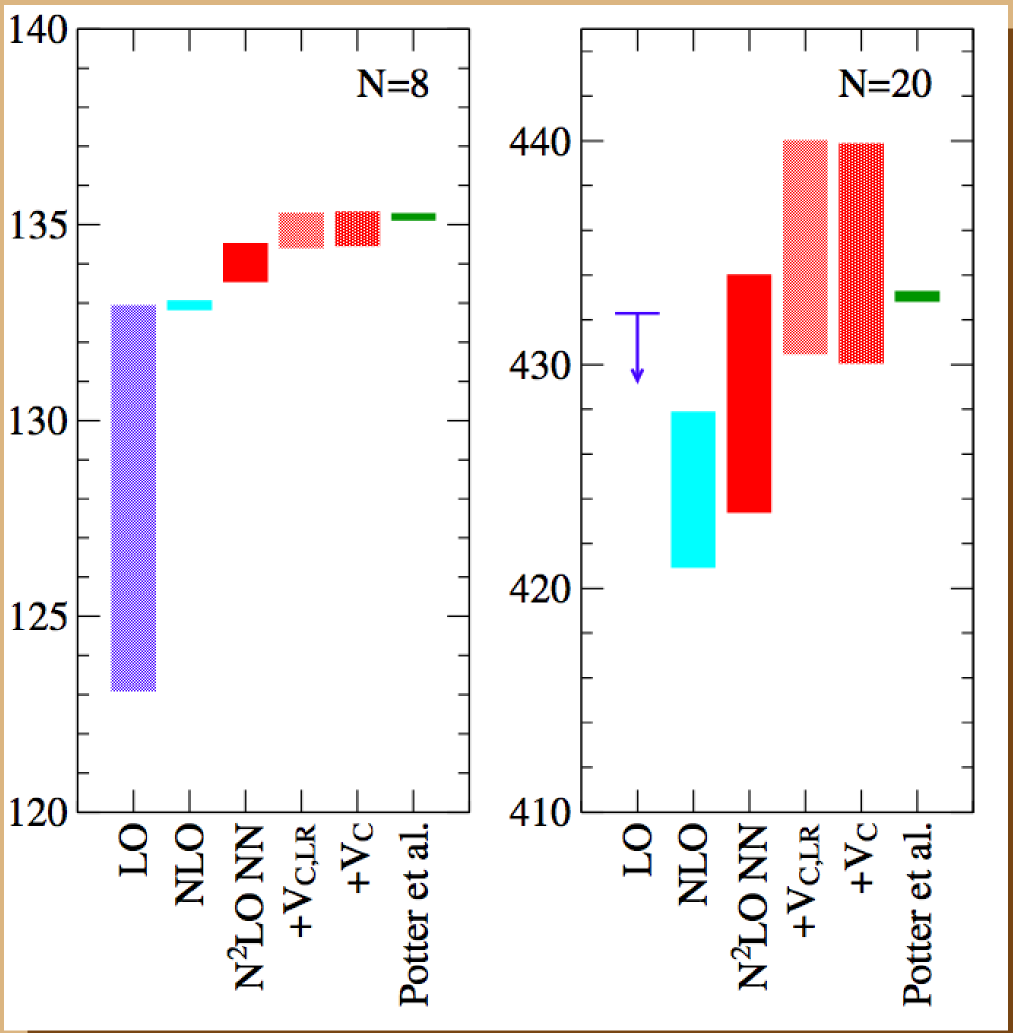
- Overall agreement across methods
- QMC band result of using more than one cutoff
- Band width essentially understood

NEUTRONS

Now turn to neutron drops

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

Neutron drops with NN+3NF chiral forces



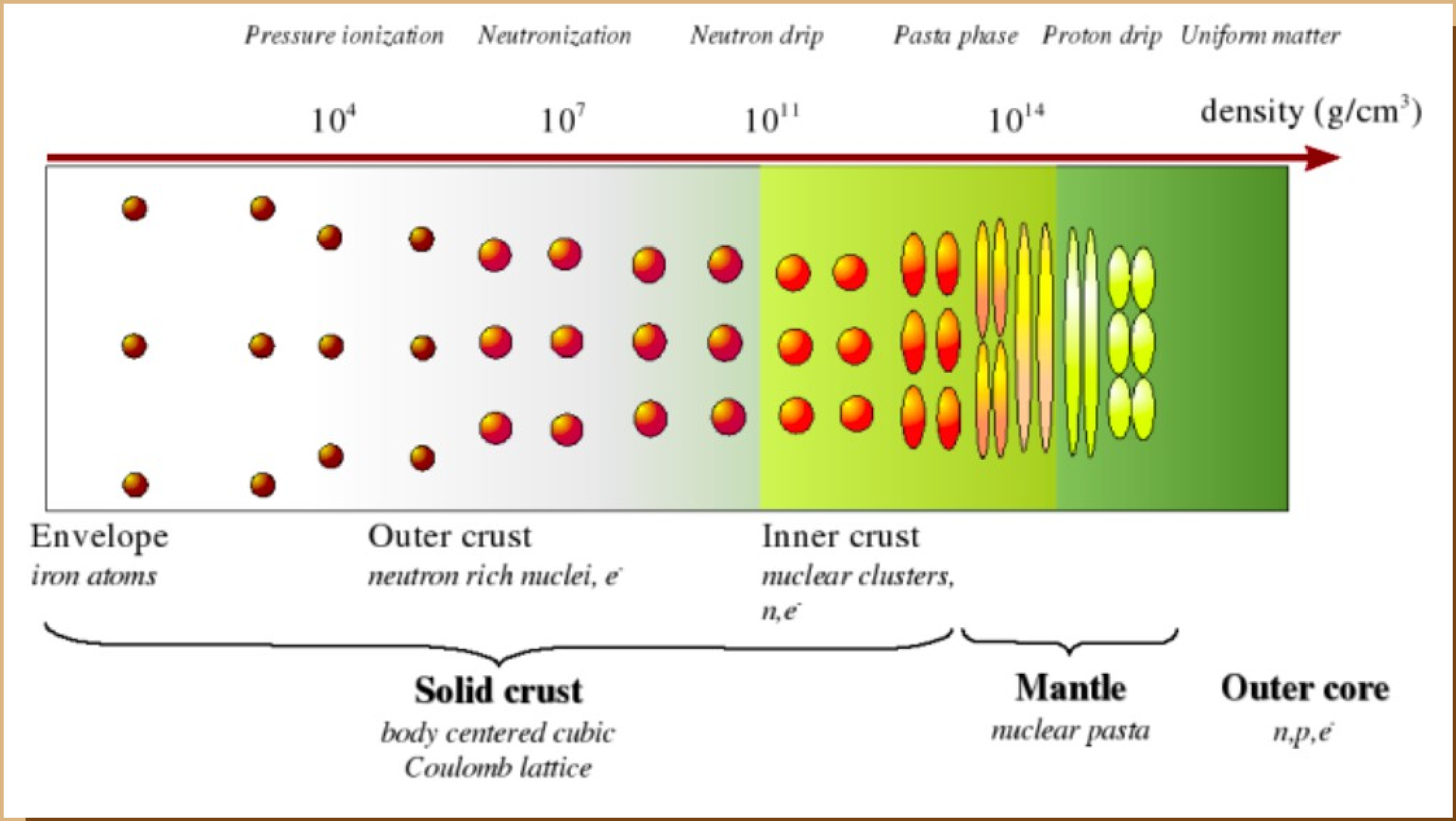
- 10 MeV harmonic oscillator trap
- Order-by-order systematics studied
- Soft LO potential leads to very low energies, especially in larger systems
- Reasonable agreement with ΛCCSD calculations

NEUTRONS

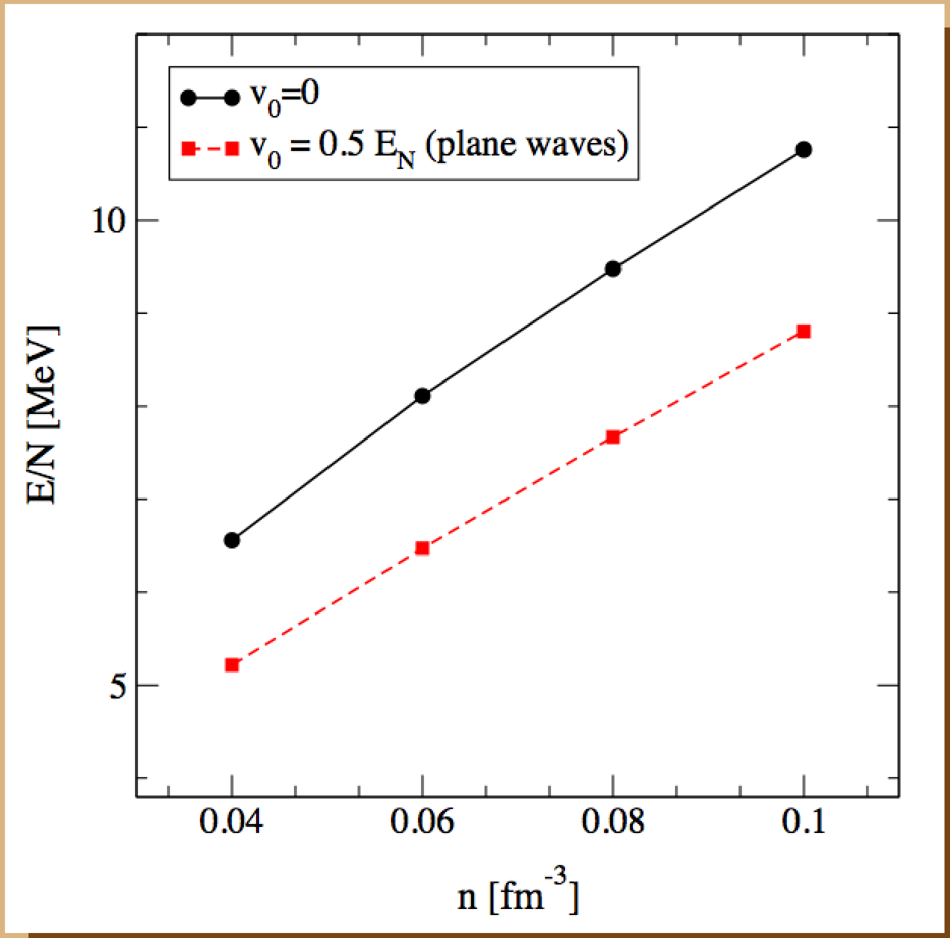
Remember that neutron-star crusts also involve a lattice of nuclei

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

Neutron star crusts more than PNM



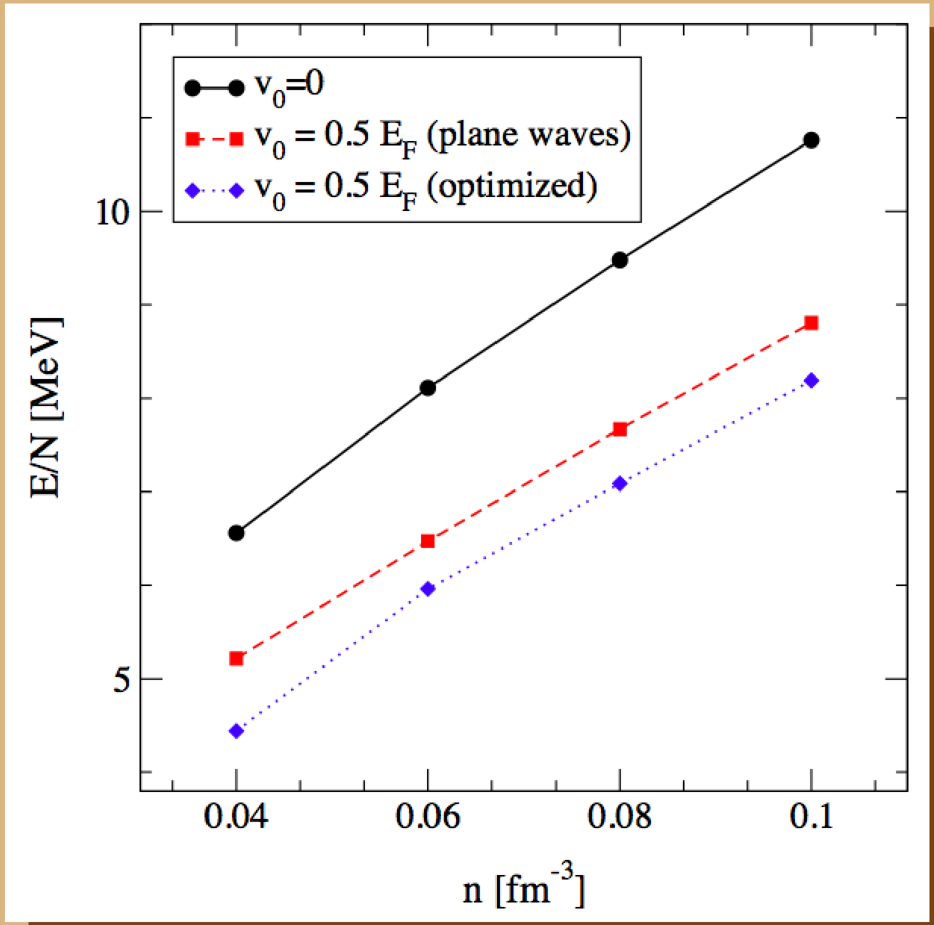
Static response of neutron matter



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

NEUTRONS

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

NEUTRONS

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

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- Evgeny Epelbaum (Bochum)
- Stefano Gandolfi (LANL)
- Kai Hebeler (Darmstadt)
- Achim Schwenk (Darmstadt)
- **Ingo Tews** (Darmstadt)

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Lecturers and Topics:

Klaus Blaum (MPI Heidelberg) – Nuclear mass measurements

Pierre Capel (EP Brussels) – Introduction to nuclear reactions

Alexandra Gade (Michigan State University) – Experiments with exotic nuclei

Jason Holt (TRIUMF) – Ab initio approaches to medium-mass nuclei

Augusto Macchiavelli (Lawrence Berkeley National Lab) – Nuclear spectroscopy

Alfredo Poves (University of Madrid) – The shell model and nuclear structure

Sofia Quaglioni (Lawrence Livermore National Lab) – Ab initio many-body theory of nuclear reactions

Robert Roth (TU Darmstadt) – Ab initio approaches to light nuclei

Olivier Sorlin (GANIL) – Shell evolution and nuclear forces

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