Quantum Monte Carlo calculations of neutron matter with Chiral Effective Field Theory interactions



Ingo Tews, In collaboration with J. Carlson, S. Gandolfi, A. Gezerlis, K. Hebeler, T. Krüger, J. Lynn, A. Schwenk, ...

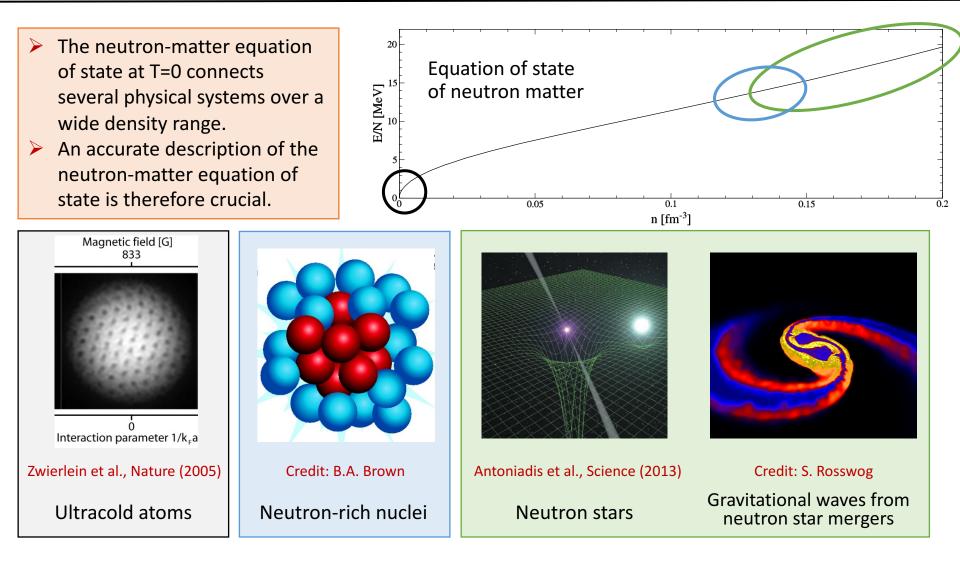
Talk, YITP program: "Nuclear Physics, Compact Stars, and Compact Star Mergers", Oct.20, 2016, Kyoto





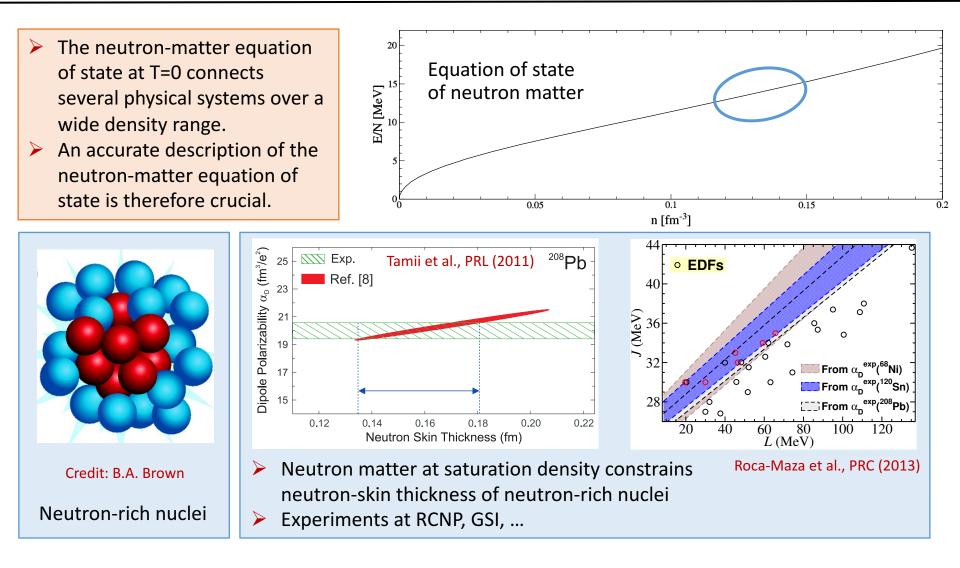
Motivation





Motivation



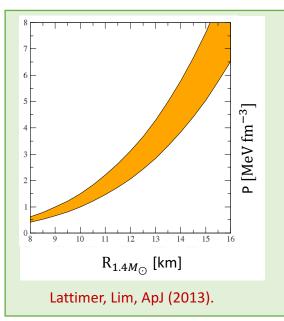


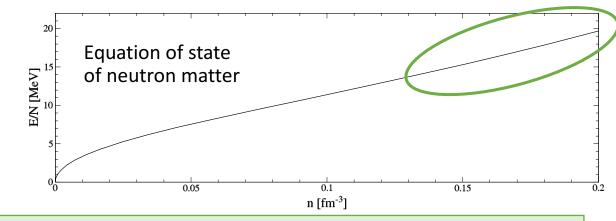
Motivation



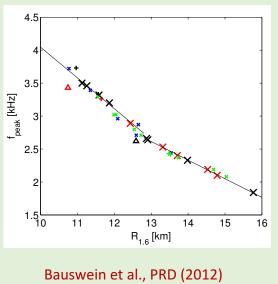
The neutron-matter equation of state at T=0 connects several physical systems over a wide density range.

An accurate description of the neutron-matter equation of state is therefore crucial.

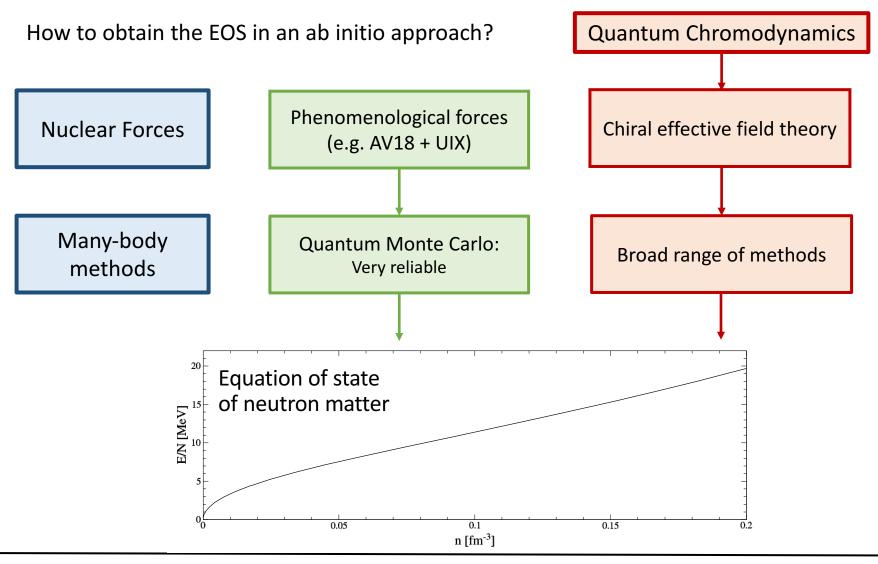




- Neutron matter equation of state at saturation density and above determines mass-radius relation of neutron stars and gravitationalwave signal of neutron-star mergers
- EOS properties at saturation density are correlated with neutron-star radii and gravitational wave peak frequency







Outline



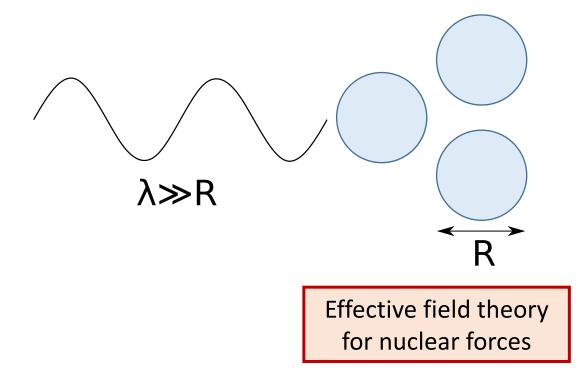
Chiral effective field theory: Epelbaum et al., PPNP (2006) and RMP (2009)

- Systematic basis for low-energy nuclear forces, connected to QCD
- naturally includes many-body forces
- Very successful in calculations of nuclei and nuclear matter
- Ab-initio calculations using chiral EFT can be used to constrain equation of state of neutron matter
- Neutron-matter applications: IT, Krüger, Hebeler, Schwenk, PRL & PRC & PLB (2013)
 - Symmetry energy
 - Neutron-star mass-radius relation
- Improving neutron-matter results using Quantum Monte Carlo methods Gezerlis, IT, et al., PRL & PRC (2013, 2014, 2016)

Summary



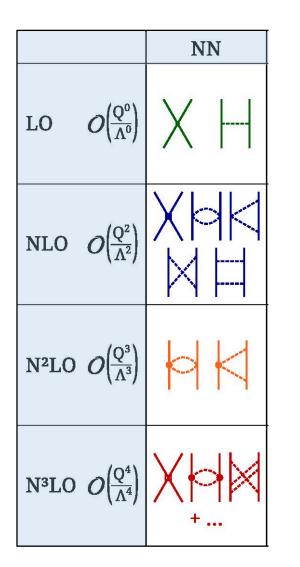
Basic principle of effective field theory:



At low energies (long wavelength) details not resolved!

- Choose relevant degrees of freedom for low-energy processes
- Systematic expansion of interactions constrained by symmetries





Explicit degrees of freedom:

Pions and nucleons

Write most general Lagrangian consistent with the symmetries of QCD

Separation of scales:

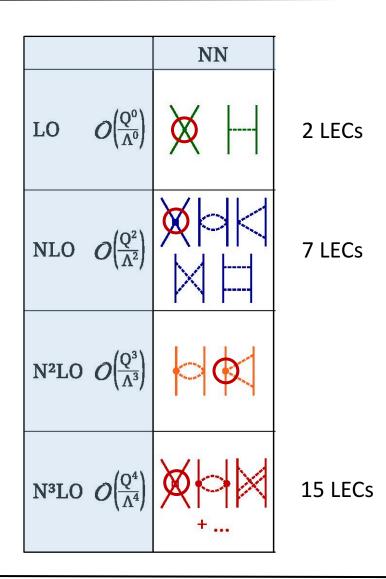
- Low momenta Q << breakdown scale A_b
- > Expand in powers of $\left(\frac{Q}{\Lambda_h}\right)^{\nu} \sim \left(\frac{1}{3}\right)^{\nu}$

Power counting:

- $\succ v = 0$: leading order (LO),
- $\succ v = 2$: next-to-leading order (NLO), ...

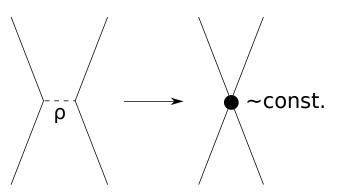
Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...





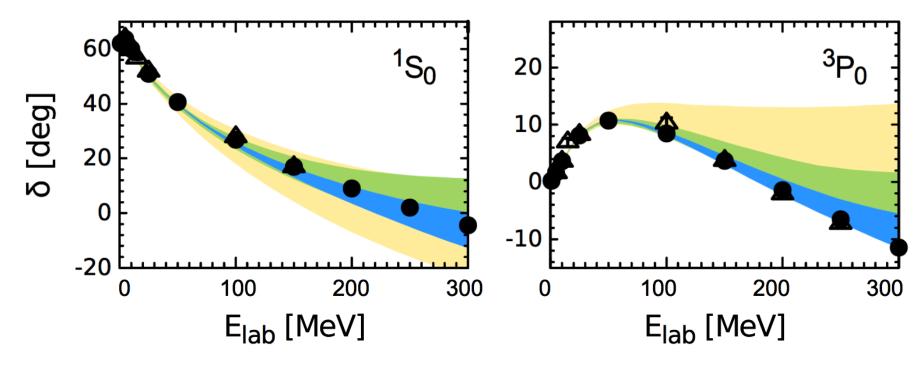
Explicit degrees of freedom:

- Pions and nucleons
- Long-range physics explicit
- Short-range physics expanded in general operator basis
- High-momentum physics absorbed into short-range couplings, fit to experiment (phase shifts)



Second scale: cutoff Λ (resolution):
➢ Interactions Λ-dependent



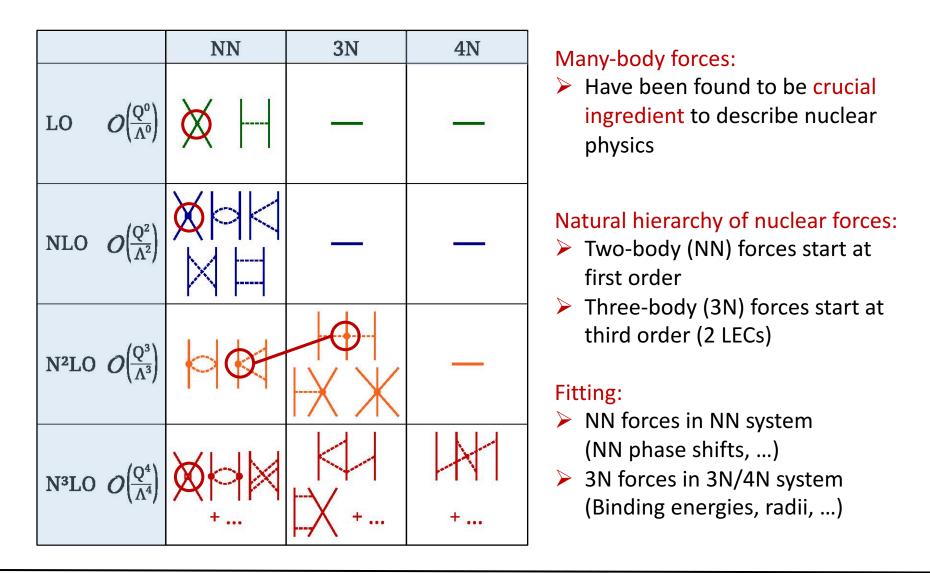


Epelbaum et al., Eur. Phys. J (2015)

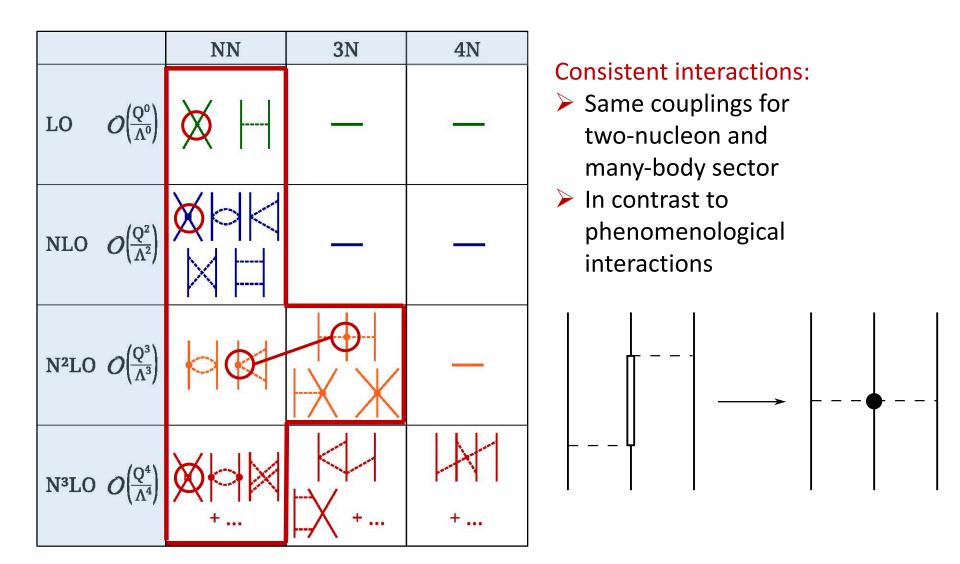
Systematic expansion of the nuclear forces:

- Can work to desired accuracy
- Can obtain systematic error estimates



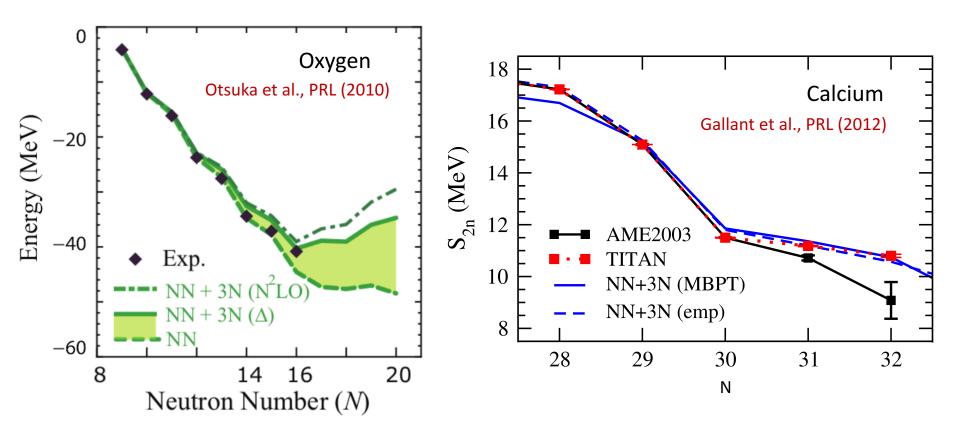








Many-body forces are crucial:



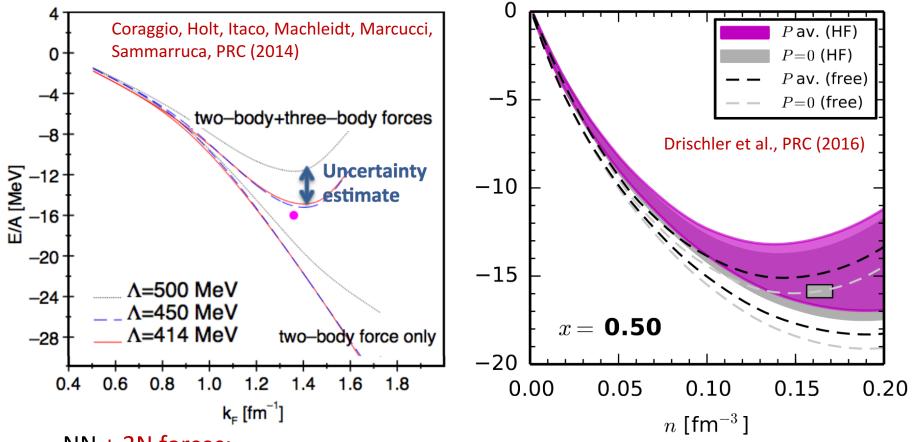
NN + 3N forces:

Give correct physics of neutron-rich nuclei

See also Hebeler et al., ARNPS (2015)



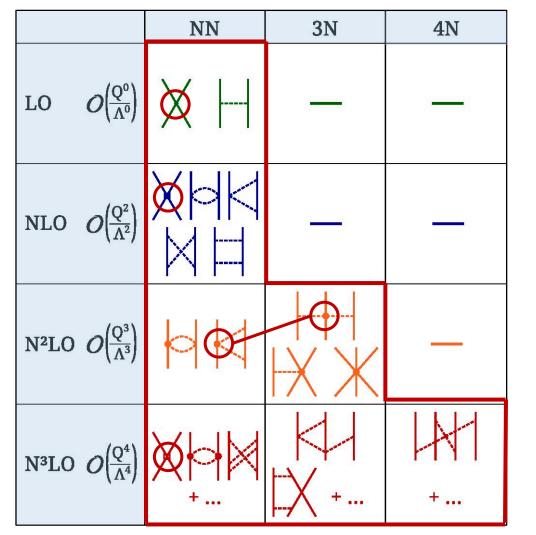
Many-body forces are crucial:



NN + 3N forces:

Give correct saturation with theoretical uncertainties in nuclear matter Drischler et al., PRC (2016)





Neutron matter:

 Complete calculation at N³LO using many-body perturbation theory (MBPT)

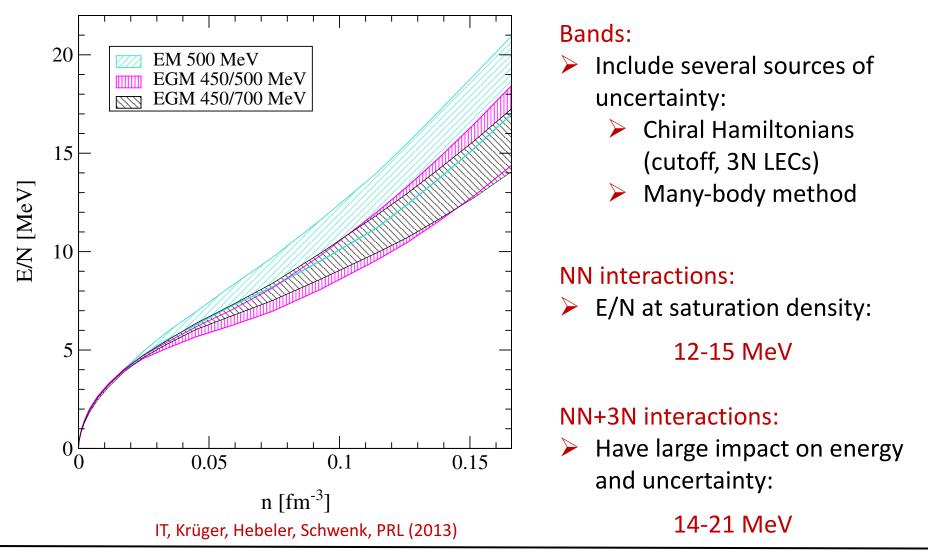
IT, Krüger, Hebeler, Schwenk, PRL (2013)

Calculation is simpler in neutron matter:

- Only certain parts of the manybody forces contribute
- Chiral many-body forces completely predicted from NN sector

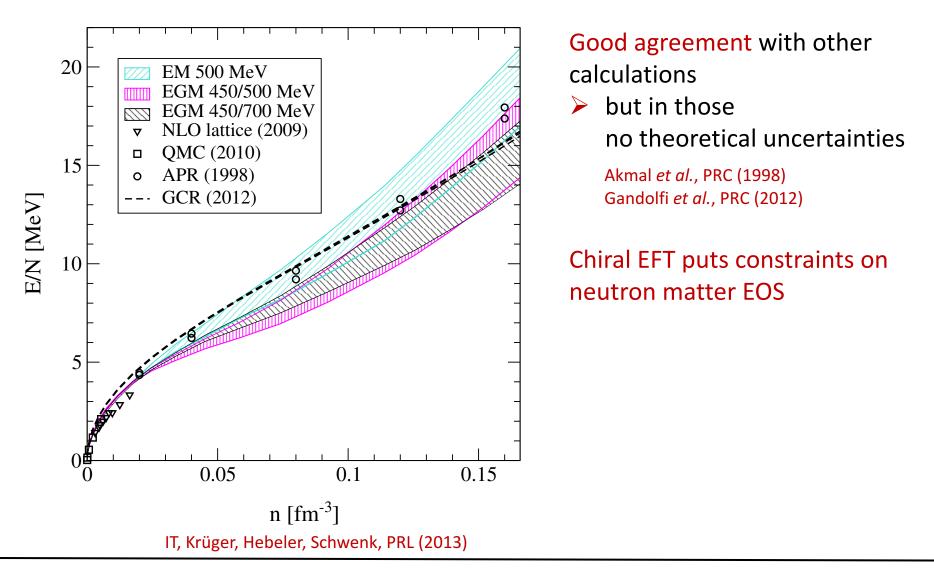
Neutron matter





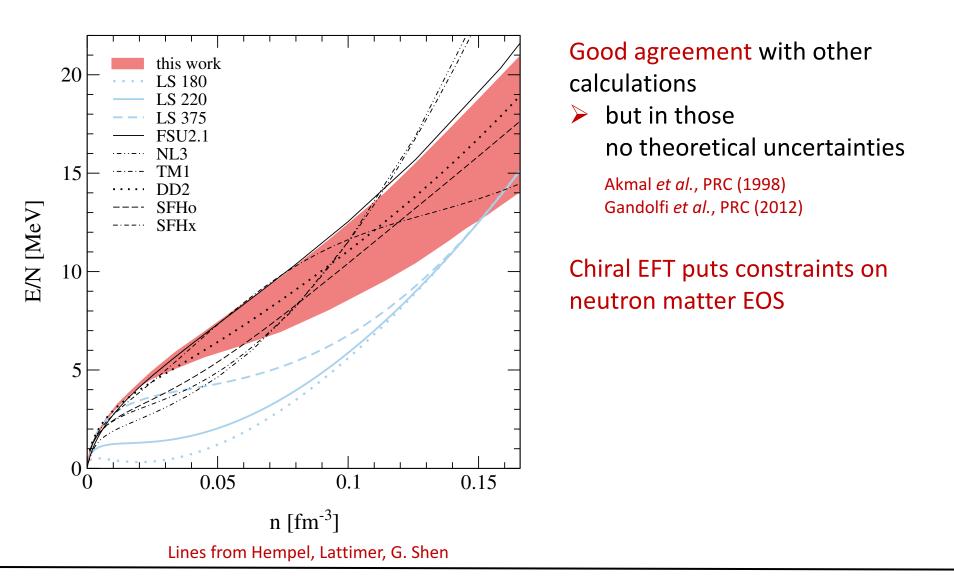
Neutron matter





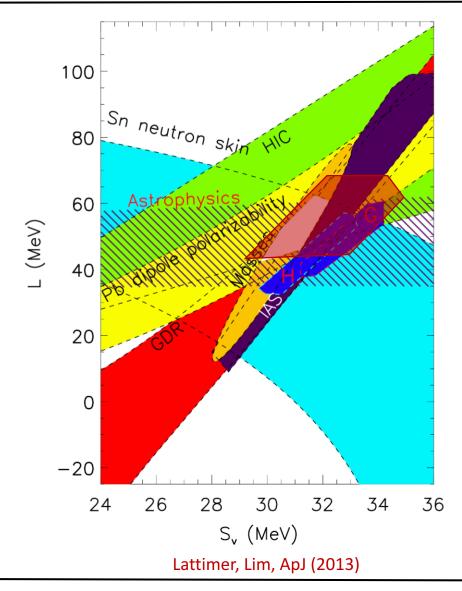
Neutron matter





Symmetry energy and L parameter





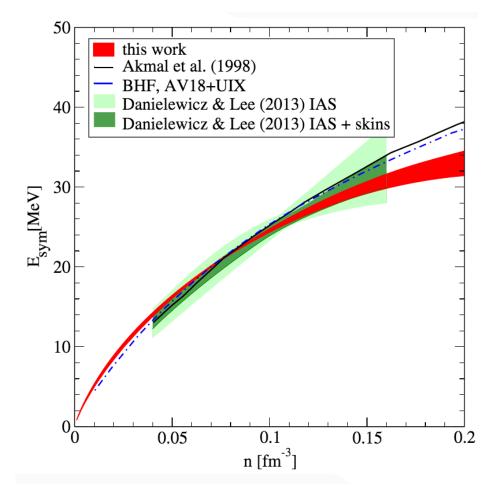
Put constraints on symmetry energy and its density dependence L:

$$S_{v}(n) = \frac{1}{8} \frac{\partial^{2}}{\partial x^{2}} \frac{E}{A}(n, x) \Big|_{x=1/2} ,$$
$$L(n_{0}) = 3n_{0} \frac{\partial}{\partial n} S_{V}(n) \Big|_{n_{0}} ,$$

S_V =
$$28.9 - 34.9$$
 MeV
L = $43.0 - 66.6$ MeV

Good agreement with experimental constraints





Drischler, Soma, Schwenk, PRC (2014)

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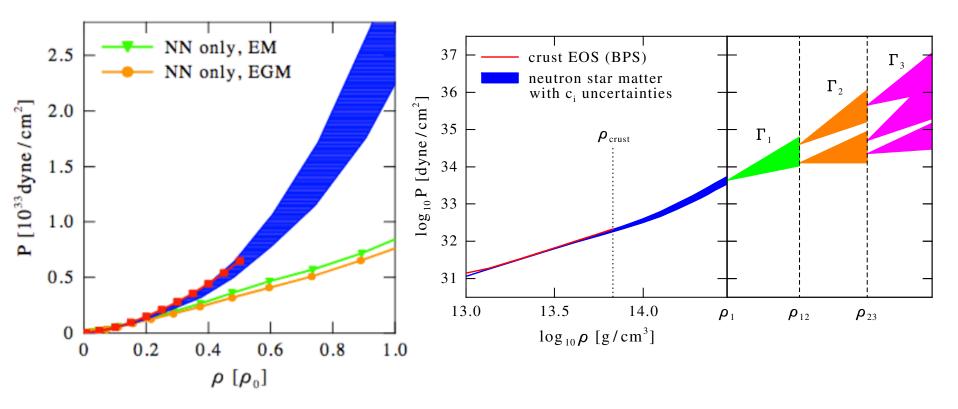
S_V =
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Good agreement with experimental constraints



Equation of state for neutron star matter: extend results to small $Y_{e,p}$

Hebeler, Lattimer, Pethick, Schwenk, PRL (2010) and APJ (2013)

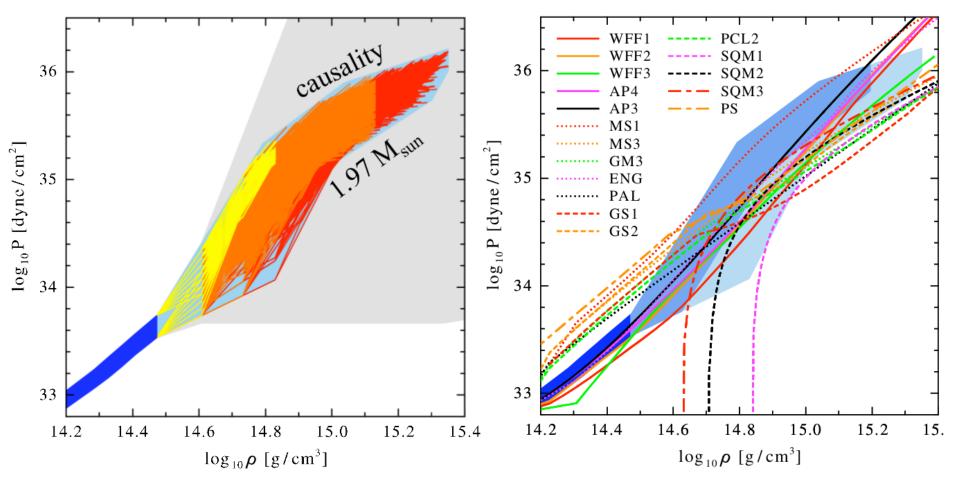


Agrees with standard crust EOS after inclusion of many-body forces

Extend to higher densities using polytropic expansion



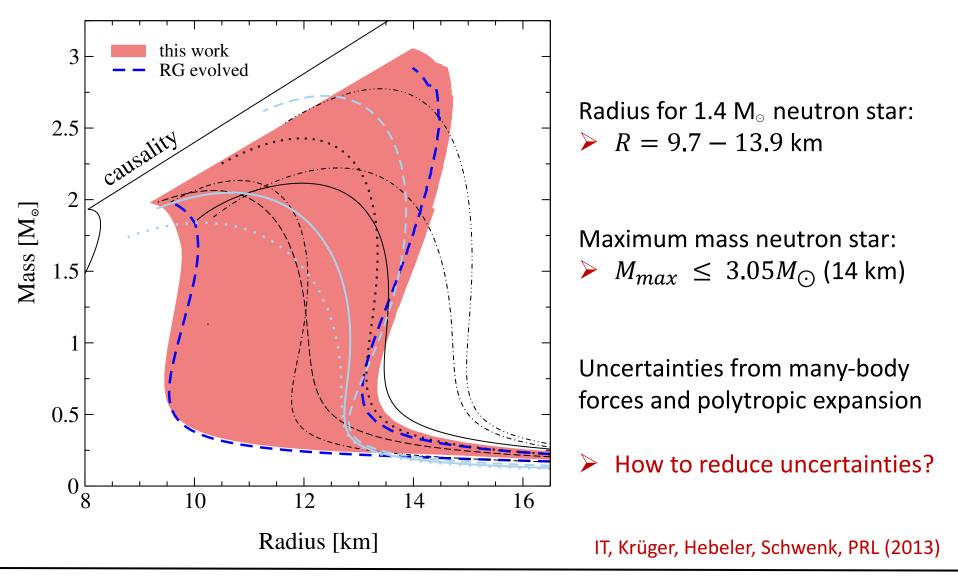
Constrain resulting EOS: causality and observed 1.97 M_{\odot} neutron star



Hebeler, Lattimer, Pethick, Schwenk, PRL (2010) and APJ (2013)

Neutron Stars





Neutron Stars



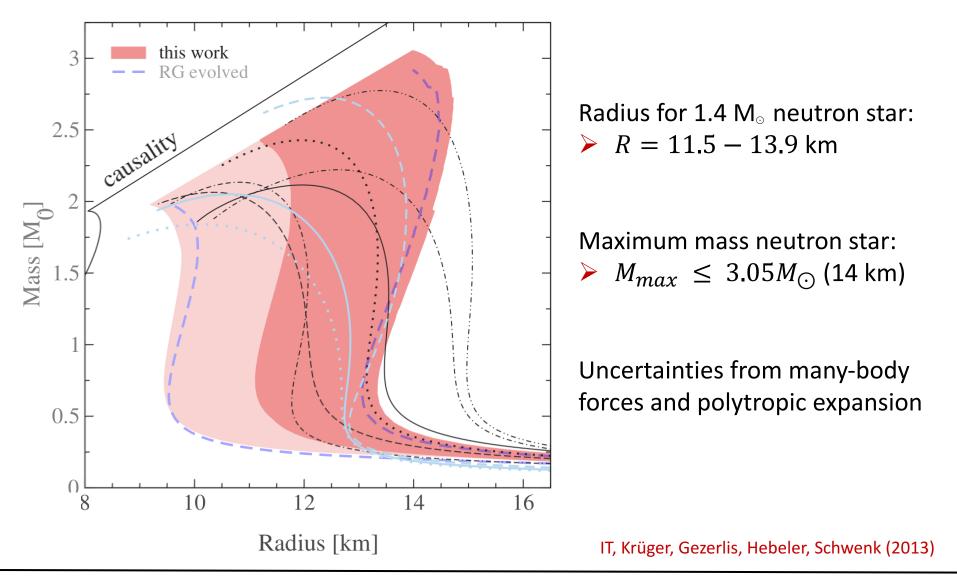
PCL2 WFF1 WFF2 SQM1 36 36 SQM2 WFF3 SQM3 AP4 PS AP3 MS1 MS3 $\log_{10} P [dyne/cm^2]$ $\log_{10} P [dyne/cm^2]$ GM3 35 35 ENG PAL GS1 GS2 34 34 33 33 14.4 14.6 14.8 15.0 15.2 15.4 14.214.2 14.4 14.6 14.8 15.0 15.2 15.4 $\log_{10}\rho$ [g/cm³] $\log_{10}\rho$ [g/cm³]

If a 2.4 M_o neutron star was observed:

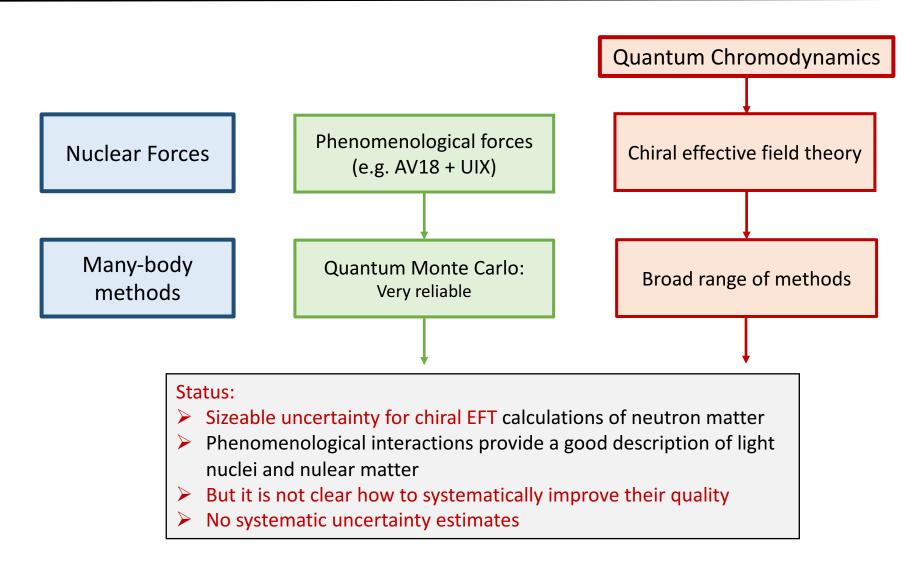
Hebeler et al., PRL (2010) and APJ (2013)

Neutron Stars

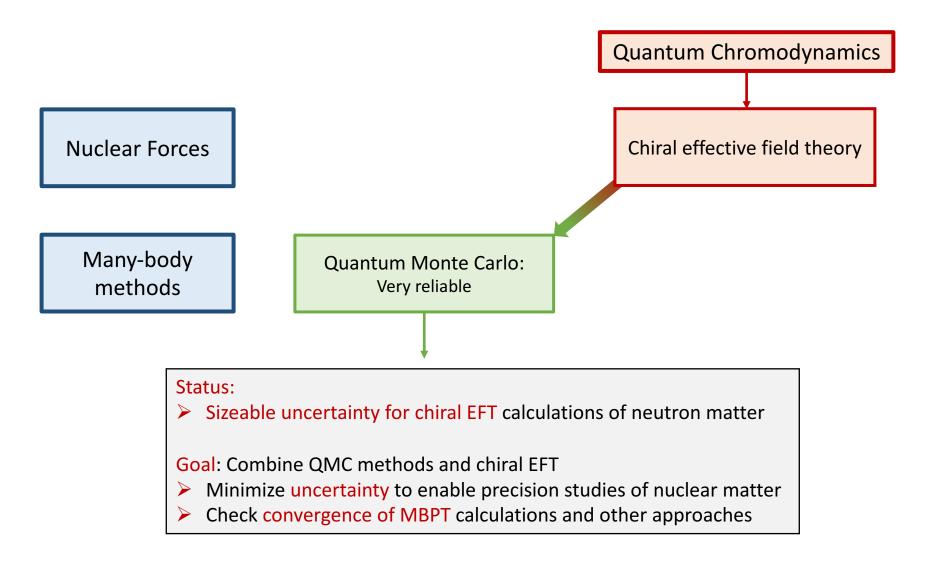






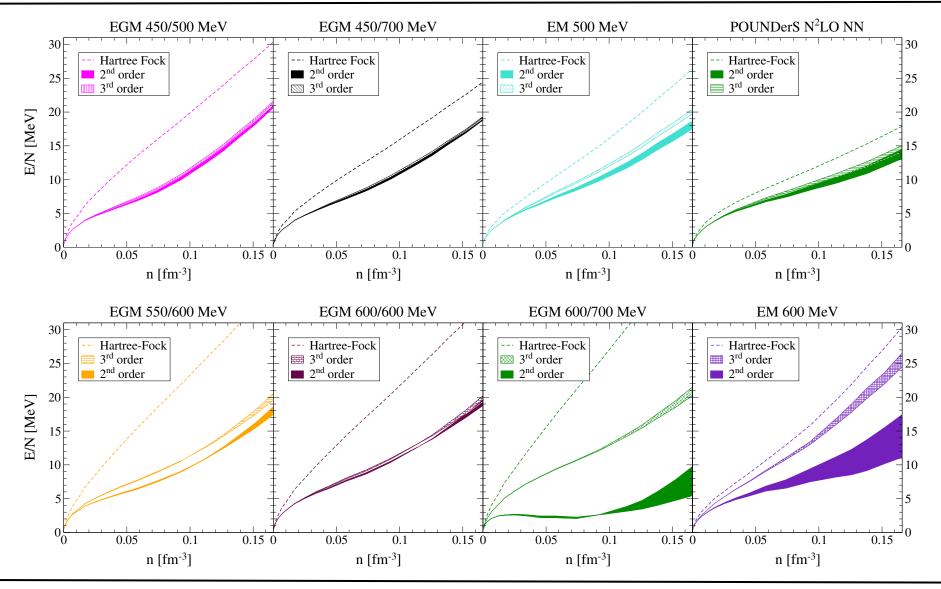






Improving neutron-matter band







Solve the many-body Schrödinger equation

$$H |\psi\rangle = -\frac{\partial}{\partial \tau} |\psi\rangle, \qquad \tau = it$$

$$\psi(R,\tau) = \int dR'^{3N} \langle R| e^{-(T+V)\tau} |R'\rangle \psi(R',0)$$

Basic steps:

Choose trial wavefunction which overlaps with the ground state

$$|\psi(R,0)\rangle = |\psi_T(R,0)\rangle = \sum_i c_i |\phi_i\rangle \to \sum_i c_i e^{-(E_i - E_0)\tau} |\phi_i\rangle$$

- > Evaluate propagator for small timestep $\Delta \tau$, feasible only for local potentials
- Make consecutive small time steps using Monte Carlo techniques to project out ground state

$$|\psi(R,\tau)\rangle \to |\phi_0\rangle \quad \text{for} \quad \tau \to \infty$$

More details:

Carlson, Gandolfi, Pederiva, Pieper, Schiavilla, Schmidt, Wiringa, RMP (2015)

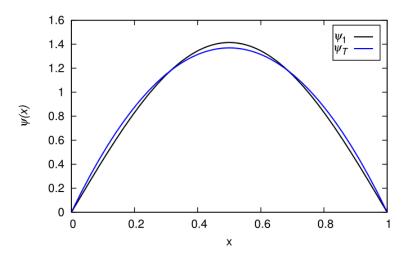


Particle in a 1D box, solution:

$$\psi_n(x) = \sqrt{2}\sin(n\pi x), \quad E_n = \frac{n^2\pi^2}{2}$$

Basic steps:

Choose parabolic trial wavefunction which overlaps with the ground state Animation by Joel Lynn, TU Darmstadt



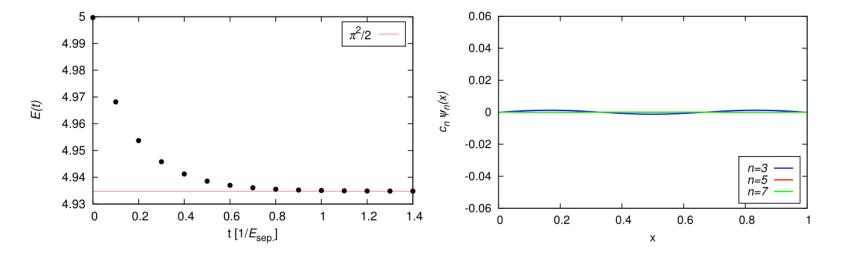


Particle in a 1D box, solution:

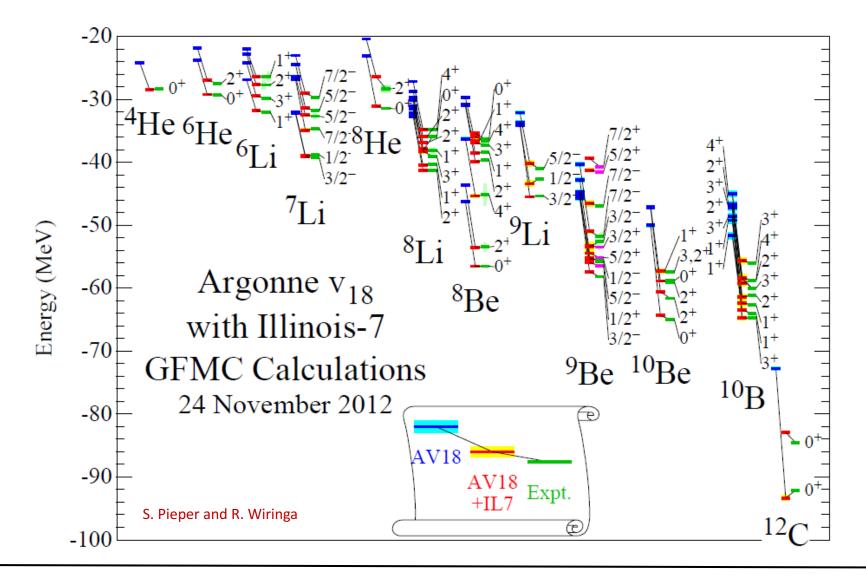
$$\psi_n(x) = \sqrt{2}\sin(n\pi x), \quad E_n = \frac{n^2\pi^2}{2}$$

► Make consecutive small timesteps,
$$\tau = 1.4 \left(\frac{1}{E_{sep}}\right)$$

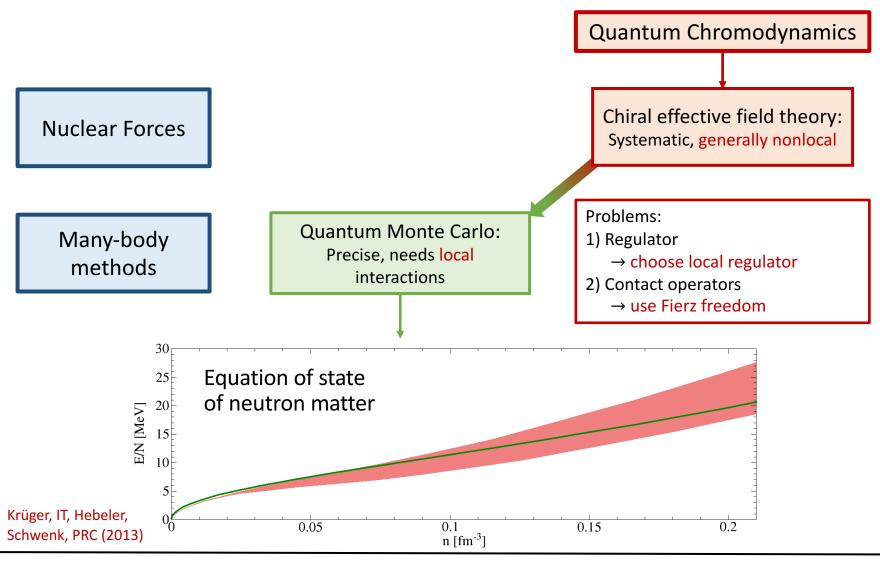
Animation by Joel Lynn, TU Darmstadt





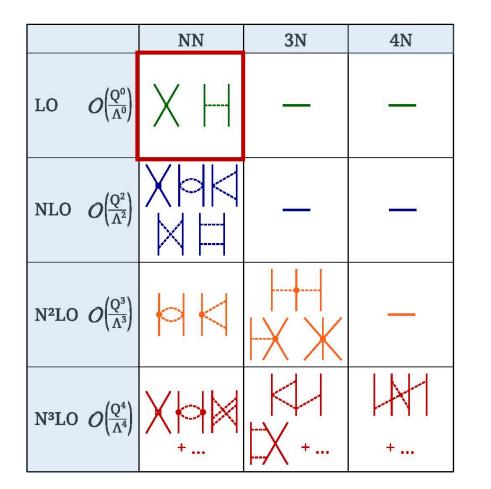






Oct. 20, 2016





Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...

• Leading order
$$V^{(0)} = V_{\text{cont}}^{(0)} + V^{\text{OPE}}$$

➢ Pion exchange local → local regulator

 $f_{\rm long}(r) = 1 - \exp(-r^4/R_0^4)$

Contact potential:

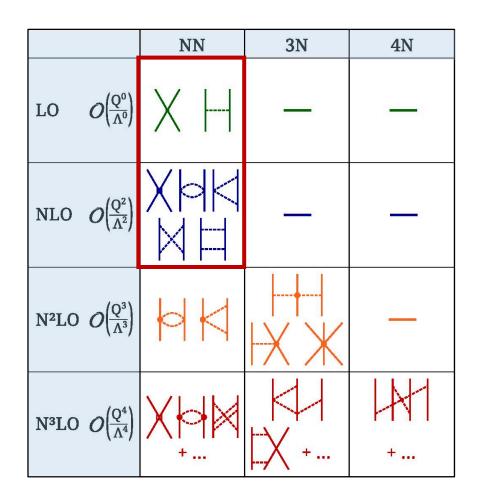
$$V_{\text{cont}}^{(0)} = \alpha_1 \mathbf{1} + \alpha_2 \sigma_1 \cdot \sigma_2 + \alpha_3 \tau_1 \cdot \tau_2 + \alpha_4 \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2$$

→ Only two independent (Pauli principle)

$$V_{\rm cont}^{(0)} = C_S \mathbf{1} + C_T \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2}$$

$$f_{\rm short}(r) = \alpha \exp(-r^4/R_0^4)$$



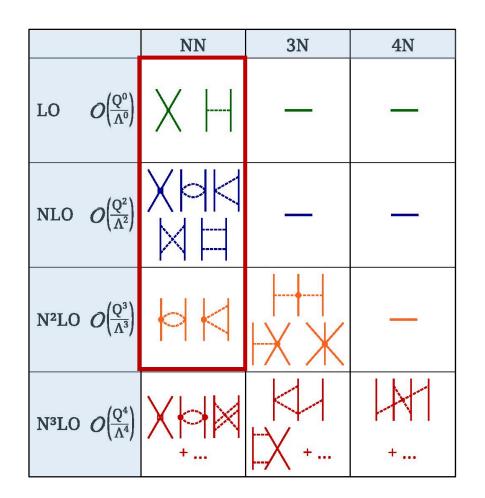


 Choose local set of short-range operators at NLO (7 out of 14)

$$V_{\text{cont}}^{(2)} = \begin{array}{l} \gamma_1 q^2 + \gamma_2 q^2 \sigma_1 \cdot \sigma_2 + \gamma_3 q^2 \tau_1 \cdot \tau_2 \\ + \gamma_4 q^2 \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2 \\ + \gamma_5 k^2 + \gamma_6 k^2 \sigma_1 \cdot \sigma_2 + \gamma_7 k^2 \tau_1 \cdot \tau_2 \\ + \gamma_8 k^2 \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2 \\ + \gamma_9 (\sigma_1 + \sigma_2) (\mathbf{q} \times \mathbf{k}) \\ + \gamma_{10} (\sigma_1 + \sigma_2) (\mathbf{q} \times \mathbf{k}) \tau_1 \cdot \tau_2 \\ + \gamma_{11} (\sigma_1 \cdot \mathbf{q}) (\sigma_2 \cdot \mathbf{q}) \\ + \gamma_{12} (\sigma_1 \cdot \mathbf{q}) (\sigma_2 \cdot \mathbf{q}) \tau_1 \cdot \tau_2 \\ + \gamma_{13} (\sigma_1 \cdot \mathbf{k}) (\sigma_2 \cdot \mathbf{k}) \\ + \gamma_{14} (\sigma_1 \cdot \mathbf{k}) (\sigma_2 \cdot \mathbf{k}) \tau_1 \cdot \tau_2 . \end{array}$$

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...





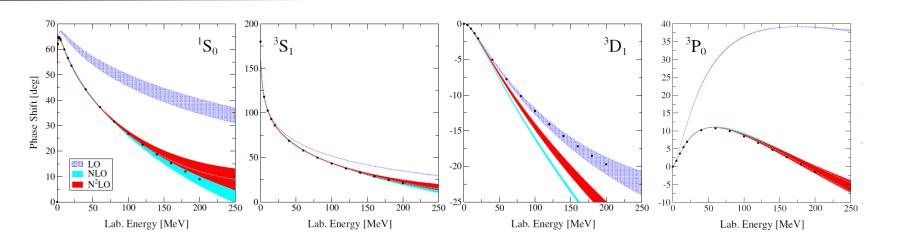
- Choose local set of short-range operators at NLO (7 out of 14)
- Pion exchanges up to N²LO are local
- This freedom can be used to remove all nonlocal operators up to N²LO

Gezerlis, IT, Epelbaum, Gandolfi, Hebeler, Nogga, Schwenk, PRL (2013) Gezerlis, IT, Epelbaum, Freunek, Gandolfi, Hebeler, Nogga, Schwenk, PRC (2014)

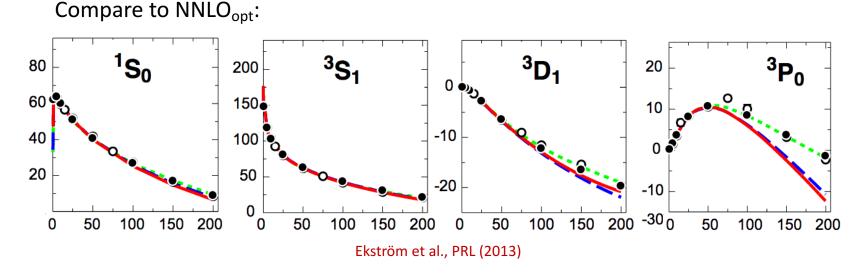
LECs fit to phase shifts

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...

Phaseshifts for local potentials



Gezerlis, IT, Epelbaum, Freunek, Gandolfi, Hebeler, Nogga, Schwenk, PRC (2014)

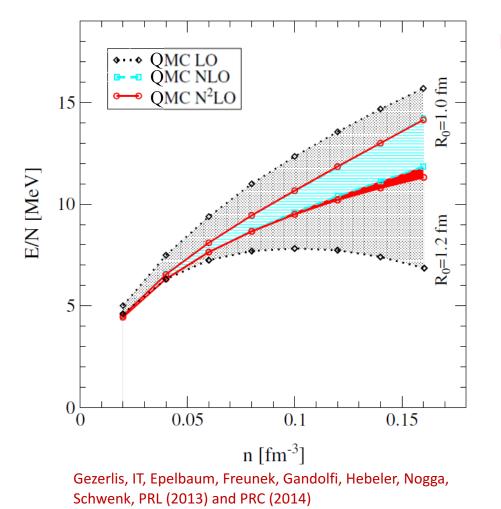


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NUCLEAR THEORY





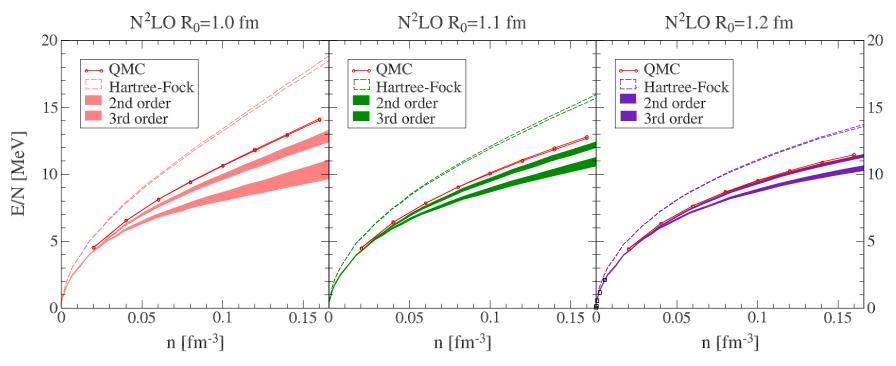
NN-only calculation:

QMC: Statistical uncertainty of points negligible

➢ Bands include NN cutoff variation $R_0 = 1.0 - 1.2 \text{ fm}$

Order-by-order convergence up to saturation density



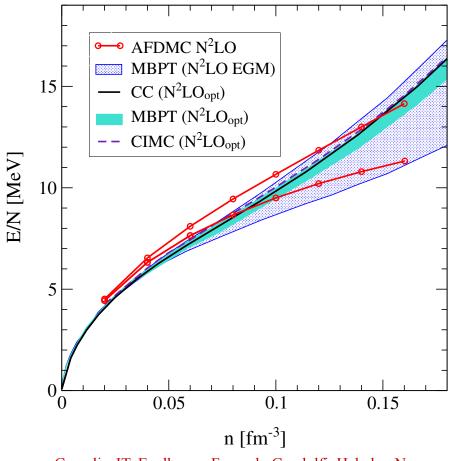


Gezerlis, IT, Epelbaum, Freunek, Gandolfi, Hebeler, Nogga, Schwenk, PRC (2014)

Many-body perturbation theory:

- Excellent agreement with QMC for soft potentials ($R_0 = 1.2$ fm)
- Validates perturbative calculations for those interactions





Gezerlis, IT, Epelbaum, Freunek, Gandolfi, Hebeler, Nogga, Schwenk, PRC (2014)

NN-only calculation

Good agreement with other approaches:

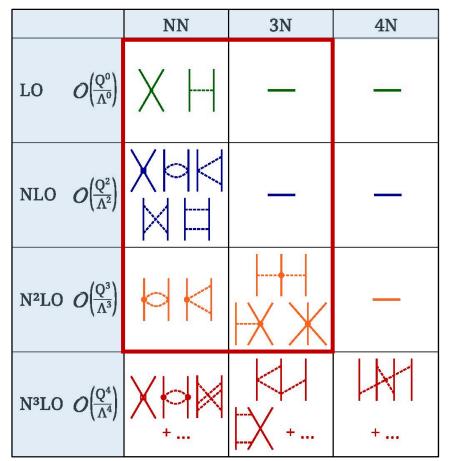
MBPT with N²LO EGM IT, Krüger, Hebeler, Schwenk, PRL (2013)

CC with N²LO_{opt} Hagen, Papenbrock, Ekström, Wendt, Baardsen, Gandolfi, Hjorth-Jensen, Horowitz, PRC (2013)

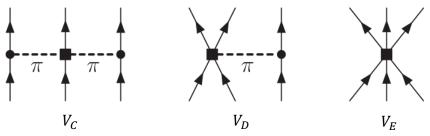
MBPT with N²LO_{opt} IT, Krüger, Gezerlis, Hebeler, Schwenk, NTSE (2013)

CIMC with N²LO_{opt} Roggero, Mukherjee, Pederiva, PRL (2014)





Next: inclusion of leading 3N forces



Three topologies:

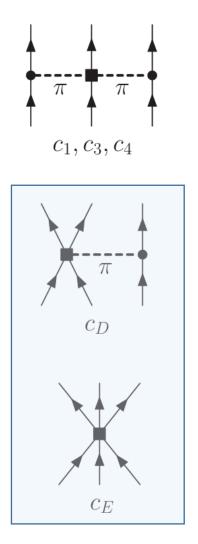
- \succ Two-pion exchange V_C
- \triangleright One-pion-exchange contact V_D
- \succ Three-nucleon contact V_E

Only two new couplings: c_D and c_E

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...

QMC with chiral 3N forces



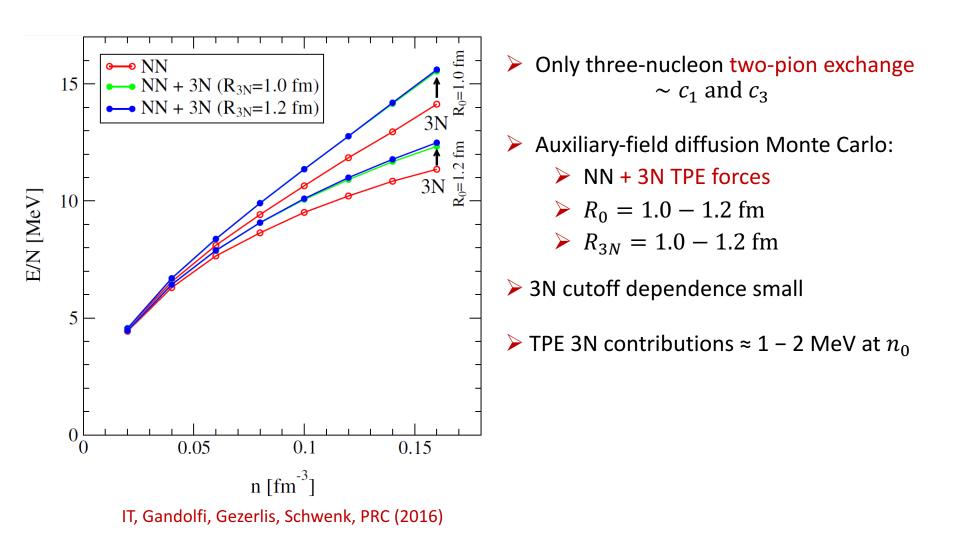


 c_1 term: Tucson-Melbourn S-wave interaction $c_{3,4}$ term: Fujita-Miyazawa interaction

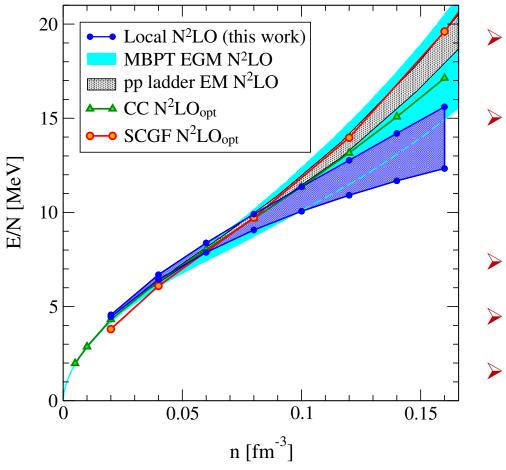
Two-pion-exchange most important in PNM, usually V_D and V_E vanish in neutron matter: c_D due to spin-isospin structure, c_E due to Pauli principle see also Hebeler, Schwenk, PRC (2010)

Only true for regulator symmetric in particle labels like commonly used nonlocal regulators, not for local regulators









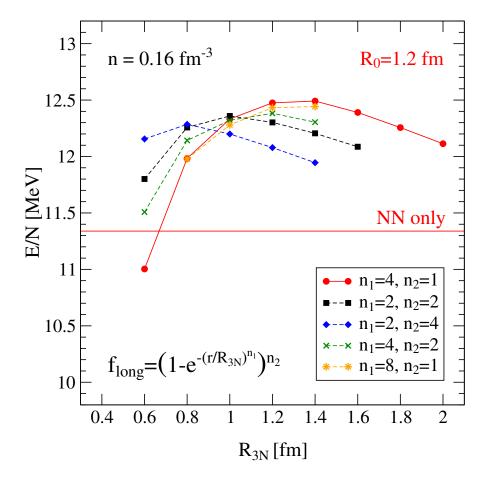
IT, Gandolfi, Gezerlis, Schwenk, PRC (2016)

• Only three-nucleon two-pion exchange $\sim c_1$ and c_3

- Auxiliary-field diffusion Monte Carlo:
 - > NN + 3N TPE forces
 - \triangleright $R_0 = 1.0 1.2 \text{ fm}$
 - $R_{3N} = 1.0 1.2 \text{ fm}$
- > 3N cutoff dependence small
- ▶ TPE 3N contributions $\approx 1 2$ MeV at n_0

smaller than for nonlocal regulators





IT, Gandolfi, Gezerlis, Schwenk, PRC (2016)

Only three-nucleon two-pion exchange $\sim c_1$ and c_3

- > Auxiliary-field diffusion Monte Carlo:
 - > NN + 3N TPE forces
 - $ightarrow R_0 = 1.0 1.2 \, \text{fm}$
 - $> R_{3N} = 1.0 1.2 \text{ fm}$
- 3N cutoff dependence small
- ▶ TPE 3N contributions $\approx 1 2$ MeV at n_0
- smaller than for nonlocal regulators
- Independent of exact regulator form



Example: two-body regulators at Hartree-Fock:

$$f_{\text{reg}}^{MSL} = \exp\left(-\left(\frac{q}{\Lambda}\right)^{2n}\right), \qquad f_{\text{reg}}^{MSNL} = \exp\left(-2\left(\frac{p}{\Lambda}\right)^{2n}\right)$$

After antisymmetrization we have a direct and an exchange term.

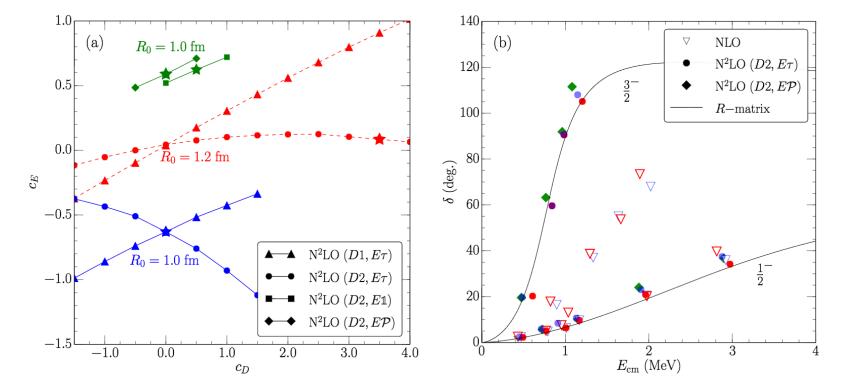
Direct term: $q = p - p' = 0 \rightarrow f_{reg}^{MSL} = 1, \quad f_{reg}^{MSNL} = \exp\left(-2\left(\frac{p}{\Lambda}\right)^{2n}\right)$ Exchange term: $q = p - p' = 2p \rightarrow f_{reg}^{MSL} = \exp\left(-\left(\frac{2p}{\Lambda}\right)^{2n}\right), f_{reg}^{MSNL} = \exp\left(-2\left(\frac{p}{\Lambda}\right)^{2n}\right)$

Spin-dependent interactions at Hartree-Fock: only exchange term survives

Effective cutoff smaller for local regulators!



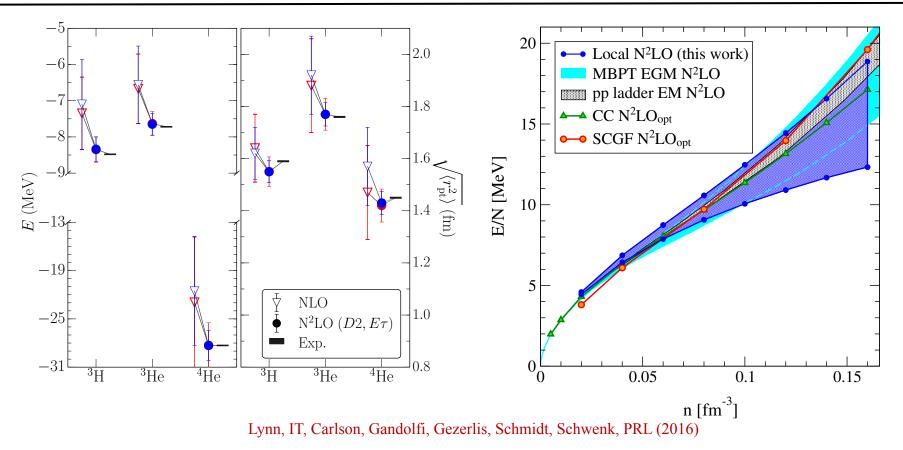
 \succ Fit c_E and c_D to ⁴He binding energy and n- α scattering



Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, PRL (2016)

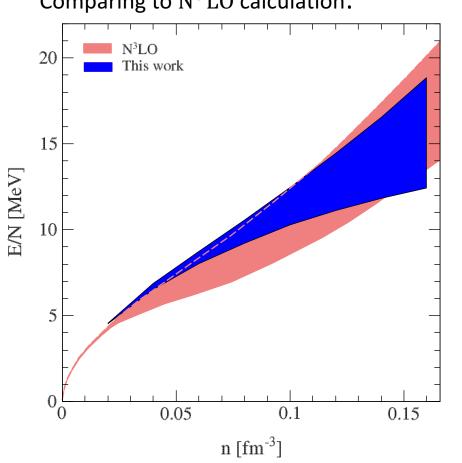
Results





- Chiral interactions at N²LO simultaneously reproduce the properties of A=3, 4, 5 systems and of neutron matter
- Commonly used phenomenological 3N interactions fail for neutron matter Sarsa, Fantoni, Schmidt, Pederiva, PRC (2003)





Comparing to N^3LO calculation:

IT, Krüger, Hebeler, Schwenk, PRL (2013) Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, PRL (2016) Chiral EFT forces with the Quantum Monte Carlo method:

- Energies agree well with MBPT result within uncertainty bands
- Many-body uncertainty negligible
- uncertainties comparable but QMC band only at N²LO and includes also hard interactions
- Improve local chiral interactions:
 Develop N³LO potentials



Improve local chiral interactions:

- Develop maximally local N³LO potentials
- Inclusion of Delta degree of freedom

Problem: only 8 out of 30 possible operators local

$$V_{\text{cont}}^{(4)} = D_{1} q^{4} + D_{2} q^{4} \tau_{1} \cdot \tau_{2} + D_{3} q^{4} \sigma_{1} \cdot \sigma_{2} + D_{4} q^{4} \sigma_{1} \cdot \sigma_{2} \tau_{1} \cdot \tau_{2}$$

$$+ D_{5} k^{4} + D_{6} k^{4} \tau_{1} \cdot \tau_{2} + D_{7} k^{4} \sigma_{1} \cdot \sigma_{2} + D_{8} k^{4} \sigma_{1} \cdot \sigma_{2} \tau_{1} \cdot \tau_{2}$$

$$+ D_{9} q^{2} k^{2} + D_{10} q^{2} k^{2} \tau_{1} \cdot \tau_{2} + D_{11} q^{2} k^{2} \sigma_{1} \cdot \sigma_{2} + D_{12} q^{2} k^{2} \sigma_{1} \cdot \sigma_{2} \tau_{1} \cdot \tau_{2}$$

$$+ D_{13} (q \times k)^{2} + D_{14} (q \times k)^{2} \tau_{1} \cdot \tau_{2} + D_{15} (q \times k)^{2} \sigma_{1} \cdot \sigma_{2} + D_{16} (q \times k)^{2} \sigma_{1} \cdot \sigma_{2} \tau_{1} \cdot \tau_{2}$$

$$+ \frac{i}{2} D_{17} q^{2} (\sigma_{1} + \sigma_{2}) \cdot (q \times k) + \frac{i}{2} D_{18} q^{2} (\sigma_{1} + \sigma_{2}) \cdot (q \times k) \tau_{1} \cdot \tau_{2}$$

$$+ \frac{i}{2} D_{19} k^{2} (\sigma_{1} + \sigma_{2}) \cdot (q \times k) + \frac{i}{2} D_{20} k^{2} (\sigma_{1} + \sigma_{2}) \cdot (q \times k) \tau_{1} \cdot \tau_{2}$$

$$+ D_{21} q^{2} \sigma_{1} \cdot q \sigma_{2} \cdot q + D_{22} q^{2} \sigma_{1} \cdot q \sigma_{2} \cdot q \tau_{1} \cdot \tau_{2}$$

$$+ D_{25} q^{2} \sigma_{1} \cdot k \sigma_{2} \cdot k + D_{26} q^{2} \sigma_{1} \cdot k \sigma_{2} \cdot k \tau_{1} \cdot \tau_{2}$$

$$+ D_{27} k^{2} \sigma_{1} \cdot k \sigma_{2} \cdot k + D_{28} k^{2} \sigma_{1} \cdot k \sigma_{2} \cdot k \tau_{1} \cdot \tau_{2}$$

$$+ D_{29} ((\sigma_{1} + \sigma_{2}) \cdot (q \times k))^{2} + D_{30} ((\sigma_{1} + \sigma_{2}) \cdot (q \times k))^{2} \tau_{1} \cdot \tau_{2}$$

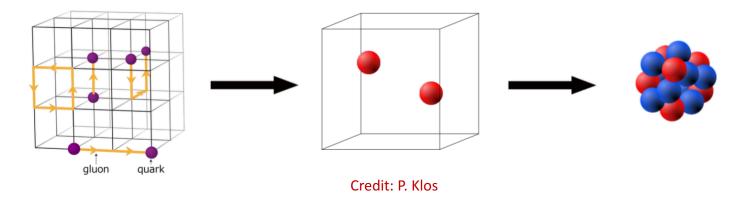
$$(34)$$

But: work in progress!



Motivation:

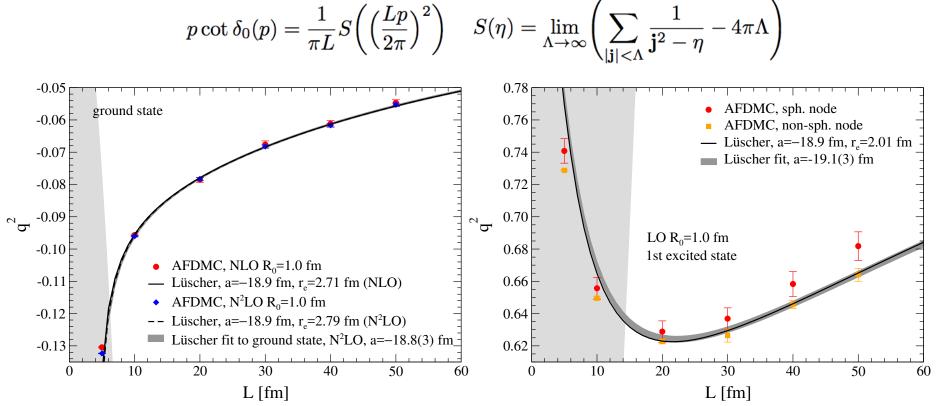
- Lattice QCD is the only ab initio method available to solve QCD directly at low energies but computational costs too high to compute more than a few particles
- Connect ab-initio nuclear physics to the underlying theory of QCD by studying, e.g., few-neutron systems in a box



Long-term goal: Matching of chiral EFT couplings to lattice QCD results

> Enable chiral EFT predictions from first principles

Use Luescher formula to extract infinite-volume scattering data from finite volume calculations:



Klos, Lynn, IT, Gandolfi, Gezerlis, Hammer, Hoferichter, Schwenk, arXiv:1604:01387, accepted for PRC

Easy to extend to larger systems or, e.g., systems with hyperons

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Summary



Chiral effective field theory:

- Provides constraints on symmetry energy, neutron star EOS
- Improvement of neutron-matter EOS work in progress
- Using QMC methods with higher order interactions expected to reduce theoretical uncertainties by a factor of two Gezerlis, IT, Epelbaum, Gandolfi, Hebeler, Nogga, Schwenk, PRL (2013) & PRC (2014)
 IT, Gandolfi, Gezerlis, Schwenk, PRC (2016)
 Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, PRL (2016)

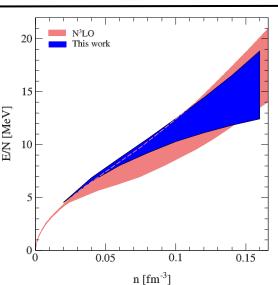
Constraints on symmetry energy and neutron stars:

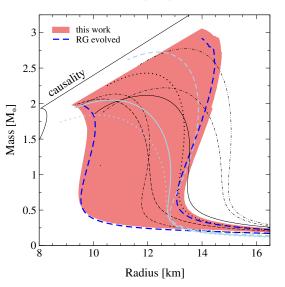
 $\succ S_V = 28.9 - 34.9 \text{ MeV}$

 \blacktriangleright L = 43.0 - 66.6 MeV

 \blacktriangleright Radius for 1.4 M $_{\odot}$ neutron star: 9.7 – 13.9 km

IT, Krüger, Hebeler, Schwenk, PRL & PRC (2013)





Thanks

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ありがとうございました!