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

- 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.
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-rich nuclei

- Neutron matter at saturation density constrains neutron-skin thickness of neutron-rich nuclei
- Experiments at RCNP, GSI, ...

Credit: B.A. Brown

Roca-Maza et al., PRC (2013)

Equation of state of neutron matter

Credit: B.A. Brown

Neutron-rich nuclei

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.

Equation of state of neutron matter

- Neutron matter equation of state at saturation density and above determines mass-radius relation of neutron stars and gravitational-wave signal of neutron-star mergers.

EOS properties at saturation density are correlated with neutron-star radii and gravitational wave peak frequency.


Bauswein et al., PRD (2012)
Motivation

How to obtain the EOS in an ab initio approach?

- Nuclear Forces
- Phenomenological forces (e.g. AV18 + UIX)
- Quantum Monte Carlo: Very reliable
- Quantum Chromodynamics
  - Chiral effective field theory
  - Broad range of methods

Equation of state of neutron matter
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**

- **Summary**
Chiral effective field theory for nuclear forces

Basic principle of **effective field theory**:

\[ \lambda \gg R \]

At low energies (long wavelength) details not resolved!

- Choose **relevant degrees of freedom** for low-energy processes
- Systematic expansion of interactions constrained by symmetries
Chiral effective field theory for nuclear forces

Explicit degrees of freedom:
- Pions and nucleons

Write most general Lagrangian consistent with the symmetries of QCD

Separation of scales:
- Low momenta $Q \ll$ breakdown scale $\Lambda_b$
- Expand in powers of $\left(\frac{Q}{\Lambda_b}\right)^\nu \sim \left(\frac{1}{3}\right)^\nu$

Power counting:
- $\nu = 0$: leading order (LO),
- $\nu = 2$: next-to-leading order (NLO), ...

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ...
Chiral effective field theory for nuclear forces

<table>
<thead>
<tr>
<th></th>
<th>NN</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>LO</td>
<td>$O\left(\frac{Q^0}{\Lambda^0}\right)$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NLO</td>
<td>$O\left(\frac{Q^2}{\Lambda^2}\right)$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N^2LO</td>
<td>$O\left(\frac{Q^3}{\Lambda^3}\right)$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N^3LO</td>
<td>$O\left(\frac{Q^4}{\Lambda^4}\right)$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2 LECs</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>7 LECs</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>15 LECs</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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)

$\rho \sim \text{const.}$

Second scale: cutoff $\Lambda$ (resolution):
- Interactions $\Lambda$-dependent
Chiral effective field theory for nuclear forces

Systematic expansion of the nuclear forces:
- Can work to desired accuracy
- Can obtain systematic error estimates

### Chiral effective field theory for nuclear forces

<table>
<thead>
<tr>
<th>Order</th>
<th>$O(Q^0/A^0)$</th>
<th>$O(Q^2/A^2)$</th>
<th>$O(Q^3/A^3)$</th>
<th>$O(Q^4/A^4)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO</td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
</tr>
<tr>
<td>NLO</td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
</tr>
<tr>
<td>N^2LO</td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
</tr>
<tr>
<td>N^3LO</td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
<td><img src="#" alt="Diagram" /></td>
</tr>
</tbody>
</table>

**Many-body forces:**
- Have been found to be crucial ingredient to describe nuclear physics

**Natural hierarchy of nuclear forces:**
- Two-body (NN) forces start at first order
- Three-body (3N) forces start at third order (2 LECs)

**Fitting:**
- NN forces in NN system (NN phase shifts, ...)
- 3N forces in 3N/4N system (Binding energies, radii, ...)
## Chiral effective field theory for nuclear forces

<table>
<thead>
<tr>
<th></th>
<th>NN</th>
<th>3N</th>
<th>4N</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LO</strong></td>
<td>$O(\frac{Q^0}{\Lambda^0})$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><img src="LO_diagram.png" alt="Diagram" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>NLO</strong></td>
<td>$O(\frac{Q^2}{\Lambda^2})$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><img src="NLO_diagram.png" alt="Diagram" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>N^2LO</strong></td>
<td>$O(\frac{Q^3}{\Lambda^3})$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><img src="N2LO_diagram.png" alt="Diagram" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>N^3LO</strong></td>
<td>$O(\frac{Q^4}{\Lambda^4})$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><img src="N3LO_diagram.png" alt="Diagram" /></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Consistent interactions:
- Same couplings for two-nucleon and many-body sector
- In contrast to phenomenological interactions

Oct. 20, 2016

Ingo Tews, NPCS M workshop
Chiral effective field theory for nuclear forces

Many-body forces are crucial:

**Oxygen**

- Otsuka et al., PRL (2010)

**Calcium**

- Gallant et al., PRL (2012)

**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)
# Chiral effective field theory for nuclear forces

<table>
<thead>
<tr>
<th></th>
<th>NN</th>
<th>3N</th>
<th>4N</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO</td>
<td>$O(Q^0 \Lambda^0)$</td>
<td><img src="image1" alt="Diagram" /></td>
<td><img src="image2" alt="Diagram" /></td>
</tr>
<tr>
<td>NLO</td>
<td>$O(Q^2 \Lambda^2)$</td>
<td><img src="image4" alt="Diagram" /></td>
<td><img src="image5" alt="Diagram" /></td>
</tr>
<tr>
<td>N^2LO</td>
<td>$O(Q^3 \Lambda^3)$</td>
<td><img src="image7" alt="Diagram" /></td>
<td><img src="image8" alt="Diagram" /></td>
</tr>
<tr>
<td>N^3LO</td>
<td>$O(Q^4 \Lambda^4)$</td>
<td><img src="image10" alt="Diagram" /></td>
<td><img src="image11" alt="Diagram" /></td>
</tr>
</tbody>
</table>

**Neutron matter:**
- Complete calculation at N^3LO using many-body perturbation theory (MBPT)
  - IT, Krüger, Hebeler, Schwenk, PRL (2013)

**Calculation is simpler in neutron matter:**
- Only certain parts of the many-body forces contribute
- Chiral many-body forces completely predicted from NN sector
Neutron matter

Bands:
- Include several sources of uncertainty:
  - Chiral Hamiltonians (cutoff, 3N LECs)
  - Many-body method

NN interactions:
- E/N at saturation density:
  12-15 MeV

NN+3N interactions:
- Have large impact on energy and uncertainty:
  14-21 MeV
Neutron matter

Good agreement with other calculations
➤ but in those
no theoretical uncertainties

Akmal et al., PRC (1998)
Gandolfi et al., PRC (2012)

Chiral EFT puts constraints on neutron matter EOS
Neutron matter

Good agreement with other calculations

but in those

no theoretical uncertainties

Akmal et al., PRC (1998)
Gandolfi et al., PRC (2012)

Chiral EFT puts constraints on neutron matter EOS

Lines from Hempel, Lattimer, G. Shen
Put constraints on *symmetry energy* and its density dependence $L$:

\[
S_v(n) = \frac{1}{8} \frac{\partial^2}{\partial x^2} \frac{E}{A} (n, x) \bigg|_{x=1/2},
\]

\[
L(n_0) = 3n_0 \frac{\partial}{\partial n} S_v(n) \bigg|_{n_0},
\]

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

Good agreement with experimental constraints

Put constraints on symmetry energy and its density dependence $L$:

$$S_V(n) = \frac{1}{8} \frac{\partial^2}{\partial x^2} \frac{E}{A} (n, x) \bigg|_{x=1/2},$$

$$L(n_0) = 3n_0 \frac{\partial}{\partial n} S_V(n) \bigg|_{n_0},$$

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

Good agreement with experimental constraints

Drischler, Soma, Schwenk, PRC (2014)
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

Radius for 1.4 M⊙ neutron star:
- $R = 9.7 - 13.9$ km

Maximum mass neutron star:
- $M_{\text{max}} \leq 3.05M_\odot$ (14 km)

Uncertainties from many-body forces and polytropic expansion
- How to reduce uncertainties?

IT, Krüger, Hebeler, Schwenk, PRL (2013)
If a $2.4 \, M_\odot$ neutron star was observed:

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

Radius for $1.4 \, M_{\odot}$ neutron star:

$R = 11.5 - 13.9 \, \text{km}$

Maximum mass neutron star:

$M_{\text{max}} \leq 3.05 \, M_{\odot} \, (14 \, \text{km})$

Uncertainties from many-body forces and polytropic expansion

IT, Krüger, Gezerlis, Hebeler, Schwenk (2013)
Improving neutron-matter band

Nuclear Forces

Many-body methods

Phenomenological forces (e.g. AV18 + UIX)

Quantum Monte Carlo: Very reliable

Quantum Chromodynamics

Chiral effective field theory

Broad range of methods

Status:
- Sizeable uncertainty for chiral EFT calculations of neutron matter
- Phenomenological interactions provide a good description of light nuclei and nuclear matter
- But it is not clear how to systematically improve their quality
- No systematic uncertainty estimates
Improving neutron-matter band

Status:
- Sizeable uncertainty for chiral EFT calculations of neutron matter

Goal: Combine QMC methods and chiral EFT
- Minimize uncertainty to enable precision studies of nuclear matter
- Check convergence of MBPT calculations and other approaches
Improving neutron-matter band

EGM 450/500 MeV

EGM 450/700 MeV

EM 500 MeV

POUNDerS N^2LO NN

EGM 550/600 MeV

EGM 600/600 MeV

EGM 600/700 MeV

EM 600 MeV
Quantum Monte Carlo method

Solve the many-body Schrödinger equation

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

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

Basic steps:

- Choose trial wavefunction which overlaps with the ground state

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

- 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

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

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
Quantum Monte Carlo method

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, $\tau = 1.4 \left( \frac{1}{E_{\text{sep}}} \right)$

Animation by Joel Lynn, TU Darmstadt
Quantum Monte Carlo method

Argonne v$_{18}$ with Illinois-7

GFMC Calculations
24 November 2012

S. Pieper and R. Wiringa

Av18
Av18 + IL7
Expt.
Local chiral interactions

Nuclear Forces

Many-body methods

Quantum Monte Carlo: Precise, needs local interactions

Quantum Chromodynamics

Chiral effective field theory: Systematic, generally nonlocal

Problems:
1) Regulator → choose local regulator
2) Contact operators → use Fierz freedom

Equation of state of neutron matter

Krüger, IT, Hebeler, Schwenk, PRC (2013)
Local chiral interactions

<table>
<thead>
<tr>
<th>Order</th>
<th>Term</th>
<th>NN</th>
<th>3N</th>
<th>4N</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO</td>
<td>$\mathcal{O}(\frac{Q^0}{\Lambda^0})$</td>
<td><img src="" alt="Diagram" /></td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>NLO</td>
<td>$\mathcal{O}(\frac{Q^2}{\Lambda^2})$</td>
<td><img src="" alt="Diagram" /></td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>N^2LO</td>
<td>$\mathcal{O}(\frac{Q^3}{\Lambda^3})$</td>
<td><img src="" alt="Diagram" /></td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>N^3LO</td>
<td>$\mathcal{O}(\frac{Q^4}{\Lambda^4})$</td>
<td><img src="" alt="Diagram" /></td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

- **Leading order** $V^{(0)} = V_{\text{cont}}^{(0)} + V^{\text{OPE}}$
- **Pion exchange** local $\rightarrow$ local regulator

\[
f_{\text{long}}(r) = 1 - \exp(-r^4/R_0^4)
\]

- **Contact potential:**

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

$\rightarrow$ Only two independent (Pauli principle)

\[
V_{\text{cont}}^{(0)} = C_S \mathbf{1} + C_T \sigma_1 \cdot \sigma_2
\]

\[
f_{\text{short}}(r) = \alpha \exp(-r^4/R_0^4)
\]

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

<table>
<thead>
<tr>
<th>Order</th>
<th>Operator</th>
<th>NN</th>
<th>3N</th>
<th>4N</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO $O^{(Q^0)}_{A^0}$</td>
<td>$\times$ $H$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>NLO $O^{(Q^2)}_{A^2}$</td>
<td>$\times$ $H$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>N$^2$LO $O^{(Q^3)}_{A^3}$</td>
<td>$\times$ $H$</td>
<td>$-$</td>
<td>$-$</td>
<td></td>
</tr>
<tr>
<td>N$^3$LO $O^{(Q^4)}_{A^4}$</td>
<td>$\times$ $H$</td>
<td>$-$</td>
<td>$-$</td>
<td></td>
</tr>
</tbody>
</table>

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

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

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißen, Hammer ...
**Local chiral interactions**

<table>
<thead>
<tr>
<th>Order (LO, NLO, N²LO, N³LO)</th>
<th>NN</th>
<th>3N</th>
<th>4N</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO $\mathcal{O}(Q^0/A^0)$</td>
<td>X</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>NLO $\mathcal{O}(Q^2/A^2)$</td>
<td>X</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>N²LO $\mathcal{O}(Q^3/A^3)$</td>
<td>X</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>N³LO $\mathcal{O}(Q^4/A^4)$</td>
<td>X</td>
<td>+</td>
<td>+</td>
</tr>
</tbody>
</table>

- 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)

Compare to NNLO_{opt}:

Ekström et al., PRL (2013)
QMC results for NN forces

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, PRL (2013) and PRC (2014)
Many-body perturbation theory:
- Excellent agreement with QMC for soft potentials ($R_0 = 1.2$ fm)
- Validates perturbative calculations for those interactions
QMC results for NN forces

NN-only calculation

- Good agreement with other approaches:
  
  **MBPT with $N^2LO$ EGM**
  IT, Krüger, Hebeler, Schwenk, PRL (2013)

  **CC with $N^2LO_{opt}$**
  Hagen, Papenbrock, Ekström, Wendt, Baardsen, Gandolfi, Hjorth-Jensen, Horowitz, PRC (2013)

  **MBPT with $N^2LO_{opt}$**
  IT, Krüger, Gezerlis, Hebeler, Schwenk, NTSE (2013)

  **CIMC with $N^2LO_{opt}$**
  Roggero, Mukherjee, Pederiva, PRL (2014)

Graph showing comparison of AFDMC, MBPT, CC, and CIMC results for NN forces.
QMC with chiral 3N forces

Next: inclusion of leading 3N forces

Three topologies:
- Two-pion exchange $V_C$
- One-pion-exchange contact $V_D$
- 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

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

see also Hebeler, Schwenk, PRC (2010)
QMC results with 3N TPE

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

- Auxiliary-field diffusion Monte Carlo:
  - NN + 3N TPE forces
  - \( R_0 = 1.0 - 1.2 \text{ fm} \)
  - \( R_{3N} = 1.0 - 1.2 \text{ fm} \)

- 3N cutoff dependence small

- TPE 3N contributions \( \approx 1 - 2 \text{ MeV at } n_0 \)

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
  - \( R_0 = 1.0 - 1.2 \text{ fm} \)
  - \( R_{3N} = 1.0 - 1.2 \text{ fm} \)

3N cutoff dependence small

TPE 3N contributions \( \approx 1 - 2 \text{ MeV at } n_0 \)

smaller than for nonlocal regulators

IT, Gandolfi, Gezerlis, Schwenk, PRC (2016)
QMC results with 3N TPE

- Only three-nucleon two-pion exchange $\sim c_1$ and $c_3$
- Auxiliary-field diffusion Monte Carlo:
  - NN + 3N TPE forces
  - $R_0 = 1.0 - 1.2$ fm
  - $R_{3N} = 1.0 - 1.2$ 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

$E/N$ [MeV] vs $R_{3N}$ [fm]

$n = 0.16$ fm$^{-3}$

$R_0 = 1.2$ fm

$N$N only

$E/N = (1 - e^{-(R_{3N}/R_{3N})^{n_1}})^{n_2}$

$n_1 = 4$, $n_2 = 1$

$n_1 = 2$, $n_2 = 2$

$n_1 = 2$, $n_2 = 4$

$n_1 = 4$, $n_2 = 2$

$n_1 = 8$, $n_2 = 1$

IT, Gandolfi, Gezerlis, Schwenk, PRC (2016)
Local NN forces in HF

- Example: two-body regulators at Hartree-Fock:
  \[ f_{\text{reg}}^{MSL} = \exp\left(-\left(\frac{q}{\Lambda}\right)^{2n}\right), \quad f_{\text{reg}}^{MSNL} = \exp\left(-2\left(\frac{p}{\Lambda}\right)^{2n}\right) \]

- After antisymmetrization we have a direct and an exchange term.

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

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

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

- Effective cutoff smaller for local regulators!
**Fits of 3N LECs**

- **Fit** $c_E$ and $c_D$ to $^4$He binding energy and n-$\alpha$ scattering

![Graphs showing fits of 3N LECs](image)

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

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

- Chiral interactions at N$^2$LO simultaneously reproduce the properties of A=3, 4, 5 systems and of neutron matter
- Commonly used phenomenological 3N interactions fail for neutron matter

Results

Comparing to \( N^3\text{LO} \) calculation:

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 \( N^2\text{LO} \) and includes also hard interactions

- Improve local chiral interactions:
  - Develop \( N^3\text{LO} \) potentials

IT, Krüger, Hebeler, Schwenk, PRL (2013)
Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, PRL (2016)
Next step: \(N^3\)LO

Improve local chiral interactions:
- Develop maximally local \(N^3\)LO potentials
- Inclusion of Delta degree of freedom

- Problem: only 8 out of 30 possible operators local

\[
V^{(4)}_{\text{cont}} = D_1 q^4 + D_2 q^4 \tau_1 \cdot \tau_2 + D_3 q^4 \sigma_1 \cdot \sigma_2 + D_4 q^4 \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2
+ D_5 k^4 + D_6 k^4 \tau_1 \cdot \tau_2 + D_7 k^4 \sigma_1 \cdot \sigma_2 + D_8 k^4 \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2
+ D_9 q^2 k^2 + D_{10} q^2 k^2 \tau_1 \cdot \tau_2 + D_{11} q^2 k^2 \sigma_1 \cdot \sigma_2 + D_{12} q^2 k^2 \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2
+ D_{13} (q \times k)^2 + D_{14} (q \times k)^2 \tau_1 \cdot \tau_2 + D_{15} (q \times k)^2 \sigma_1 \cdot \sigma_2 + D_{16} (q \times k)^2 \sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2
+ \frac{i}{2} D_{17} q^2 (\sigma_1 + \sigma_2) \cdot (q \times k) + \frac{i}{2} D_{18} q^2 (\sigma_1 + \sigma_2) \cdot (q \times k) \tau_1 \cdot \tau_2
+ \frac{i}{2} D_{19} k^2 (\sigma_1 + \sigma_2) \cdot (q \times k) + \frac{i}{2} D_{20} k^2 (\sigma_1 + \sigma_2) \cdot (q \times k) \tau_1 \cdot \tau_2
+ D_{21} q^2 \sigma_1 \cdot q \sigma_2 \cdot q + D_{22} q^2 \sigma_1 \cdot q \sigma_2 \cdot q \tau_1 \cdot \tau_2
+ D_{23} k^2 \sigma_1 \cdot q \sigma_2 \cdot q + D_{24} k^2 \sigma_1 \cdot q \sigma_2 \cdot q \tau_1 \cdot \tau_2
+ D_{25} q^2 \sigma_1 \cdot k \sigma_2 \cdot k + D_{26} q^2 \sigma_1 \cdot k \sigma_2 \cdot k \tau_1 \cdot \tau_2
+ D_{27} k^2 \sigma_1 \cdot k \sigma_2 \cdot k + D_{28} k^2 \sigma_1 \cdot k \sigma_2 \cdot k \tau_1 \cdot \tau_2
+ D_{29} ((\sigma_1 + \sigma_2) \cdot (q \times k))^2 + D_{30} ((\sigma_1 + \sigma_2) \cdot (q \times k))^2 \tau_1 \cdot \tau_2
\]

- 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:

\[ p \cot \delta_0(p) = \frac{1}{\pi L} S \left( \left( \frac{Lp}{2\pi} \right)^2 \right) \quad S(\eta) = \lim_{\Lambda \to \infty} \left( \sum_{|j|<\Lambda} \frac{1}{j^2 - \eta} - 4\pi \Lambda \right) \]

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
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

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

Constraints on symmetry energy and neutron stars:

- $S_V = 28.9 - 34.9$ MeV
- $L = 43.0 - 66.6$ MeV
- Radius for $1.4 \, M_\odot$ neutron star: $9.7 - 13.9$ km

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

Thanks to my collaborators:

- Technische Universität Darmstadt: H.-W. Hammer, K. Hebeler, P. Klos, J. Lynn, A. Schwenk
- Universität Bochum: E. Epelbaum
- Ohio State University: A. Dyhdalo, D. Furnstahl
- Los Alamos National Laboratory: J. Carlson, S. Gandolfi
- University of Guelph: A. Gezerlis
- Forschungszentrum Jülich: A. Nogga
- Institute for Nuclear Theory: M. Hoferichter

Thanks to FZ Jülich for computing time and NIC excellence project.

ありがとうございます！

Oct. 20, 2016
Ingo Tews, NPCSM workshop