#### Quantum Monte Carlo calculations of the equation of state of neutron matter with chiral EFT interactions

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## Outline



#### Motivation

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

- Systematic basis for nuclear forces, naturally includes many-body forces
- Very successful in calculations of nuclei and nuclear matter
- Quantum Monte Carlo method
  - Very precise for strongly interacting systems
  - Need of local interactions (depend only on  $r = |\mathbf{r}_i \mathbf{r}_j|$  )

Local chiral interactions Gezerlis, IT, et al., PRL & PRC (2013, 2014, 2016)

• Can be constructed up to N<sup>2</sup>LO

> Results for neutron matter, light nuclei, and n-alpha scattering

S and L constraints from lower bound of neutron matter





To obtain the equation of state we need:

- A theory for the strong interactions among nucleons
  - → Phenomenological forces or Chiral EFT
- An ab initio method to solve the many-body Schrödinger equation
  - → Many-body Pert. Theory (MBPT), Quantum Monte Carlo (QMC), Coupled Cluster, ...

#### Motivation





Good agreement with experimental constraints

#### Motivation





#### Status:

- Sizeable uncertainty for chiral EFT calculations of neutron matter
- Quantum Monte Carlo: very precise method for strongly interacting systems
- Phenomenological interactions provide a good description of light nuclei and nuclear matter, but it is not clear how to systematically improve their quality, no uncertainty estimates

#### QMC calculations with local chiral EFT interactions

# Chiral effective field theory for nuclear forces





Systematic expansion of nuclear forces in low momenta Q over breakdown scale  $\Lambda_b$ :

- Pions and nucleons as explicit degrees of freedom
- Long-range physics explicit, short-range physics expanded in general operator basis, couplings (LECs) fit to experiment

Separation of scales:

Expand in powers of  $\left(\frac{Q}{\Lambda_h}\right)^{\nu} \sim \left(\frac{1}{3}\right)^{\nu}$ 

- Power counting scheme
- Can work to desired accuracy with systematic error estimates

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

# Chiral effective field theory for nuclear forces



#### Many-body forces:

- Crucial for nuclear physics
- Natural hierarchy of nuclear forces
- Fitting: NN forces in NN system (NN phase shifts), 3N forces in 3N/4N system (Binding energies, radii)
- Consistent interactions: Same couplings for two-nucleon and manybody sector



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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

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

- $\blacktriangleright$  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:

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







Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, in preparation.







To evaluate the propagator for small timesteps  $\Delta \tau$  we need local potentials:

$$\langle r' | \hat{V} | r \rangle = \begin{cases} V(r) \, \delta(r - r'), & \text{if local} \\ V(r', r), & \text{if nonlocal} \end{cases}$$

Chiral Effective Field Theory interactions generally nonlocal:

- > Momentum transfer  $q \rightarrow p' p$
- > Momentum transfer in the exchange channel  $k = \frac{1}{2}(p + p')$
- Fourier transformation:  $q \rightarrow r, k \rightarrow$  Derivatives

Sources of nonlocalities:

Usual regulator in relative momenta

$$f(p) = e^{-(p/\Lambda)^{2n}}$$

k-dependent contact operators

Solutions:

Choose local regulators:

$$V_{\text{long}}(r) \rightarrow V_{\text{long}}(r) \left(1 - e^{-(r/R_0)^4}\right)$$
$$\delta_{R_0}(\mathbf{r}) = \alpha e^{-(r/R_0)^4}$$

Use Fierz freedom to choose local set of contact operators

## Local chiral interactions



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



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

 $\blacktriangleright$  Pion exchange local  $\rightarrow$  local regulator

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

Contact potential:

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

#### $\rightarrow$ 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)

$$\begin{split} V_{\text{cont}}^{(2)} = & \gamma_1 q^2 + \gamma_2 q^2 \, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \gamma_3 q^2 \, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ & + \gamma_4 q^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ & + \gamma_5 k^2 + \gamma_6 k^2 \, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \gamma_7 k^2 \, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ & + \gamma_8 k^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ & + \gamma_9 (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) (\mathbf{q} \times \mathbf{k}) \\ & + \gamma_{10} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) (\mathbf{q} \times \mathbf{k}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ & + \gamma_{11} (\boldsymbol{\sigma}_1 \cdot \mathbf{q}) (\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\ & + \gamma_{12} (\boldsymbol{\sigma}_1 \cdot \mathbf{q}) (\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\ & + \gamma_{13} (\boldsymbol{\sigma}_1 \cdot \mathbf{k}) (\boldsymbol{\sigma}_2 \cdot \mathbf{k}) \\ & + \gamma_{14} (\boldsymbol{\sigma}_1 \cdot \mathbf{k}) (\boldsymbol{\sigma}_2 \cdot \mathbf{k}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \,. \end{split}$$

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



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 N<sup>2</sup>LO are local
- This freedom can be used to remove all nonlocal operators up to N<sup>2</sup>LO

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

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

LECs fit to phase shifts







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

## **Benchmark of MBPT**





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

Many-body perturbation theory:

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





Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ... Inclusion of leading 3N forces:



Three topologies:

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

Only two new couplings:  $c_D$  and  $c_E$ .

Fit to uncorrelated observables:

- Probe properties of light nuclei: <sup>4</sup>He E<sub>B</sub>
- > Probe T=3/2 physics: n- $\alpha$  scattering

## QMC with chiral 3N forces





Usually Two-pion-exchange most important in PNM:  $c_1$  term: Tucson-Melbourn S-wave interaction  $c_{3,4}$  term: Fujita-Miyazawa interaction

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
  - $> R_0 = 1.0 1.2 \text{ fm}$
  - $\succ R_{3N} = 1.0 1.2 \text{ fm}$
- > 3N cutoff dependence small
- ▶ TPE 3N contributions  $\approx$  1 2 MeV at  $n_0$

smaller than for nonlocal regulators



#### Fit $c_E$ and $c_D$ to <sup>4</sup>He binding energy and n- $\alpha$ scattering



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





- Less repulsion from TPE, but additional contributions due to shorter-range 3N forces
- After inclusion of all contributions we find agreement of various approaches (different way of uncertainty estimate, see EKM, PRC 2015)





- Chiral interactions at N<sup>2</sup>LO simultaneously reproduce the properties of A ≤ 5 systems and of neutron matter (uncertainty estimate as in E. Epelbaum et al, EPJ (2015))
- Commonly used phenomenological 3N interactions fail for neutron matter Sarsa, Fantoni, Schmidt, Pederiva, PRC (2003)





Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, in preparation.

Chiral interactions at N<sup>2</sup>LO simultaneously reproduce the properties of A≤5 systems and of neutron matter (uncertainty estimate as in E. Epelbaum et al, EPJ (2015))
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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 N<sup>2</sup>LO and includes also hard interactions

Improve local chiral interactions:
 Develop N<sup>3</sup>LO potentials

## Next step: N<sup>3</sup>LO



Improve local chiral interactions:

- > Develop maximally local N<sup>3</sup>LO 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!



# **Now**: Constraints on S and L from lower bound of neutron matter energy

Kolomeitsev, Lattimer, Ohnishi, IT, arXiv:1611.07133

# S and L constraints from lower bound of neutron matter energy





#### Kolomeitsev, Lattimer, Ohnishi, IT, arXiv:1611.07133

#### Empirical observation:

Unitary gas energy seems to be lower bound to neutron-matter energy

Constraints on S and L

#### Unitary gas:

- Gas interacting via two-body interactions with infinite scattering length and vanishing effective range
- Then, system has no scale except density, and can be described by a dimensionless parameter, ξ (Bertsch parameter)
- Details of the interaction become irrelevant (universality)
- > Experiment and theory:  $\xi \approx 0.37$

#### S and L constraints from lower bound of neutron matter energy





Kolomeitsev, Lattimer, Ohnishi, IT, arXiv:1611.07133

#### **Empirical observation:**

Unitary gas energy seems to be lower bound to neutron-matter energy

Constraints on S and L

# S and L constraints from lower bound of neutron matter energy







Put constraints on symmetry energy S and its density dependence L.

 $S_0^{\text{LB}} = 28.14 \text{ MeV}$ , and  $L_0 = 25.28 \text{ MeV}$ .

## Summary



QMC calculations of neutron matter, light nuclei, and n-alpha scattering with local chiral potentials up to N<sup>2</sup>LO including NN and 3N forces can serve as nonperturbative benchmarks.

Gezerlis, IT, Epelbaum, Gandolfi, Hebeler, Nogga, Schwenk, PRL (2013) Gezerlis, IT, Epelbaum, Freunek, Gandolfi, Hebeler, Nogga, Schwenk, PRC (2014) IT, Gandolfi, Gezerlis, Schwenk, PRC (2016) Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, PRL (2016)

- ➤ Chiral interactions at N<sup>2</sup>LO simultaneously reproduce the properties of A≤5 systems and of neutron matter, commonly used phenomenological 3N interactions fail.
- Further improvements will allow to determine neutron-matter EOS with improved uncertainties (factor of 2).
- Constraints on symmetry energy and its slope parameter from lower bound of neutron-matter energy.

Kolomeitsev, Lattimer, Ohnishi, IT, arXiv:1611.07133



## Thanks

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## Thank you for your attention.