## Update on QMC calculations with local chiral interactions



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## Outline



- Quantum Monte Carlo method
  - Very precise for strongly interacting systems
  - Need of local interactions (depend only on relative distance r)
- Local chiral interactions
  - Can be constructed up to N<sup>2</sup>LO
- > Artifacts for local regulators: Ambiguity for NN and 3N contact interactions
- > Results for nuclei with A $\leq$ 16
  - Excellent description of binding energies and charge radii

Summary

## Quantum Monte Carlo method



Cast many-body Schrödinger equation as diffusion equation:

$$\lim_{\tau \to \infty} e^{-H\tau} |\Psi_T\rangle \to |\Psi_0\rangle$$
$$\psi(R,\tau) = \int dR'^{3N} \langle R|e^{-(T+V)\tau}|R'\rangle \psi(R',0)$$

Basic steps:

- ➤ Choose trial wavefunction which overlaps with the ground state  $|\psi(R,0)\rangle = |\psi_T(R,0)\rangle = \sum_i c_i |\phi_i\rangle \rightarrow \sum_i c_i e^{-(E_i - E_0)\tau} |\phi_i\rangle$
- $\succ$  Evaluate propagator for small timestep  $\Delta \tau$ , in practice only for local potentials
- Make consecutive small time steps using Monte Carlo techniques to project out ground state

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

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





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:

> Make consecutive small timesteps,  $\tau = 1.4 \left(\frac{1}{E_{sep}}\right)$ Animation by Joel Lynn, TU Darmstadt



## Quantum Monte Carlo method





## Quantum Monte Carlo method





- Very precise method for strongly interacting systems.
- > With transient estimates, stochastically exact.
- > Needs as input local interactions but chiral EFT generally nonlocal!





Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Machleidt, Meißner, Hammer ... Can be constructed 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)

- Two-body LECs fit to phase shifts
- Include leading 3N forces:



#### **3N LECS** fit to uncorrelated observables:

- > Probe properties of light nuclei:  ${}^{4}$ He E<sub>B</sub>
- > Probe spin-orbit splitting:  $n-\alpha$  scattering



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

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

Chiral Effective Field Theory interactions generally nonlocal:

- ightarrow Momentum transfer  $\mathbf{q}=\mathbf{p}'-\mathbf{p}$
- > Momentum transfer in the exchange channel  $\mathbf{k} = \frac{1}{2}(\mathbf{p} + \mathbf{p}')$
- hicksim Fourier transformation:  ${f q} o {f r}, \, {f k} o 
  abla_{f r}$

#### Solutions:

Choose local regulators:

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

Use Fierz freedom to choose local set of contact operators.

Sources of nonlocalities:

Usual regulator in rel. momenta

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

k-dependent contact operators







# $\begin{array}{l} \blacktriangleright \quad \mbox{Pion exchanges local} \\ V_{\rm long}(r) = V_C(r) + W_C(r) \ \tau_1 \cdot \tau_2 \\ + \left( V_S(r) + W_S(r) \ \tau_1 \cdot \tau_2 \right) \ \sigma_1 \cdot \sigma_2 \\ + \left( V_T(r) + W_T(r) \ \tau_1 \cdot \tau_2 \right) S_{12} \end{array}$

#### $\rightarrow$ local regulator

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

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)  

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

$$\delta(\mathbf{r}) \rightarrow \delta_{R_0}(\mathbf{r}) = \alpha e^{-(r/R_0)^4}$$



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





 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 ...





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



> Contact potential at LO:

$$V_{\rm cont}^{(0)} = C_1 \mathbf{1} + C_{\sigma} \sigma_{12} + C_{\tau} \tau_{12} + C_{\sigma\tau} \sigma_{12} \tau_{12}$$

Construct antisymmetrized potential:

$$V_{\rm as}(\mathbf{q}, \mathbf{k}) = \frac{1}{2} \left( V(\mathbf{q}, \mathbf{k}) - \mathcal{A}[V(\mathbf{q}, \mathbf{k})] \right)$$
$$\mathcal{A}[V(\mathbf{q}, \mathbf{k})] = \frac{1}{4} (1 + \sigma_{12})(1 + \tau_{12})V\left(\mathbf{q} \rightarrow -2\mathbf{k}, \mathbf{k} \rightarrow -\frac{1}{2}\mathbf{q}\right)$$

$$V_{\text{cont,as}}^{(0)} = \frac{1}{2} \left( 1 - \frac{1}{4} (1 + \sigma_{12}) (1 + \tau_{12}) \right) V_{\text{cont}}^{(0)}$$
$$= \tilde{C}_{S} + \tilde{C}_{T} \sigma_{12} + \left( -\frac{2}{3} \tilde{C}_{S} - \tilde{C}_{T} \right) \tau_{12} + \left( -\frac{1}{3} \tilde{C}_{S} \right) \sigma_{12} \tau_{12}$$

Only two linearly independent contact interactions!



True, only when regulator f behaves like

$$f(\mathbf{q}, \mathbf{k}) = f\left(-2\mathbf{k}, -\frac{1}{2}\mathbf{q}\right)$$

but not for local regulator  $f(\mathbf{q})$ :

$$V_{\text{cont,as}}^{(0,\text{loc})} = \tilde{C}_{S} + \tilde{C}_{T}\sigma_{12} + \left(-\frac{2}{3}\tilde{C}_{S} - \tilde{C}_{T}\right)\tau_{12} + \left(-\frac{1}{3}\tilde{C}_{S}\right)\sigma_{12}\tau_{12} + V_{\text{corr}}^{f}(\mathbf{p}\cdot\mathbf{p}')$$

Manifestation of the fact that introducing a regulator function affects potential terms beyond the order at which one is working, and should be corrected at higher order.

#### But:

Violation of Fierz ambiguity can lead to sizable contributions in 3N sector. Lynn, IT, et al., PRL (2016), Dyhdalo, Hebeler, Furnstahl, IT, PRC (2016)

Leads to mixing of different partial waves.





Violation of Fierz ambiguity sizable in the NN sector at LO but restored to a large extent by including subleading operators at NLO.

> In 3N sector, subleading corrections only at N<sup>4</sup>LO.



Cutoff  $R_0 = 1.0$  fm: Huth, IT, et al., PRC (2017)



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 Gezerlis, IT, Epelbaum, Gandolfi, Hebeler, Nogga, Schwenk, PRL (2013)
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## QMC with chiral 3N forces





 $c_1, c_3, c_4$ 



Two-pion-exchange:

- c<sub>1</sub> term: Tucson-Melbourn S-wave interaction
- c<sub>3,4</sub> term: Fujita-Miyazawa interaction

Usually only contribution to pure neutron matter.

> Usually  $V_D$  and  $V_E$  vanish in T=3/2 or S=3/2 systems:

- V<sub>D</sub> due to spin-isospin structure
- V<sub>E</sub> 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!

local 3N, see also Navratil, Few Body Syst. (2007)

## QMC with chiral 3N forces





 $\blacktriangleright$  For local regulator also V<sub>E</sub> contributes to neutron matter:

$$V_E \sim c_E \sum_{i < j < k} \sum_{\text{cyc}} \mathcal{O}_{ijk} \,\delta_{R_{3N}}(r_{ij}) \,\delta_{R_{3N}}(r_{kj})$$

Fierz ambiguity:

$$\mathcal{D}_{ijk} = \{\mathbb{1}, \, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \ \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k, \, [(\boldsymbol{\sigma}_i imes \boldsymbol{\sigma}_j) \cdot \boldsymbol{\sigma}_k] [(\boldsymbol{\tau}_i imes \boldsymbol{\tau}_j) \cdot \boldsymbol{\tau}_k] \}.$$

Epelbaum, Nogga, Gloeckle, Kamada, Meißner, Witala, PRC (2002)

No Fierz rearrangement freedom for local regulators, choose different short-range structures to estimate the impact:

$$V_{E\tau} \sim \tau_i \cdot \tau_j$$
$$V_{E\mathbb{1}} \sim \mathbb{1}$$
$$V_{E\mathcal{P}} \sim \mathcal{P}_{S=1/2, T=1/2}$$



Fit  $c_E$  and  $c_D$  to <sup>4</sup>He binding energy and  $n-\alpha$  scattering (A $\leq$ 5)



Lynn, IT, et al., PRL (2016)





- ➤ 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)

### Results





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Results for AFDMC calculations of heavier systems ( $R_0 = 1.0$  fm):

(Using the same local chiral interactions)





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Results for AFDMC calculations of heavier systems ( $R_0 = 1.2$  fm):

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Results for AFDMC calculations of heavier systems ( $R_0 = 1.2$  fm):

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## 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.
- QMC methods offer access to harder chiral interactions.
- ➤ Chiral interactions a t N<sup>2</sup>LO simultaneously reproduce the properties of A≤ 16 systems and of neutron matter, commonly used phenomenological 3N interactions fail. Extension to heavier, neutron-rich systems possible.
- Important regulator effects for local interactions.
- Further improvements necessary to reduce uncertainties.





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