Quantum Monte Carlo calculations of neutron matter with local chiral three-body forces

Ingo Tews,
In collaboration with A. Dyhdalo, D. Furnstahl, S. Gandolfi, A. Gezerlis, K. Hebeler, J. Lynn, A. Schwenk,…

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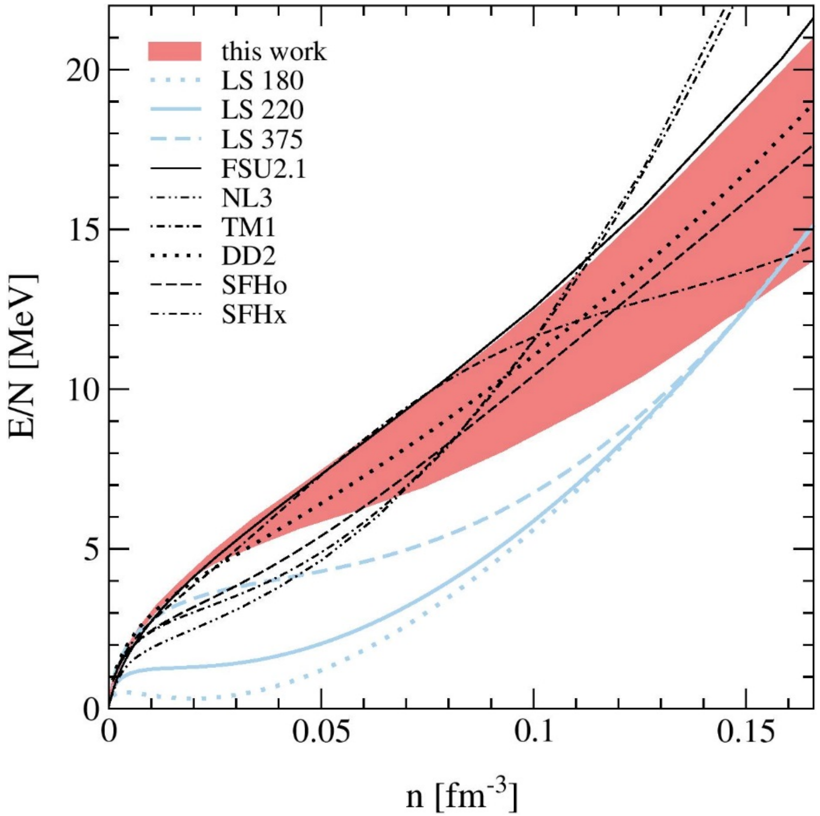
Motivation

Complete N³LO neutron matter calculation in many-body perturbation theory

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



Krüger, IT Hebeler, Schwenk, PRC (2013)

Here:

- Nonlocal regulators

Band includes:

- NN cutoff variation
- 3N cutoff variation
- Uncertainties in the c_i couplings
- Many-body uncertainty → Minimize

Motivation

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Quantum Chromodynamics

Nuclear Forces	Phenomenological forces: local	Chiral effective field theory: systematic, improveable, nonlocal
Many-body methods	Quantum Monte Carlo: reliable, need local interactions	e.g. many-body perturbation theory: only soft potentials

Status:

- Sizeable uncertainty for chiral EFT calculations of neutron matter

Motivation

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Quantum Chromodynamics

Nuclear Forces

Chiral effective field theory:
systematic, improveable,
nonlocal

Many-body methods

Quantum Monte Carlo:
reliable,
need local interactions

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

We want to:
- Combine Quantum Monte Carlo method with chiral EFT interactions
- Minimize many-body uncertainty

Motivation

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Quantum Chromodynamics

Chiral effective field theory:
systematic, improveable,
nonlocal

Nuclear Forces

Many-body methods

Quantum Monte Carlo:
reliable,
need local interactions

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

Status:
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We want to:
- Combine Quantum Monte Carlo method with chiral EFT interactions
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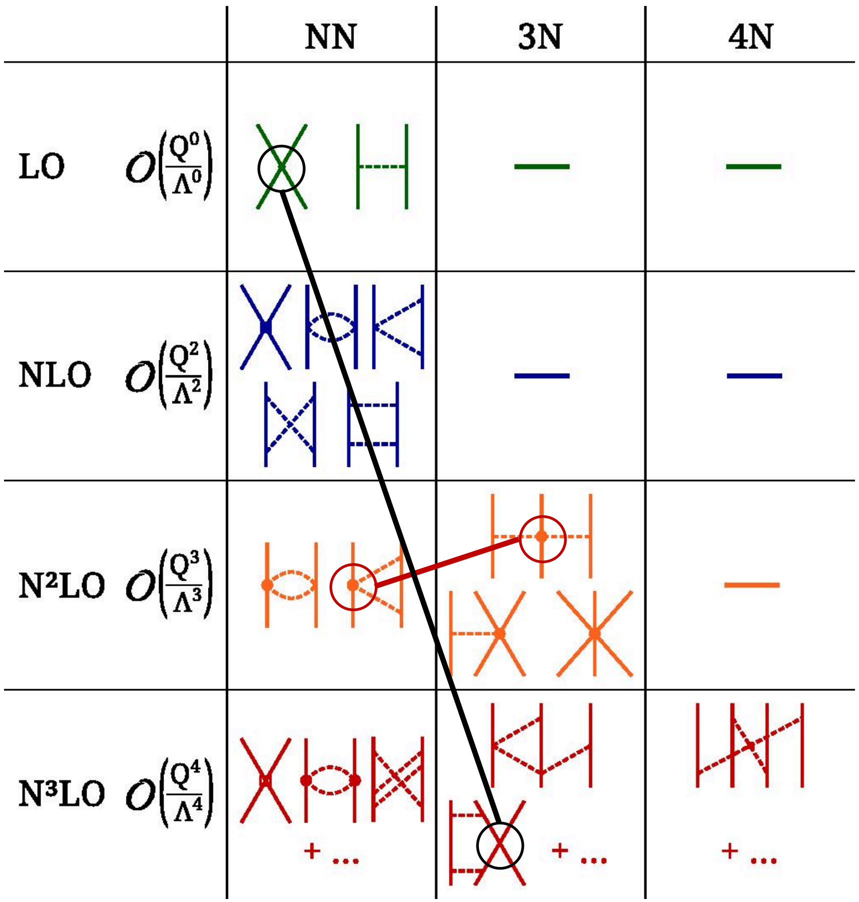
Chiral effective field theory for nuclear forces



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

Separation of scales:

- Low momenta $Q \ll$ breakdown scale Λ_b
- Expansion parameter $\left(\frac{Q}{\Lambda_b}\right)^{\nu} \sim 1/3$

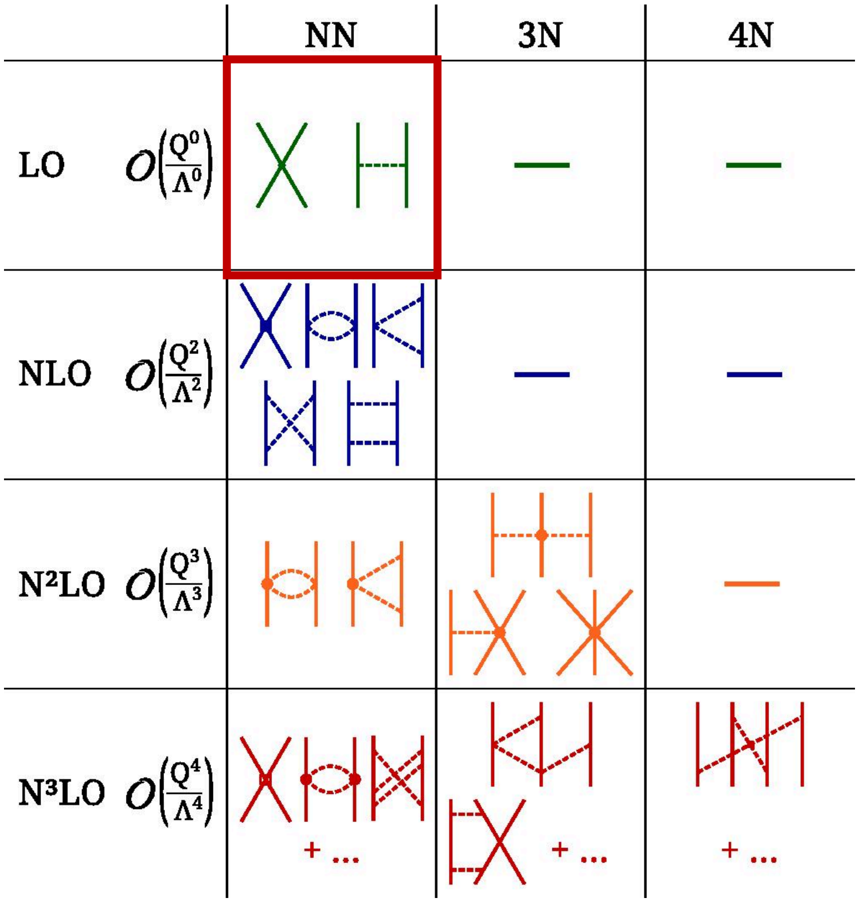
Explicit degrees of freedom:

- Pions and nucleons
- Long-range physics explicit, short-range physics expanded in general operator basis
- Couplings fit to data

Systematic:

- Can work to desired accuracy
- Obtain error estimates
- Consistent many-body interactions

Local chiral interactions



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

Example:

- Leading order $V^{(0)} = V^{(0)}_{\text{cont}} + V^{\text{OPE}}$
- Pion exchanges local → local regulator:

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

- Contact potential:

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

→ Only two independent (Pauli principle)

$$V^{(0)}_{\text{cont}} = C_S + C_T\, \sigma_1 \cdot \sigma_2$$

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

- This freedom can be used to remove all nonlocal operators up to N²LO

QMC results for NN forces

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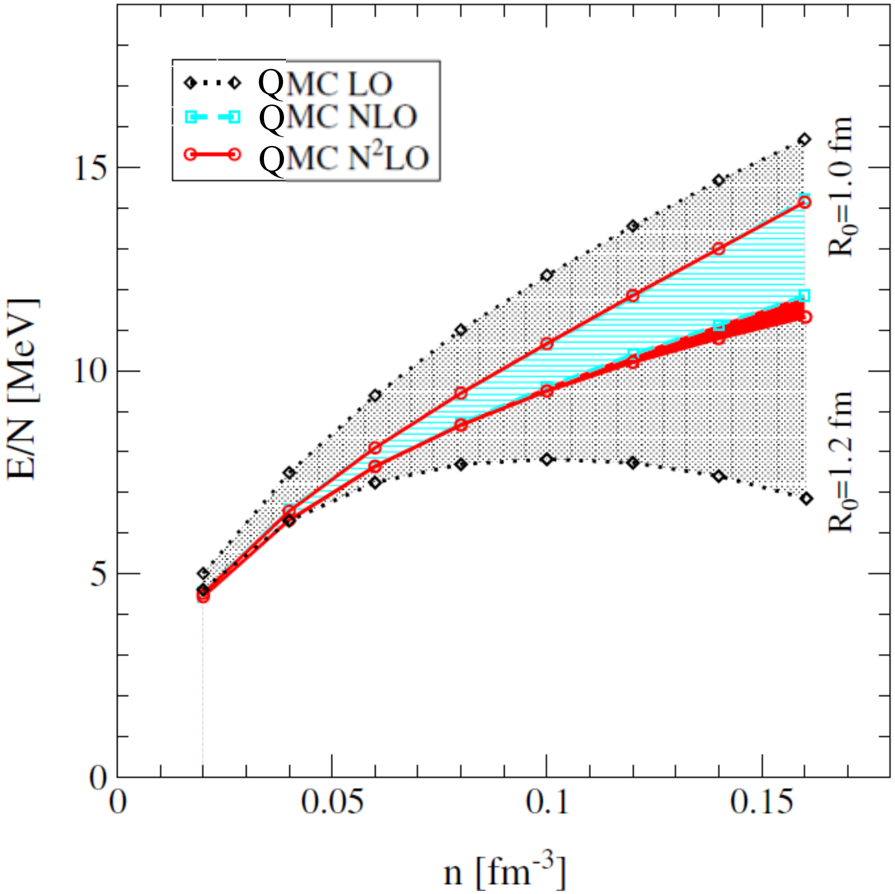
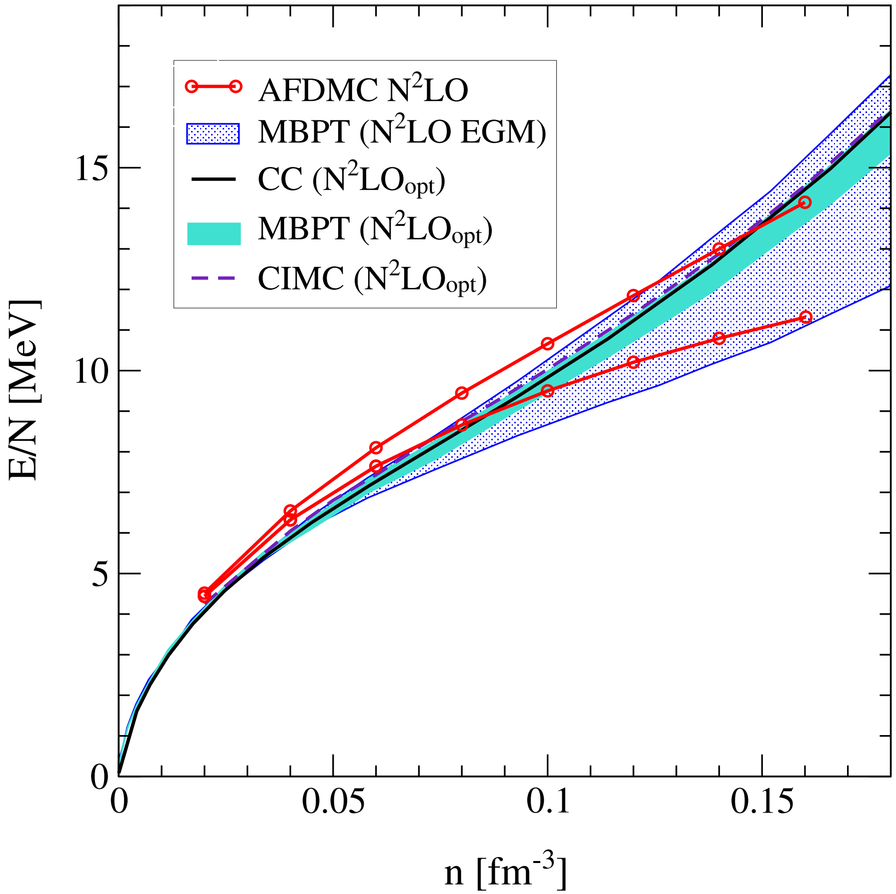


Gezerlis, IT, Epelbaum, Freunek, Gandolfi, Hebeler, Nogga, Schwenk, PRL (2013) and PRC (2014)

NN-only calculation:

- Statistical uncertainty of points negligible
- Bands include NN cutoff variation $R_0 = 1.0 - 1.2$ fm
- Order-by-order convergence up to saturation density

QMC results for NN forces



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

NN-only calculation

- Good agreement with other approaches:

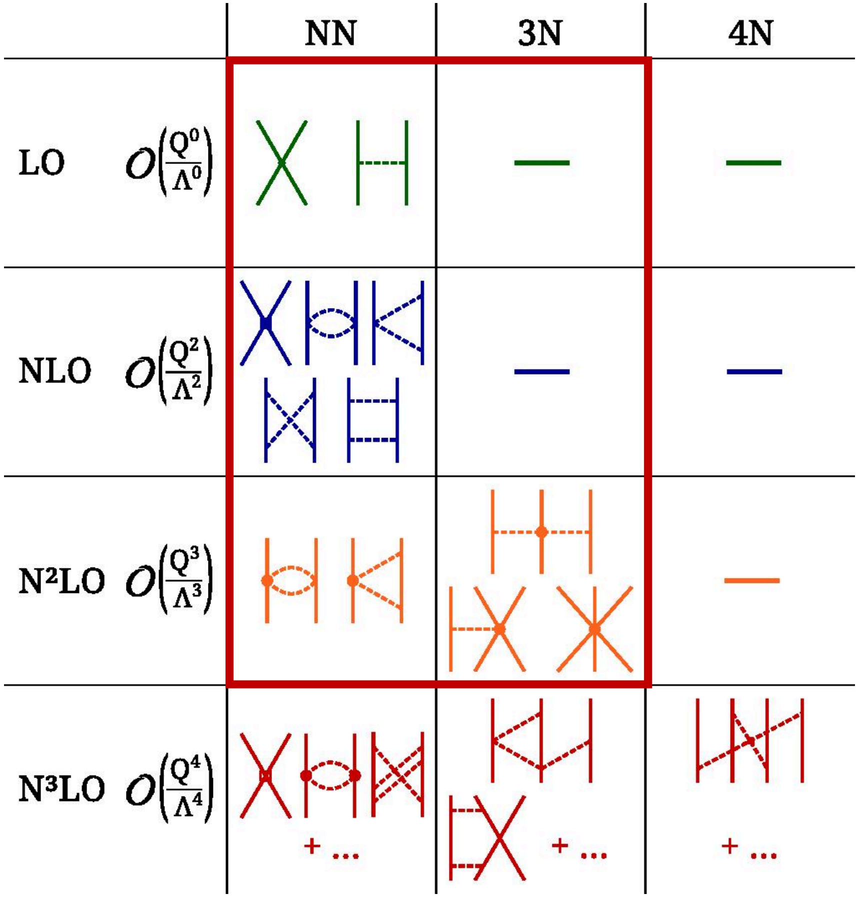
MBPT with N^2LO EGM
IT, Krüger, Hebeler, Schwenk, PRL (2013)

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

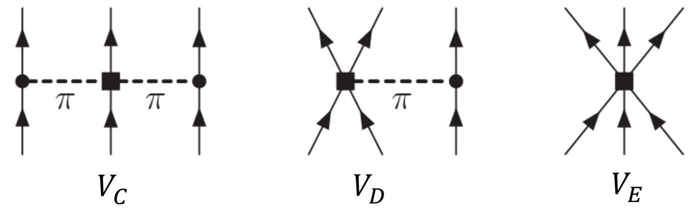
MBPT with N^2LO_{opt}
IT, Krüger, Gezerlis, Hebeler, Schwenk, NTSE (2013)

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

QMC with chiral 3N forces



Next: inclusion of leading 3N forces



Three topologies:

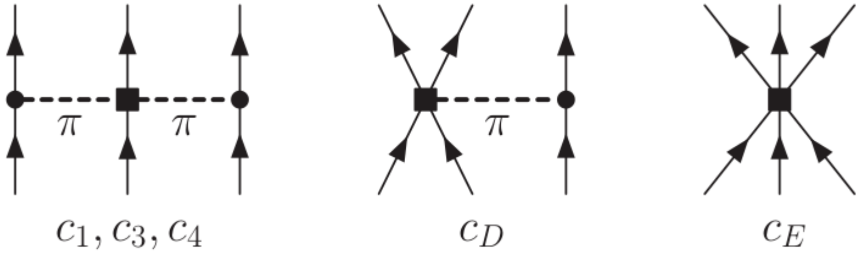
- Two-pion exchange V_C
- One-pion-exchange contact V_D
- Three-nucleon contact V_E

Only two new couplings: c_D and c_E

→ see talk by Joel Lynn

Two-pion-exchange most important in PNM:
usually V_D and V_E vanish in neutron matter
(only for regulator symmetric in particle labels)

QMC with chiral 3N forces



For local regulator all three topologies contribute to neutron matter:

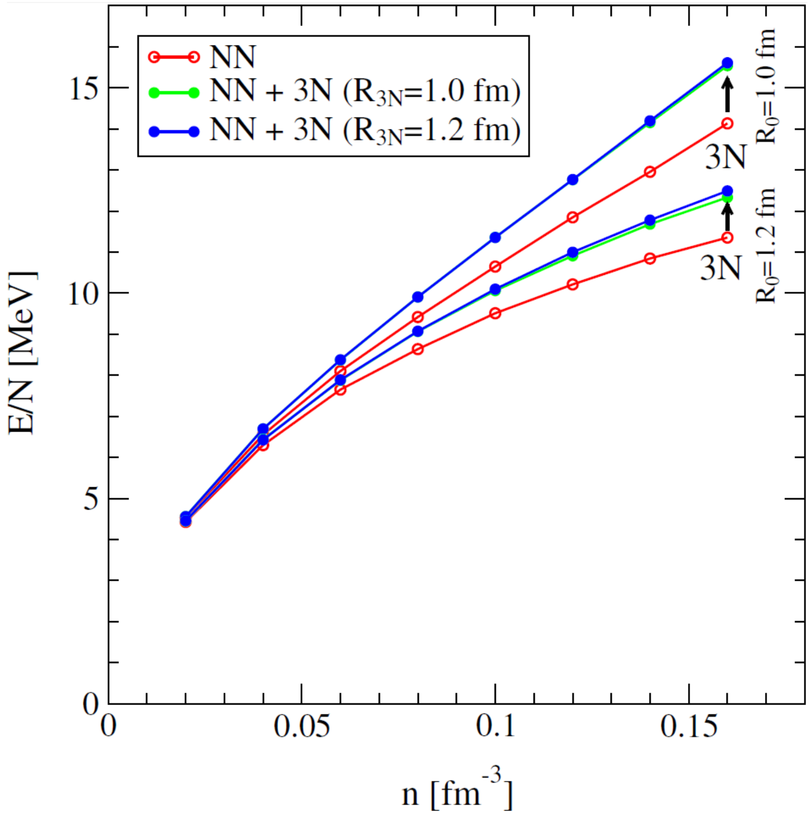
$$V_E \to \frac{c_E}{2\, f_\pi^4\, \Lambda_\chi} \sum_{\pi\{i,j,k\}} \delta_{\mathrm{r}}(r_{ij})\, \delta_{\mathrm{r}}(r_{jk})$$

$$V_D \sim c_D \sum_{\pi\{i,j,k\}} \left[\frac{m_\pi^2}{4\pi} \sum_{\pi\{i,j,k\}} \delta_{\mathrm{r}}(r_{ij})\, X_{ik}(r_{jk}) - \sigma_i \cdot \sigma_k \delta_{\mathrm{r}}(r_{ij}) \delta_{\mathrm{r}}(r_{jk}) \right]$$

$$V_C \sim c_3 \sum_{\pi\{i,j,k\}} \left[X_{ij}(r_{ij}) X_{jk}(r_{jk}) + \frac{4\pi}{m_\pi^2} X_{ik}(r_{ij}) \delta_{\mathrm{r}}(r_{jk}) + \frac{4\pi}{m_\pi^2} X_{ik}(r_{jk}) \delta_{\mathrm{r}}(r_{ij}) + \left(\frac{4\pi}{m_\pi^2}\right)^2 \sigma_i \cdot \sigma_k \delta_{\mathrm{r}}(r_{ij}) \delta_{\mathrm{r}}(r_{jk}) \right] + V(c_1)$$

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

QMC results with 3N TPE

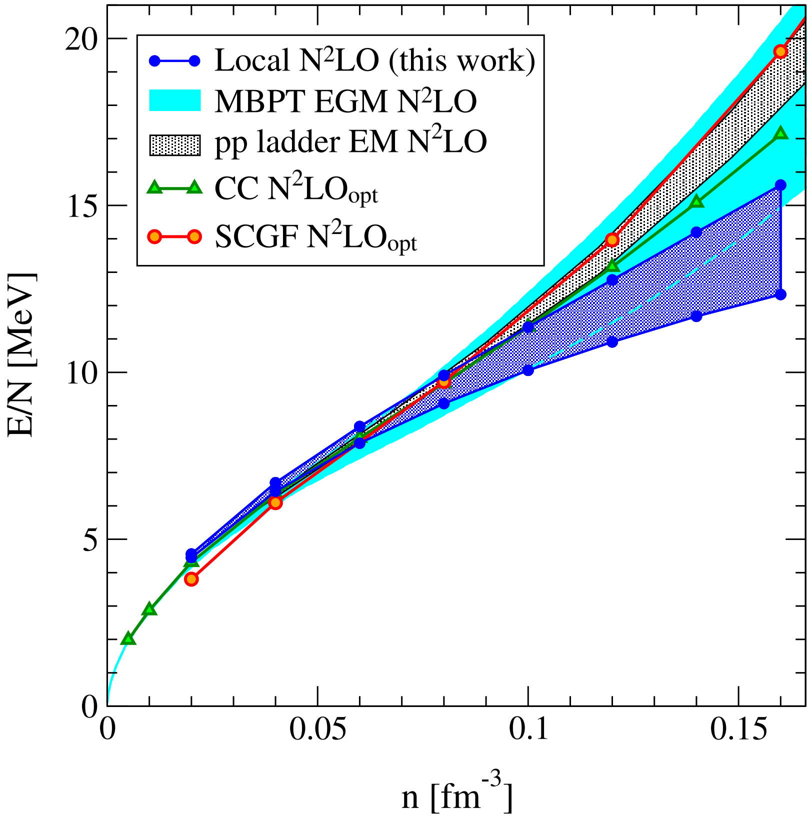


IT, Gandolfi, Gezerlis, Schwenk, PRC (2016)

- Only three-nucleon two-pion exchange $\sim c_1$ and c_3
- Auxiliary-field diffusion Monte Carlo:
  - NN + 3N forces
  - $R_0 = 1.0 - 1.2$ fm
  - $R_{3N} = 1.0 - 1.2$ fm
- TPE 3N contributions ≈ 1 – 2 MeV, smaller than for nonlocal regulators
- 3N cutoff dependence small
- Variation with $c_1 = -(0.37 - 0.81)$ and $c_3 = -(2.71 - 3.40)$ smaller 0.3 MeV

Krüger, IT Hebeler, Schwenk, PRC (2013)

QMC results with 3N TPE



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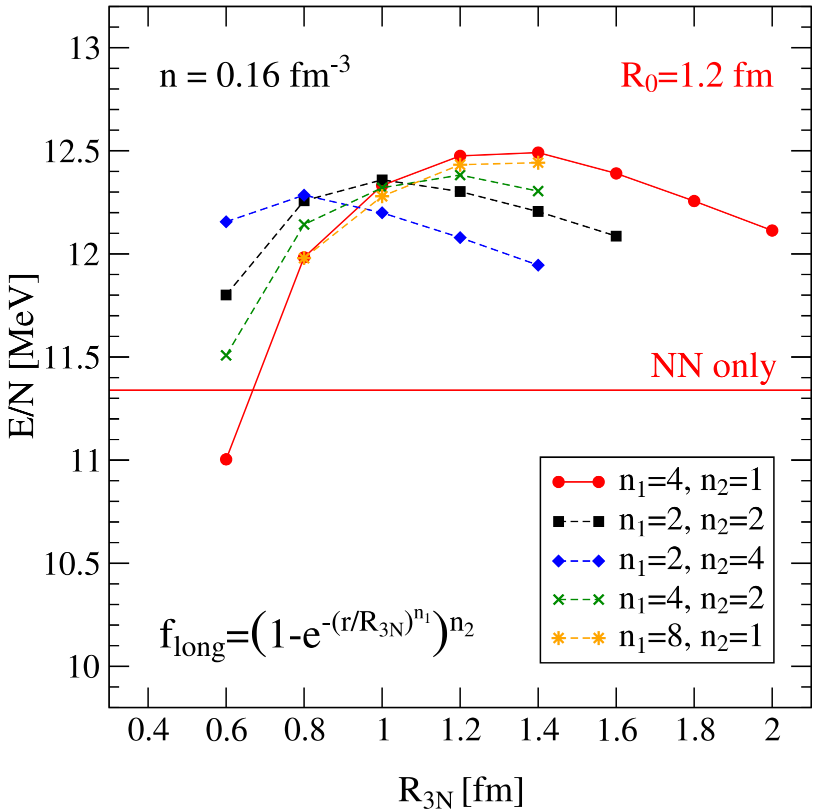

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  Krüger, IT Hebeler, Schwenk, PRC (2013)
- Independent of exact regulator form

Local 3N forces in HF

- In the following study 3N forces in Hartree-Fock
- Use the following regulators:

$$f_{\rm reg}^{QMC} = \left(1 - \exp\left(-\frac{r_{ij}^4}{R_0^4}\right)\right)\left(1 - \exp\left(-\frac{r_{jk}^4}{R_0^4}\right)\right)$$

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

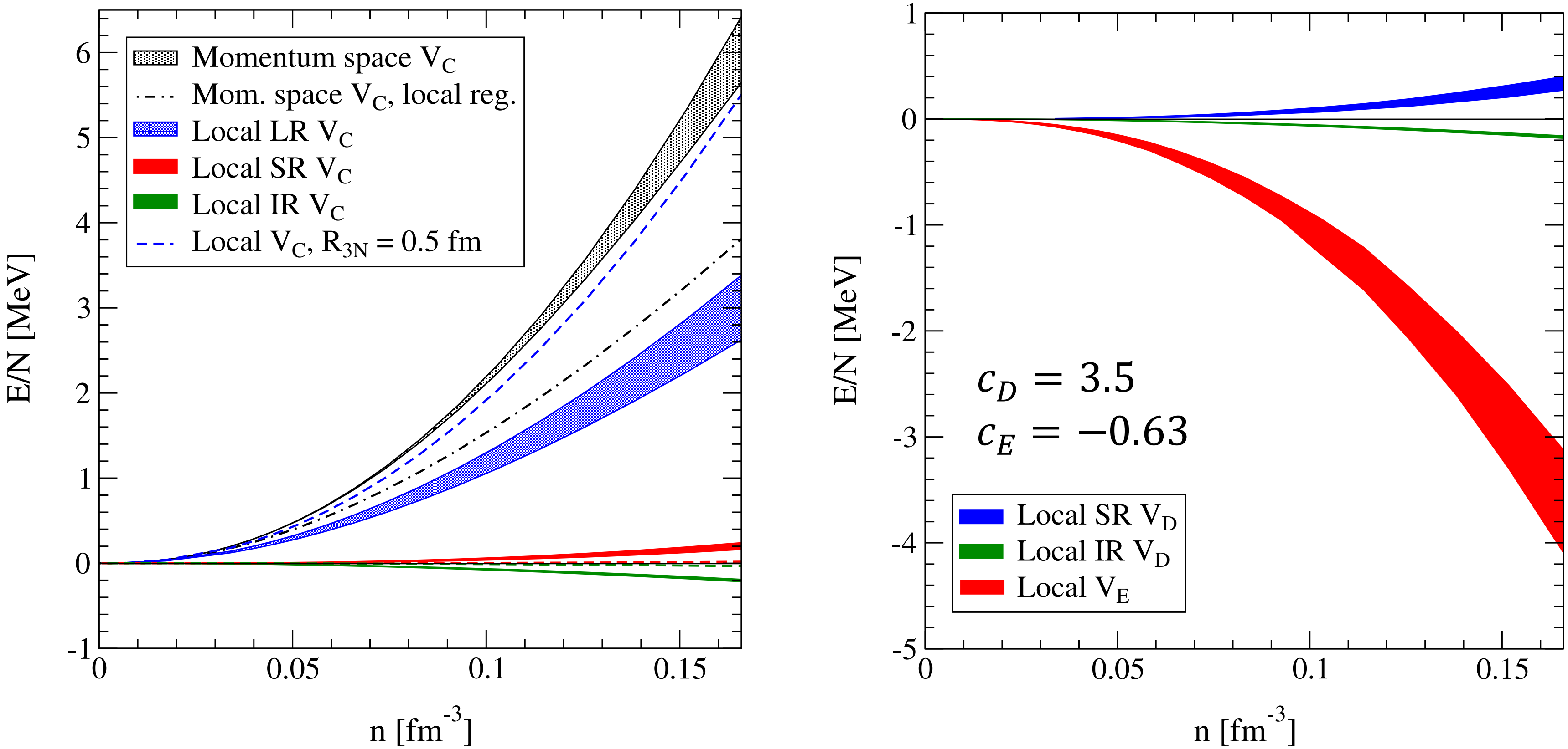
$$f_{\rm reg}^{MSL} = \exp\left(-\left(\frac{q_i}{\Lambda}\right)^{2n}\right)\exp\left(-\left(\frac{q_j}{\Lambda}\right)^{2n}\right)$$

Navratil, Few Body Syst. (2007)

$$f_{\rm reg}^{MSNL} = \exp\left(-\left(\frac{k_1^2 + k_2^2 + k_3^2 - \mathbf{k}_1 \cdot \mathbf{k}_2 - \mathbf{k}_1 \cdot \mathbf{k}_3 - \mathbf{k}_2 \cdot \mathbf{k}_3}{3\Lambda^2}\right)^{2n}\right)$$

U. van Kolck, PRC (1994), Epelbaum, Nogga, Glöckle, Kamada, Meißner, Witala, PRC (2002)

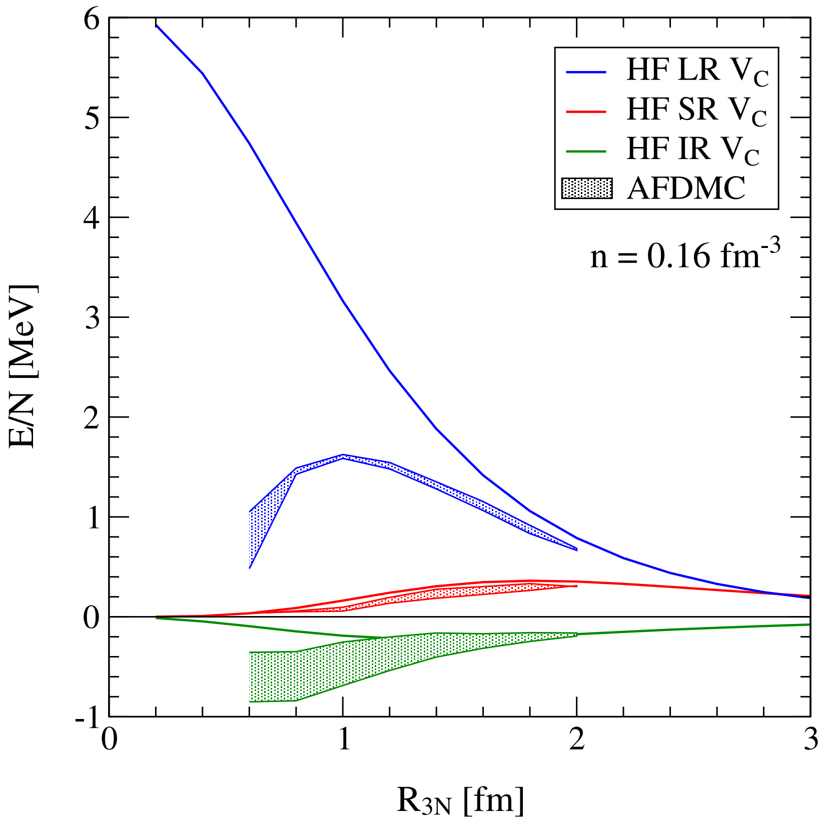
Local 3N forces in HF

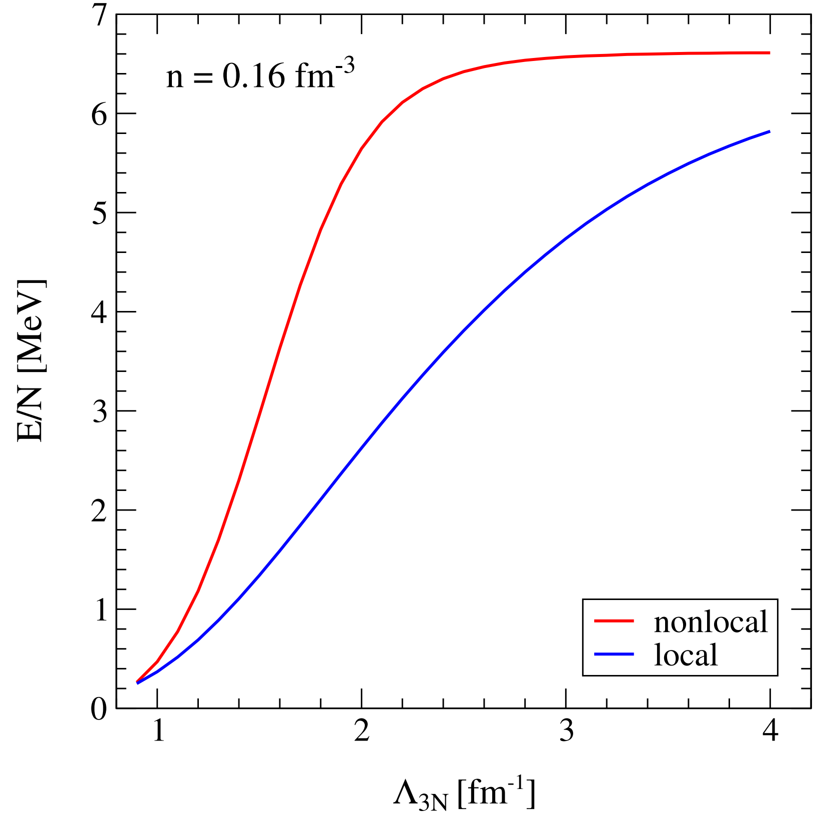


IT, Gandolfi, Gezerlis, Schwenk, PRC (2016)

- Local 3N TPE energies smaller than for nonlocal regulators already at HF level
- Also true for local momentum-space regulators
- Shorter-range parts can add sizeable contributions

Local 3N forces in HF





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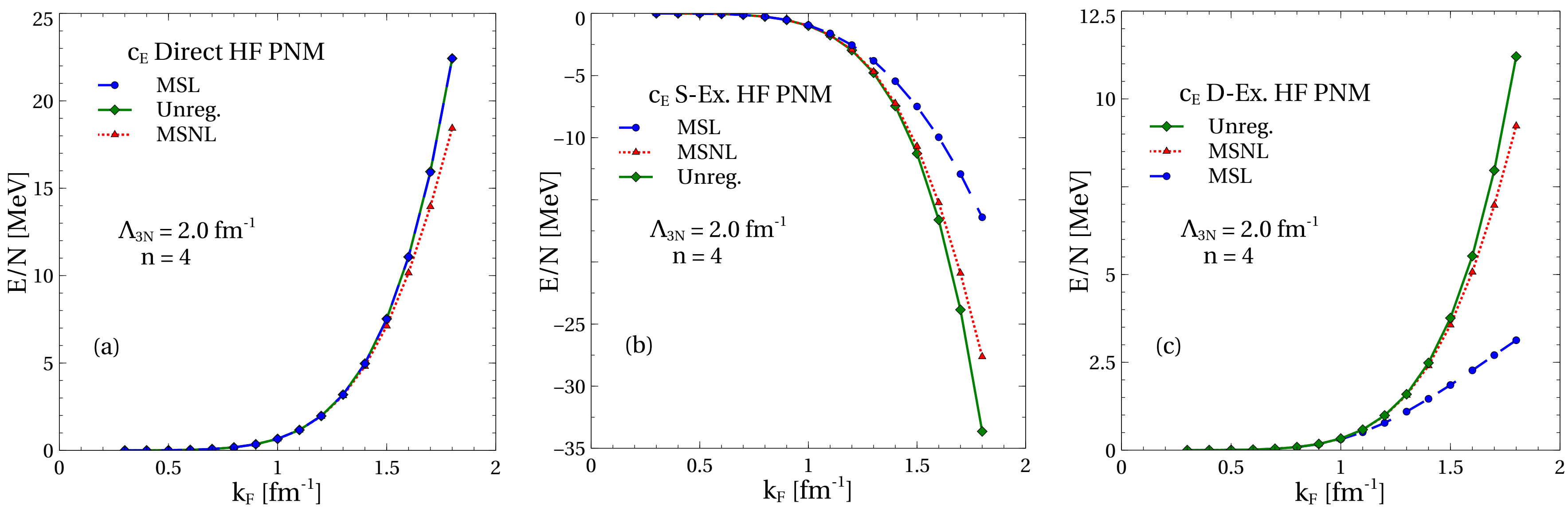
Local 3N forces in HF

Two problems:

1) Shorter-range parts can add sizeable contributions at HF
2) Local 3N TPE energies smaller than for nonlocal regulators

Focus on V_E: $$\mathcal{A}_{123} V_E = (1 - P_{12} - P_{23} - P_{13} + P_{12}P_{13} + P_{12}P_{23}) V_E = 0$$



With regulator: $\mathcal{A}_{123} V_{E,\mathrm{reg}}^{MSNL} = 0$ $\quad$ $\mathcal{A}_{123} V_{E,\mathrm{reg}}^{MSL} \neq 0$

Dyhdalo, Furnstahl, Hebeler, IT, in preparation

Local 3N forces in HF

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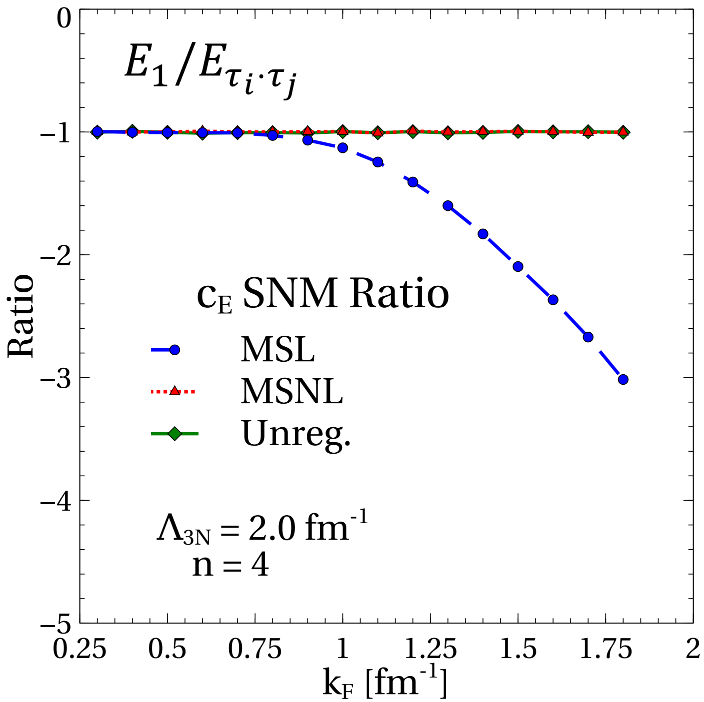

Dyhdalo, Furnstahl, Hebeler, IT, in preparation

- 6 different operator structures for V_E:

$$\beta_1 \cdot 1 + \beta_2 \sigma_i \cdot \sigma_j + \beta_3 \tau_i \cdot \tau_j + \beta_4 \sigma_i \cdot \sigma_j\, \tau_i \cdot \tau_j + \beta_5\, \sigma_i \cdot \sigma_j\, \tau_j \cdot \tau_k + \beta_6\, \sigma_i \times \sigma_j \cdot \sigma_k\, \tau_i \times \tau_j \cdot \tau_k$$

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

- Linearly dependent after antisymmetrization if regulator is symmetric in particle labels
- Not true for local regulators
  → see talk by Joel Lynn

Local 3N forces in HF

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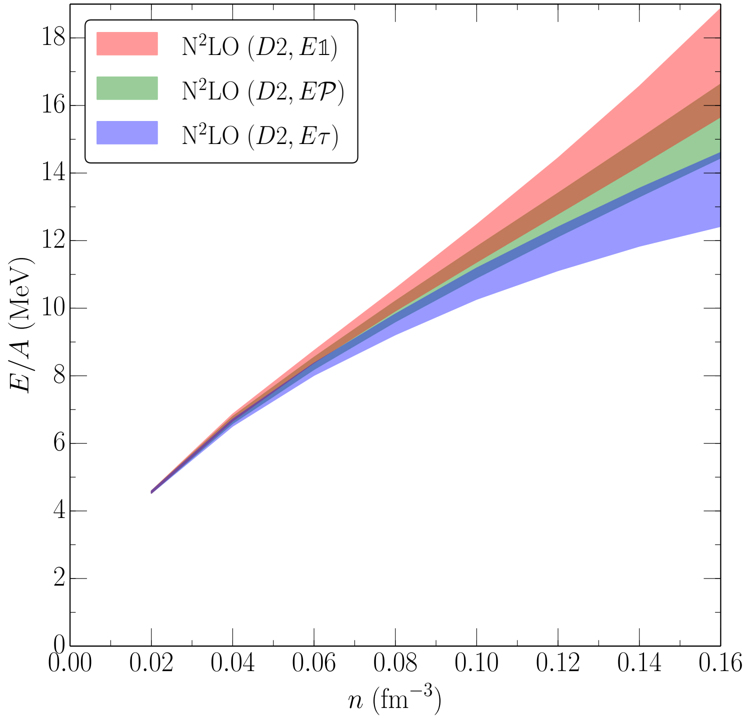

Lynn, IT, Carlson, Gandolfi, Gezerlis, Schmidt, Schwenk, PRL (2016)

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Local NN forces in HF

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Two problems:

1) Shorter-range parts can add sizeable contributions at HF
2) Local 3N TPE energies smaller than for nonlocal regulators

- Example: two-body regulators at HF:

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

Direct term:

$$q = k - k' = 0 \quad \rightarrow \quad f_{\text{reg}}^{MSL} = 1, \qquad f_{\text{reg}}^{MSNL} = \exp\left(-2\left(\frac{k}{\Lambda}\right)^{2n}\right)$$

Exchange term:

$$q = k - k' = 2k \quad \rightarrow \quad f_{\text{reg}}^{MSL} = \exp\left(-\left(\frac{2k}{\Lambda}\right)^{2n}\right), f_{\text{reg}}^{MSNL} = \exp\left(-2\left(\frac{k}{\Lambda}\right)^{2n}\right)$$

Effective cutoff smaller for local regulators and spin-dependent interactions!

Local NN forces in HF

Two problems:

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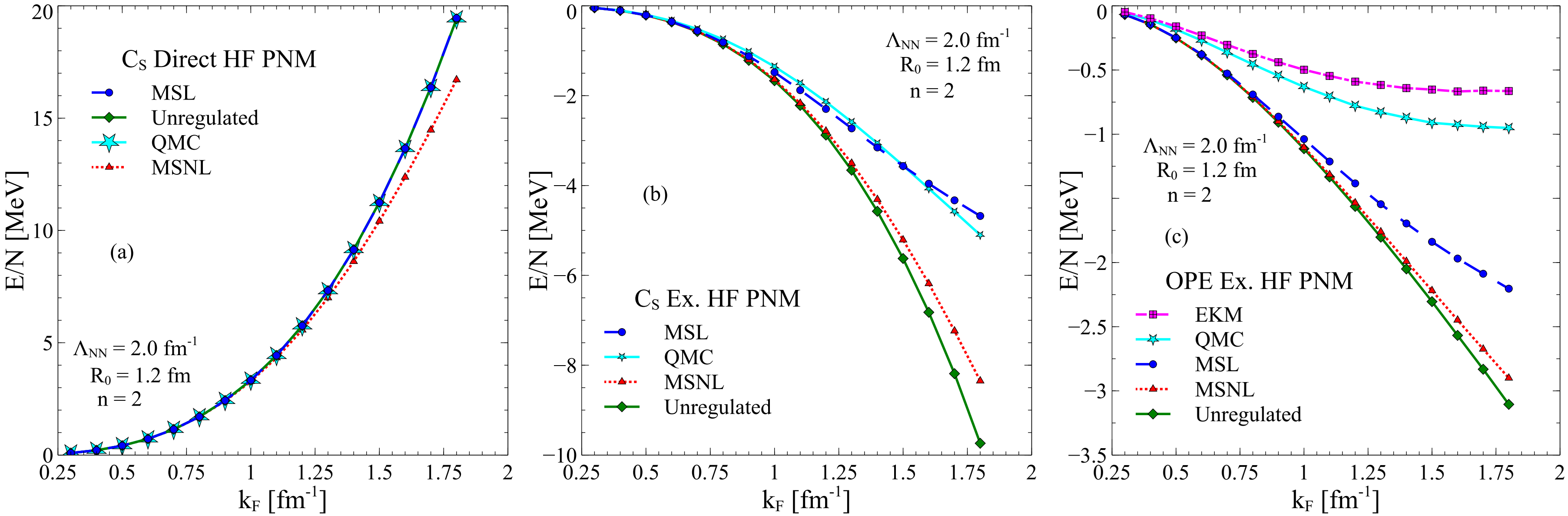
2) Local 3N TPE energies smaller than for nonlocal regulators

➢ Example: two-body regulators at HF:



Dyhdalo, Furnstahl, Hebeler, IT, in preparation

Local NN forces in HF

Two problems:

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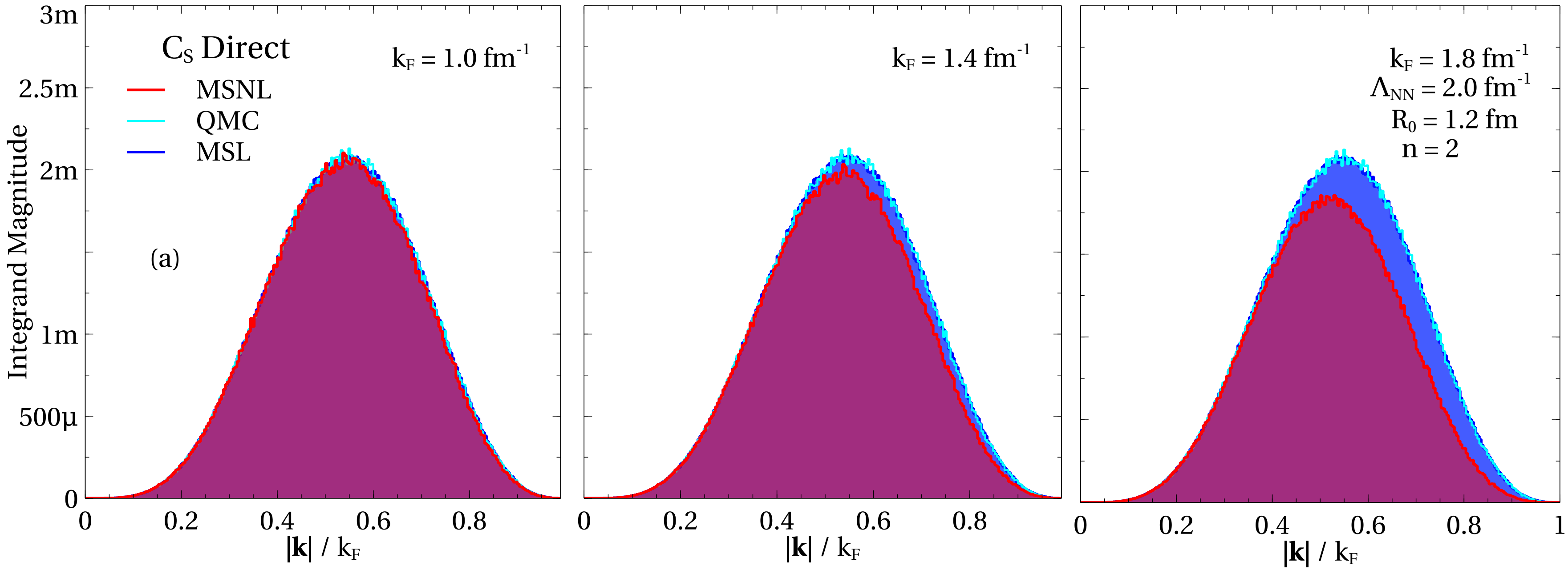
- Example: two-body regulators at HF:

  Interaction phase space for C_S direct term



Dyhdalo, Furnstahl, Hebeler, IT, in preparation

Local NN forces in HF

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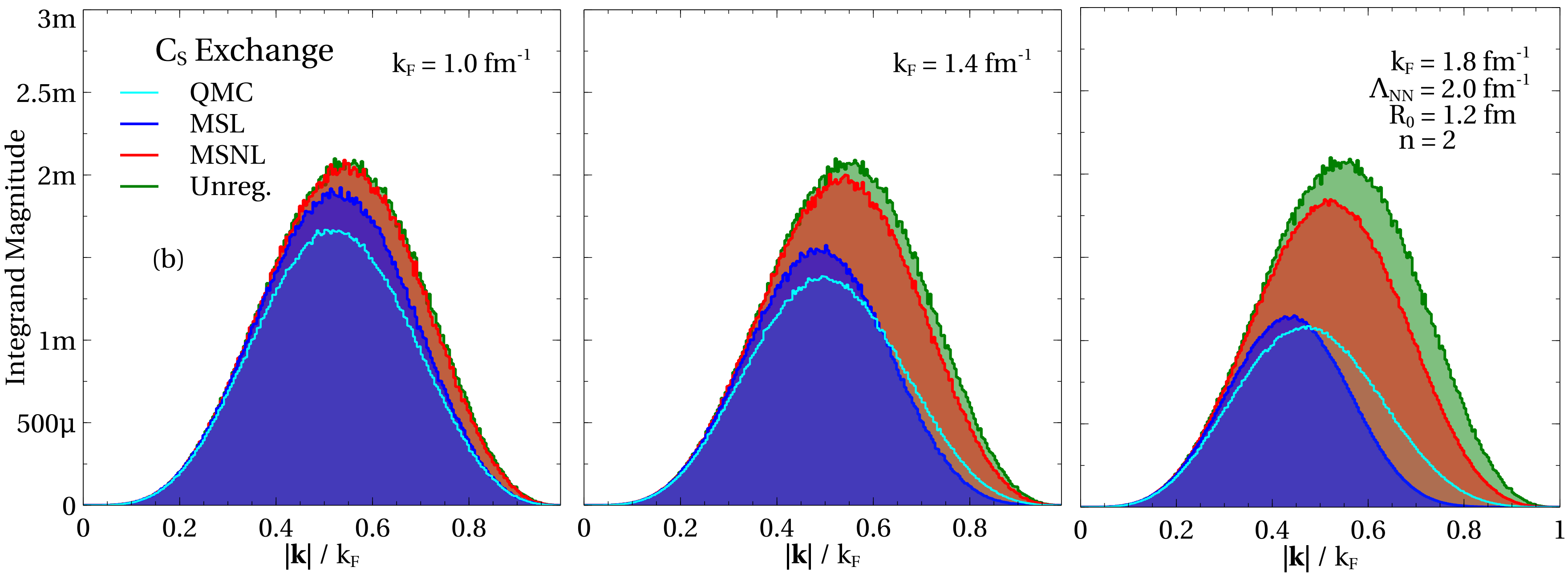

Dyhdalo, Furnstahl, Hebeler, IT, in preparation

Local NN forces in HF

Two problems:

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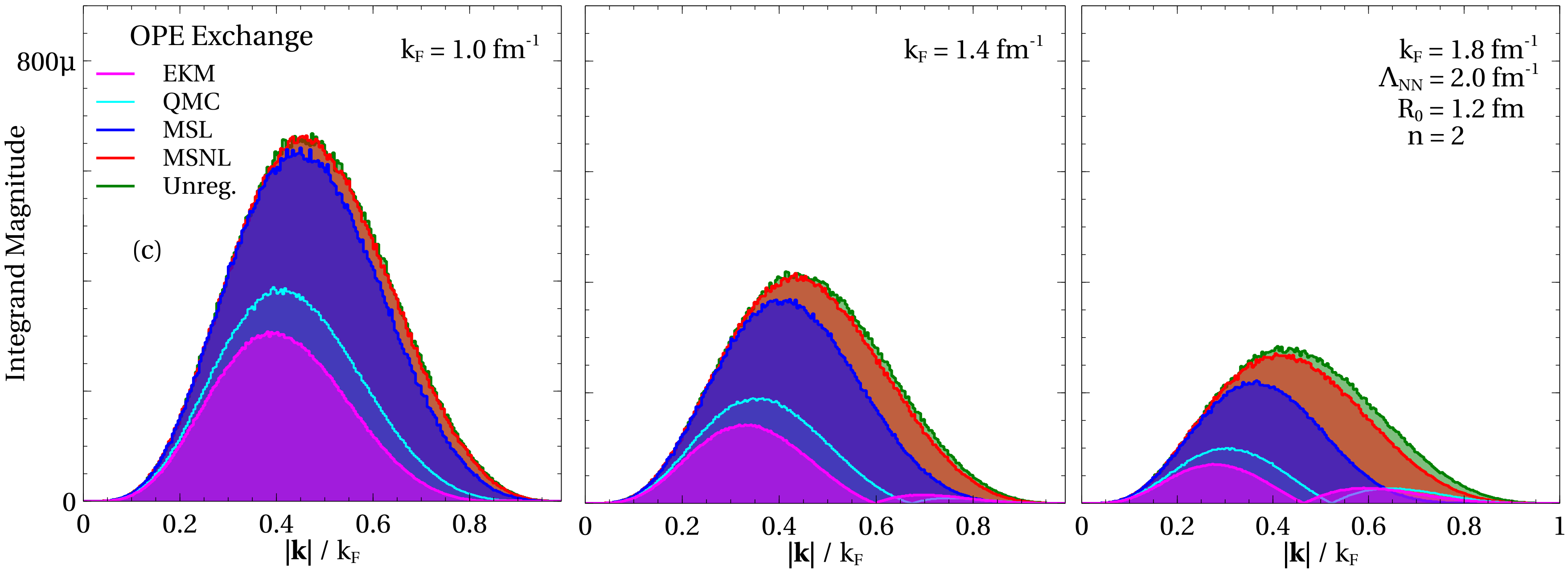
- Example: two-body regulators at HF:

  Interaction phase space for OPE exchange term



Dyhdalo, Furnstahl, Hebeler, IT, in preparation

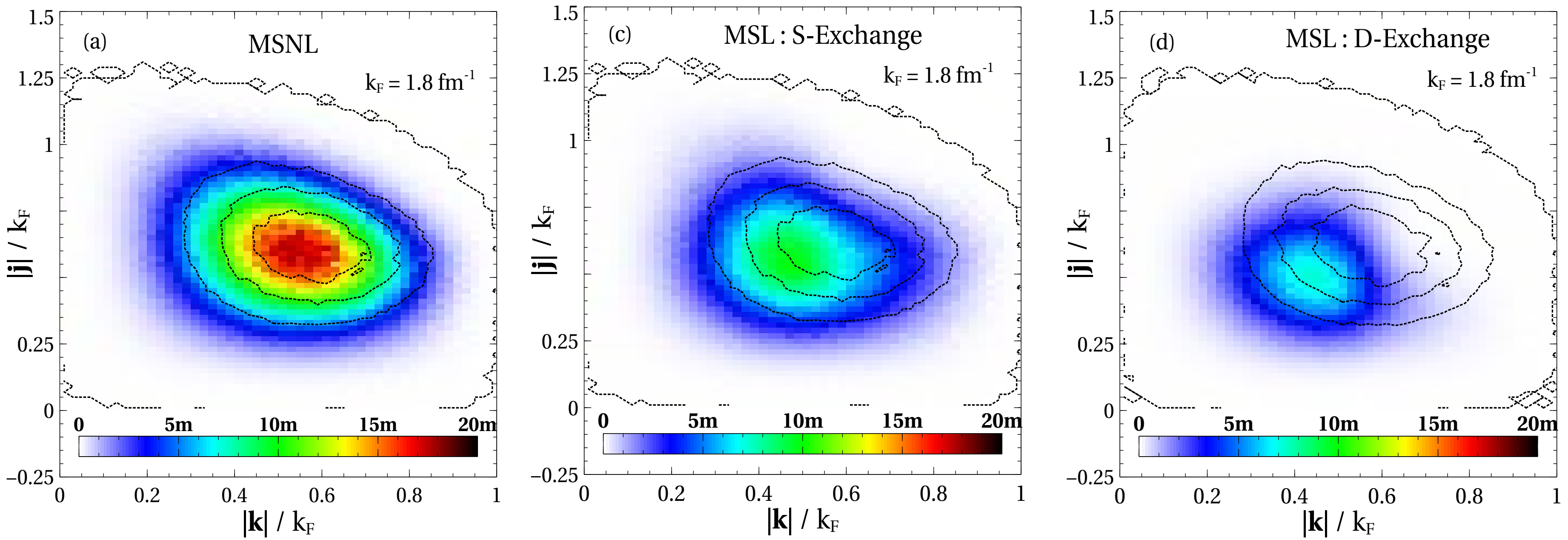
Local 3N forces in HF

Two problems:

1) Shorter-range parts can add sizeable contributions at HF
2) Local 3N TPE energies smaller than for nonlocal regulators

- Now 3N:

  Interaction phase space for 3N regulators



Dyhdalo, Furnstahl, Hebeler, IT, in preparation

Local NN forces in HF

Two problems:

1) Shorter-range parts can add sizeable contributions at HF
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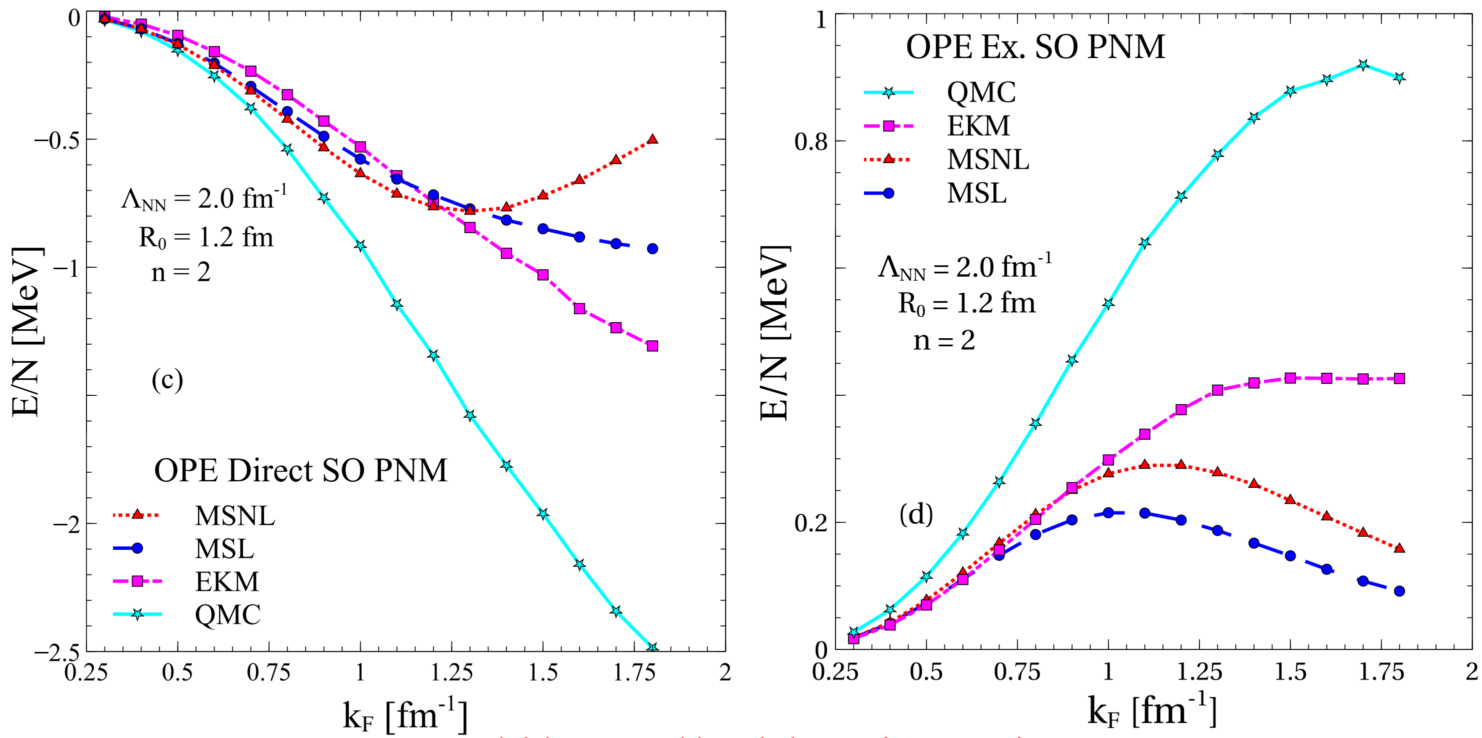
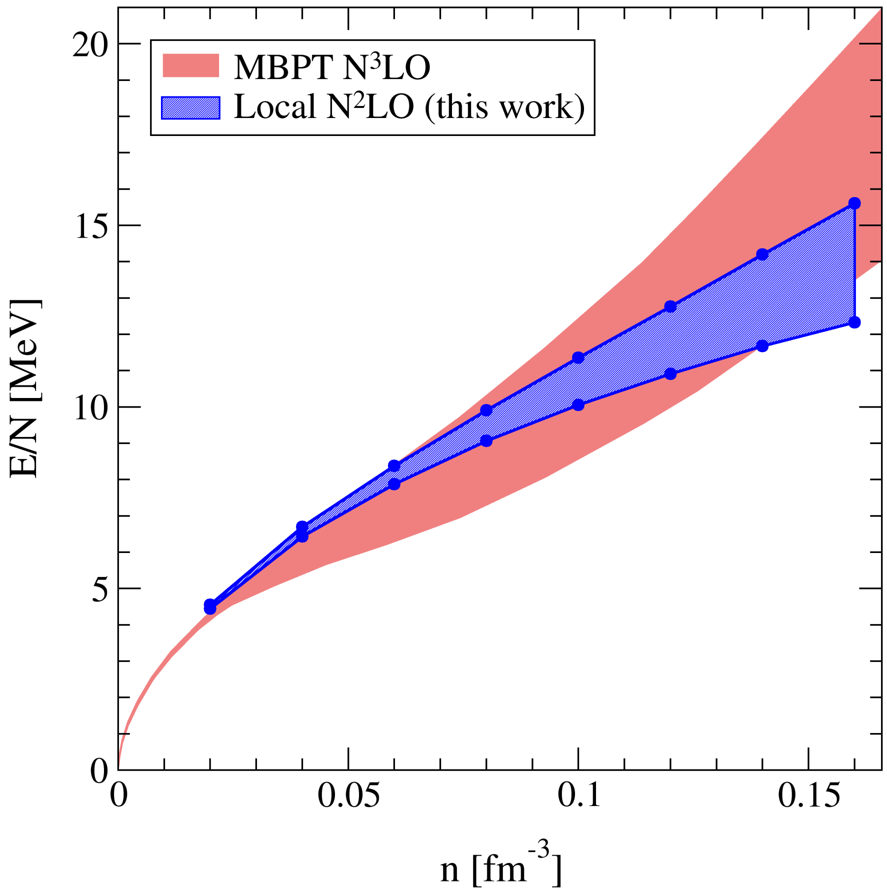
➢ Example: two-body regulators at 2nd order:



Dyhdalo, Furnstahl, Hebeler, IT, in preparation

Closing the circle

Comparing to N^3LO calculation:



Local N^2LO band includes:

- NN cutoff variation
- 3N cutoff variation → negligible
- Uncertainties in the 3N couplings → small
- Many-body uncertainty → negligible

BUT:

- Local regulators lead to less repulsion
- Additional contributions due to shorter-range 3N contributions

Summary

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- Local chiral potentials up to N^2LO including NN and 3N forces
- Local 3N two-pion-exchange contributions smaller than for nonlocal 3N forces
- Shorter-range parts can add sizeable contributions
- Different short-range operator structures lead to different results

More information on V_D and V_E:

- see talk by Joel Lynn :

  "Chiral Three-Nucleon Interactions in Light Nuclei, Neutron-Alpha Scattering, and Neutron Matter "

Important task for the future:

- Understanding of sensitivity on regularization scheme
- need to improve local regulators to minimize artifacts

Thanks

Thanks to my collaborators:

- Technische Universität Darmstadt:
  K. Hebeler, J. Lynn, A. Schwenk
- Ohio State University:
  A. Dyhdalo, D. Furnstahl
- Universität Bochum:
  E. Epelbaum
- Los Alamos National Laboratory:
  J. Carlson, S. Gandolfi
- University of Guelph:
  A. Gezerlis
- Forschungszentrum Jülich:
  A. Nogga

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Thank you!

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BACKUP

Phaseshifts for local potentials

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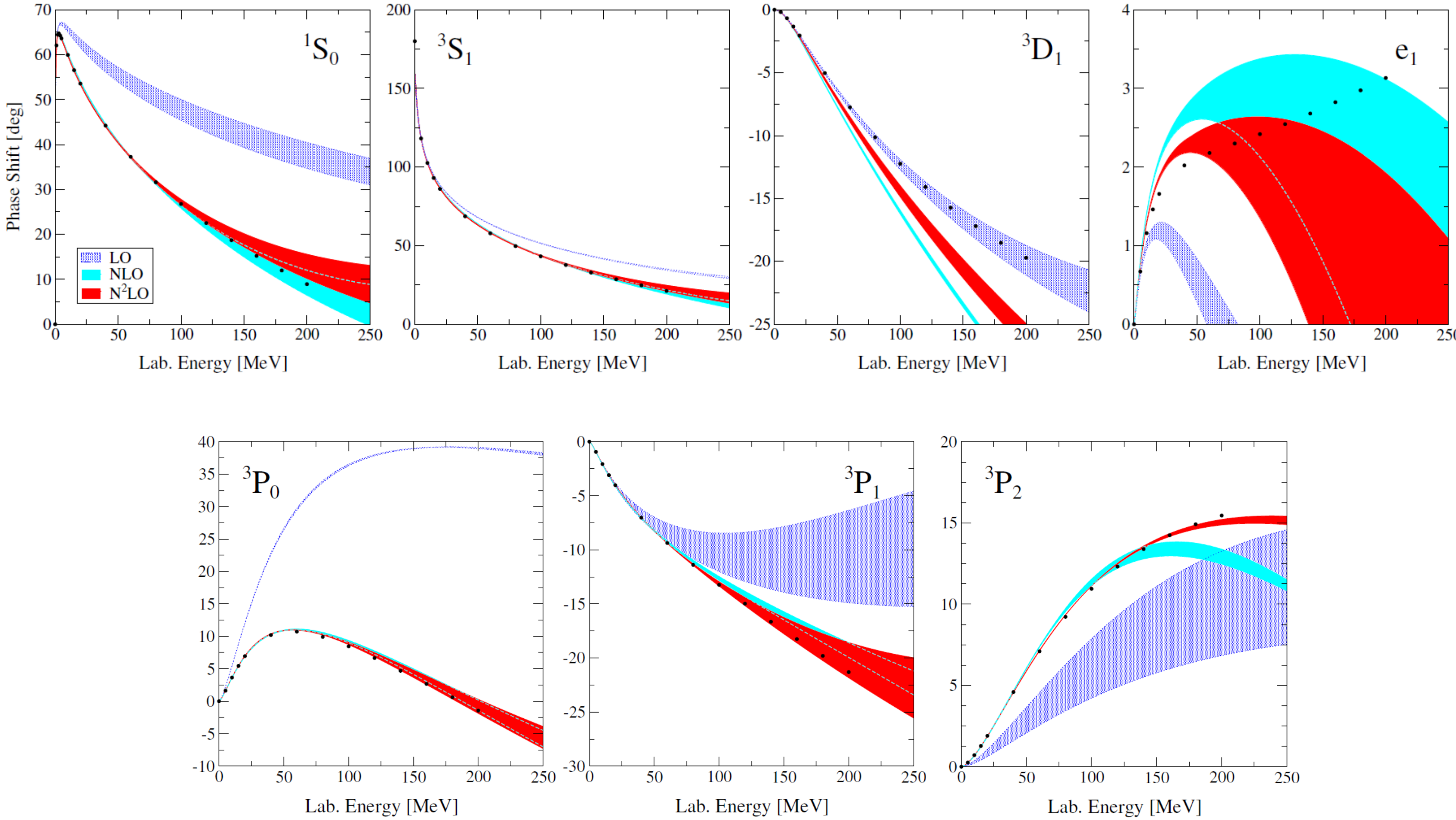
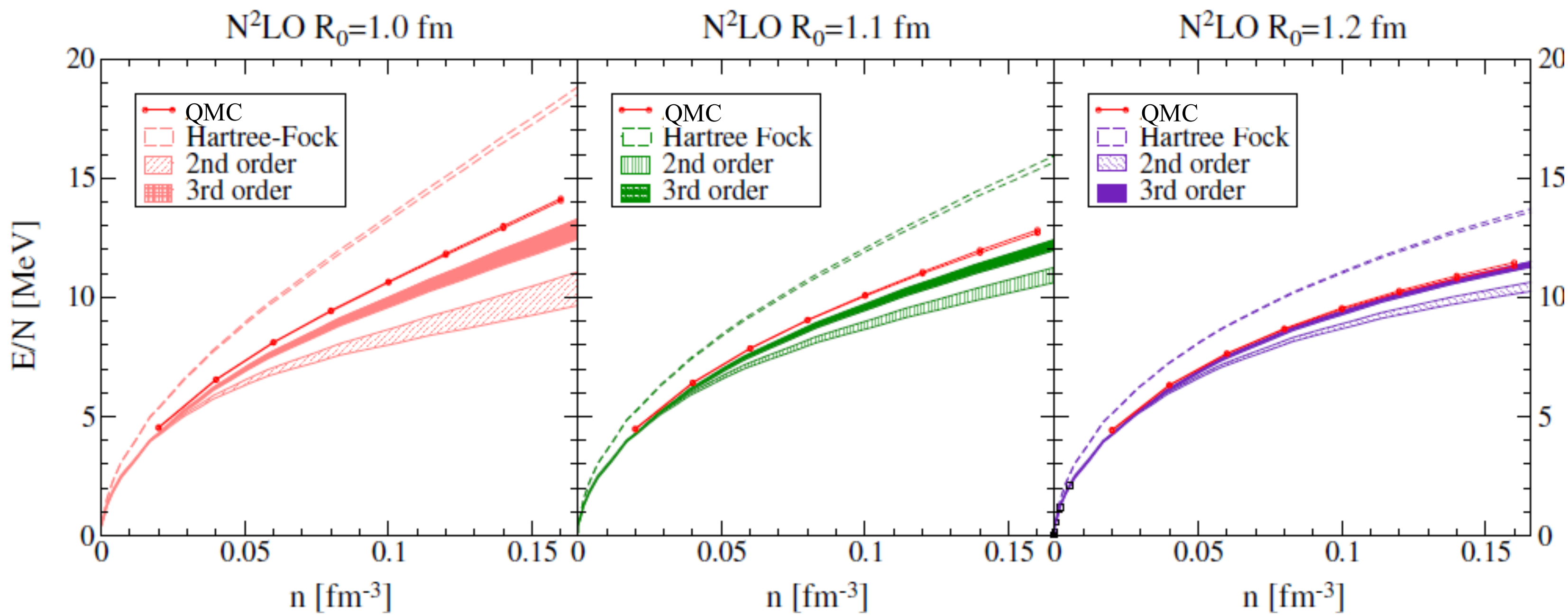


Gezerlis, IT, Epelbaum, Freunek, Gandolfi,
Hebeler, Nogga, Schwenk, PRC (2014)

Benchmark



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

Many-body perturbation theory:

- Excellent agreement with QMC for low-cutoff potentials ($R_0 = 1.2$ fm, 400 MeV)
- Validates perturbative calculations for those interactions