# Recent developments and applications of three-nucleon interactions

Kai Hebeler Vancouver, February 27, 2018

#### **Progress in Ab Initio Techniques in Nuclear Physics**







# Outline

#### Calculation of semilocal momentum space 3N matrix elements (SMS)

- \*strategy
- \*challenges
- \*status
- Few-body results A=3 and A=4
- Many-body results up to <sup>16</sup>O
   *Thomas Hüther's talk+poster*

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#### Calculation of semilocal momentum space 3N matrix elements (SMS)

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Novel efficient interface for **NN and 3N interactions** in a **non-partial-wave** basis

- First application to nuclear matter plus first fits of 3N couplings to nuclear matter
- applications to other systems and frameworks?

# Power counting in chiral 3N sector: Contributions of many-body forces at N<sup>3</sup>LO in neutron matter



0.05

0

0.1

n [fm<sup>-3</sup>]

0.15

0.05

0

0.1

 $n [fm^{-3}]$ 

0.15

0

0.05

0.1

n [fm<sup>-3</sup>]

0.15

0.2

0.15 (

0

0.05

0.1

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0.15

0.05

0.1

n [fm<sup>3</sup>]

# Power counting in chiral 3N sector: Contributions of many-body forces at N<sup>3</sup>LO in neutron matter



# 3NF power counting in 3H for different regulators



PRC 91,044001 (2015)



# 3NF power counting in 3H for different regulators



- size of N3LO contribution not suppressed for shown nonlocal interactions
- N3LO contributions suppressed for semilocal interactions
- technical challenges for semilocal interactions:
  - \* forces non-perturbative, large basis spaces/RG evolution needed
  - \* implementation of 3N forces hard, stability problems for scattering calculations
  - \* Derivation and implementation of nuclear currents hard  $\rightarrow$  Hermann's talk

Separation of long- and short-range physics



$$\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2$$
  
 $\mathbf{p}' = (\mathbf{p}'_1 - \mathbf{p}'_2)/2$   
 $\mathbf{q} = (\mathbf{p}_1 - \mathbf{p}'_1)$ 

Separation of long- and short-range physics



nonlocal 
$$V_{\rm NN}(\mathbf{p},\mathbf{p}') \to \exp\left[-\left((p^2+p'^2)/\Lambda^2\right)^n\right]V_{\rm NN}(\mathbf{p},\mathbf{p}')$$

Epelbaum, Glöckle, Meissner, NPA 747, 362 (2005) Entem, Machleidt, PRC 68, 041001 (2003)

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momentum space)

cf. Navratil, Few-body Systems 41, 117 (2007)

Separation of long- and short-range physics



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cf. Navratil, Few-body Systems 41, 117 (2007)

(coordinate space) 
$$V_{\rm NN}^{\pi}(\mathbf{r}) \rightarrow \left(1 - \exp\left[-\left(r^2/R^2\right)^n\right]\right) V_{\rm NN}^{\pi}(\mathbf{r}) \\ \delta(\mathbf{r}) \rightarrow \alpha_n \exp\left[-\left(r^2/R^2\right)^n\right]$$

Gezerlis et. al, PRL, 111, 032501 (2013)

Separation of long- and short-range physics



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semi-local

$$V_{\rm NN}(\mathbf{q}) \to \exp\left[-\left(q^2/\Lambda^2\right)^n\right] V_{\rm NN}(\mathbf{q})$$

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Epelbaum et. al, PRL, 115, 122301 (2015)

## 3NF power counting for different regulators



#### Representation of 3N interactions in momentum space

 $|pq\alpha\rangle_i \equiv |p_iq_i; [(LS)J(ls_i)j] \mathcal{J}\mathcal{J}_z(Tt_i)\mathcal{T}\mathcal{T}_z\rangle$ 



Due to the large number of matrix elements, the traditional way of computing matrix elements requires extreme amounts of computer resources.

$$N_p \simeq N_q \simeq 15$$
  

$$N_\alpha \simeq 30 - 180 \qquad \longrightarrow \quad \dim[\langle pq\alpha | V_{123} | p'q'\alpha' \rangle] \simeq 10^7 - 10^{10}$$

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**A 'new' algorithm allows efficient calculation.** KH, Krebs, Epelbaum, Golak, Skibinski, PRC 91, 044001(2015)

# Calculation of 3N forces in momentum partial-wave representation

 $\langle pq\alpha | V_{123} | p'q'\alpha' \rangle \sim \sum_{m_i} \int d\hat{\mathbf{p}} \, d\hat{\mathbf{q}} \, d\hat{\mathbf{p}}' \, d\hat{\mathbf{q}}' Y_l^m(\hat{\mathbf{p}}) Y_{\bar{l}}^{\bar{m}}(\hat{\mathbf{q}}) \, \langle \mathbf{pq}ST | V_{123} | \mathbf{p'q'}S'T' \rangle \, Y_{l'}^{m'}(\hat{\mathbf{p}}') Y_{\bar{l}'}^{\bar{m}'}(\hat{\mathbf{q}}')$ 

#### traditional method:

- reduce dimension of angular integrals from 8 to 5 by using symmetry
- discretize angular integrals and perform all sums numerically

#### much more efficient method:

- use that all interaction contributions (except rel. corr.) are local:  $\langle \mathbf{pq}|V_{123}|\mathbf{p'q'}\rangle = V_{123}(\mathbf{p} - \mathbf{p'}, \mathbf{q} - \mathbf{q'})$   $= V_{123}(p - p', q - q', \cos \theta)$ 
  - $\rightarrow$  allows to perform all except for 3 integrals analytically
- only a few small discrete internal sums need to be performed for each external momentum and angular momentum





## **Computational strategy:**

(1) calculate unregularized 3NF in sufficiently large partial-wave basis(2) fourier transform coordinate space regulator to momentum space



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$$\langle pq\alpha | V_{123}^{\rm reg} | p'q'\alpha' \rangle = \int d\tilde{q} \,\tilde{q}^2 \int d\tilde{p} \,\tilde{p}^2 \sum_{\tilde{\alpha}} \langle pq\alpha | V_{123} | \tilde{p}\tilde{q}\tilde{\alpha} \rangle \,\langle \tilde{p}\tilde{q}\tilde{\alpha} | f_{LR} | p'q'\alpha' \rangle$$



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 (2) fourier transform coordinate space regulator to momentum space
 (3) decompose regulator f<sub>LR</sub> in partial wave momentum basis
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(5) regularize short-range parts in interactions with non-local regulator



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(5) regularize short-range parts in interactions with non-local regulator(6) antisymmetrize interactions (optional)

## Semi-local regularization of 3NF (momentum space)



 $f_{\rm LR} = f_{\rm LR}(\mathbf{q}) = \exp\left[-(\mathbf{q}^2 + m_{\pi}^2)/\Lambda^2\right] \longrightarrow \text{Hermann Krebs' talk}$ 

$$V_{123} = V_{123}(p - p', q - q', \cos \theta) = V_{123}(\tilde{p}, \tilde{q}, \cos \theta)$$

**Example:** N2LO 2pi topology:  $V_{123}^{2\pi} \sim \frac{1}{(\mathbf{q}_2^2 + m_\pi^2)(\mathbf{q}_2^3 + m_\pi^2)}$  $=\frac{1}{((\mathbf{p}-\mathbf{q}/2)^2+m_{\pi}^2)((\mathbf{p}+\mathbf{q}/2)^2+m_{\pi}^2)}$  $V_{123}^{2\pi,reg} \sim \frac{f_{\rm LR}(\mathbf{q}_2)f_{\rm LR}(\mathbf{q}_3)}{(\mathbf{q}_2^2 + m_\pi^2)(\mathbf{q}_2^3 + m_\pi^2)}$ 

# Status and storage of 3NF matrix elements

- Calculation of matrix elements at N2LO completed
- all 3N topologies are calculated and stored separately, allows to easily adjust values of LECs  $c_1, c_3, c_4, c_D, c_E, C_S$  and  $C_T$
- calculated matrix elements of Faddeev components

 $\left\langle pq\alpha | V_{123}^i | p'q'\alpha' \right\rangle$ 

as well as fully and partially antisymmetrized matrix elements

$$\langle pq\alpha | (1 + P_{123} + P_{132}) V_{123}^i (1 + P_{123} + P_{132}) | p'q'\alpha' \rangle$$

$$\langle pq\alpha | V_{123}^i (1 + P_{123} + P_{132}) | p'q'\alpha' \rangle$$

• HDF5 file format for efficient I/O

First results:Thomas Hüther's talk

http://www.hdfgroup.org

Novel efficient many-body framework for nuclear matter (and other problems?)

Main code developer: Christian Drischler



#### **Problem:**

Evaluation of MBPT diagrams beyond second order in perturbation theory

becomes complicated and tedious in partial wave representation.

Present frameworks too inefficient for including matter properties in force fits.

Novel efficient many-body framework for nuclear matter (and other problems?)

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#### Strategy:

Implementation of NN and 3N forces without partial wave decomposition. Calculate MBPT diagrams in vector basis

 $|12...n\rangle = |\mathbf{k}_1 m_{s_1} m_{t_1}\rangle \otimes |\mathbf{k}_2 m_{s_2} m_{t_2}\rangle \otimes ... \otimes |\mathbf{k}_n m_{s_n} m_{t_n}\rangle$ 

using Monte-Carlo techniques. Implementation efficient and very transparent.

Drischler et al. arXiv:1710.08220 (2017)

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#### Status:

Implementation of nonlocal NN plus 3N forces up to N3LO complete. Implemented MBPT diagrams up to 4th order for state-of-the-art interactions.



# Example: Second order diagram in MBPT

$$E_{\rm NN+3N,eff}^{(2)} = \frac{1}{4} \left[ \prod_{i=1}^{4} \operatorname{Tr}_{\sigma_i} \int \frac{d\mathbf{k}_i}{(2\pi)^3} \right] \left| \langle 12 | V_{\rm as}^{(2)} | 34 \rangle \right|^2 \\ \times \frac{n_{\mathbf{k}_1} n_{\mathbf{k}_2} (1 - n_{\mathbf{k}_3}) (1 - n_{\mathbf{k}_4})}{\varepsilon_{\mathbf{k}_1} + \varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{k}_3} - \varepsilon_{\mathbf{k}_4}} (2\pi)^3 \\ \times \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4).$$



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#### Partial wave representation:

$$\begin{split} \sum_{S,M_S,M'_S} \left| \langle \mathbf{k}SM_S | V_{as}^{(2)} | \mathbf{k}'SM'_S \rangle \right|^2 \\ &= \sum_L P_L(\cos\theta_{\mathbf{k},\mathbf{k}'}) \sum_{J,l,l',S} \sum_{\widetilde{J},\widetilde{l},\widetilde{l}'} (4\pi)^2 i^{(l-l'+\widetilde{l}-\widetilde{l}')} (-1)^{\widetilde{l}+l'+L} \\ &\times \mathcal{C}_{l0\widetilde{l}'0}^{L0} \mathcal{C}_{l'0\widetilde{l}0}^{L0} \sqrt{(2l+1)(2l'+1)(2\widetilde{l}'+1)(2\widetilde{l}'+1)} \\ &\times (2J+1)(2\widetilde{J}+1) \left\{ \begin{array}{l} l & S & J \\ \widetilde{J} & L & \widetilde{l}' \end{array} \right\} \left\{ \begin{array}{l} J & S & l' \\ \widetilde{l} & L & \widetilde{J} \end{array} \right\} \\ &\times \langle k | V_{Sl'lJ}^{(2)} | k' \rangle \langle k' | V_{S\widetilde{l}'\widetilde{l}\widetilde{J}}^{(2)} | k \rangle [1-(-1)^{l+S+1}] \\ &\times [1-(-1)^{\widetilde{l}+S+1}], \end{array}$$

- hard to automatize and generalize to higher order diagrams
- prone to mistakes

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- hard to automatize and generalize to higher order diagrams
- prone to mistakes

Single-particle vector representation:

 $\frac{E_{\rm NN}^{(2)}}{V} = +\frac{1}{4} \sum_{\substack{ij\\ab}} \frac{\langle ij|\mathscr{A}_{12}V_{\rm NN}|ab\rangle \langle ab|\mathscr{A}_{12}V_{\rm NN}|ij\rangle}{D_{ijab}}$ 

- each diagram a compact single line of code
- straightforward to automatize code generation
- adaptive evaluation of integrals using Monte-Carlo techniques

# Higher-order contributions

#### example: third order (particle-particle, hole-hole, particle-hole)



#### Status:

- implemented all NN diagrams up to fourth order in MBPT, 3N interactions up to third order
- implemented all NN and 3N interactions (nonlocal) up to N3LO
- possible to also use NN matrix elements stored in partial wave basis by partial wave resummation
- interaction interface suitable for all many-body frameworks that require matrix elements in a momentum vector single-particle basis

## **Proof of principle:**

Fits of 3N interactions to saturation properties of nuclear matter

- incorporation of saturation properties in fits was not possible so far due to insufficient efficiency of many-body calculations
- performed calculations up to 4th order for set of presently used NN interactions, natural convergence pattern Drischler et al., arXiv:1710.08220 (2017)



## **Proof of principle:**

Fits of 3N interactions to saturation properties of nuclear matter

- incorporation of saturation properties in fits was not possible so far due to insufficient efficiency of many-body calculations
- performed fits for 3NF at N2LO and N3LO to 3H and matter for new family of NN forces by Entem, Machleidt and Nosyk Entem et al. PRC 96, 024004 (2017)

Drischler et al., arXiv:1710.08220 (2017)

0.5

0.0

-0.5

-1.0

-1.5

-2.0

-2.5

EMN N<sup>2</sup>LO (2017) EMN N<sup>3</sup>LO (2017)

-2

0

 $= 500 \text{ Me}^{\circ}$ 

4

2



## **Proof of principle:**

Fits of 3N interactions to saturation properties of nuclear matter

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Drischler et al., arXiv:1710.08220 (2017)

EMN N<sup>2</sup>LO (2017) EMN N<sup>3</sup>LO (2017)

-2

0

2

Δ

0.0

-0.5

-1.0

-1.5

-2.0

-2.5



Thank you!

Backup slides

#### Status of 3NF matrix element calculation



•  $N_p = 25, p_{\text{max}} = 10 \text{ fm}^{-1}$   $N_q = 25, q_{\text{max}} = 10 \text{ fm}^{-1}$ 

• Computed for cutoffs  $\Lambda=400, 450, 500, 550~{\rm MeV}$ 

• Calculation of I/m TPE expensive! need to fix values of  $\beta_8, \beta_9$ 

I. local EFT interactions, suitable for Quantum Monte Carlo calculations status: NN plus 3N up to N2LO, calculations of few-body systems and neutron matter



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Carlsson et al., PRX 6,011019 (2016)

3. fits of NN plus 3N forces to two-, few- and many-body observables status: NN plus 3N up to N2LO, NN phase shifts fitted up to T<sub>lab</sub>~35 MeV



3. fits of NN plus 3N forces to two-, few- and many-body observables status: NN plus 3N up to N2LO, NN phase shifts fitted up to T<sub>lab</sub>~35 MeV



4. semilocal NN forces, development of improved method to estimate uncertainties

status: NN up to N4LO, 3N interactions up to N3LO



3. fits of NN plus 3N forces to two-, few- and many-body observables status: NN plus 3N up to N2LO, NN phase shifts only fitted up to T<sub>lab</sub>~35 MeV



4. semilocal NN forces, development of improved method to estimate uncertainties status: NN up to N4LO, 3NF up to N3LO



Epelbaum, Krebs, Meißner, PRL 115, 122301 (2015)

Binder et al., PRC 93, 044002 (2016)

# Equation of state of symmetric nuclear matter: nuclear saturation









"Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density. In particular, a substantial tensor force is required."

Hans Bethe (1971)





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Reproduction of saturation point without readjusting parameters!



-18

0.13

0.14

0.15

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Hans Bethe (1971)

Drischler, KH, Schwenk, PRC93, 054314 (2016)

0.16 0.17

 $n_0 \, [{\rm fm}^{-3}]$ 

1.8/2.0 (1

0.18 0.19

# Ab initio calculations of heavier nuclei





# Ab initio calculations of heavier nuclei



NLO  $O\left(\frac{q^2}{32}\right)$ 

- spectacular increase in range of applicability of ab initio many body frameworks
- significant discrepancies to experimental data for heavy nuclei for

(most of) presently used nuclear interactions

• need to quantify theoretical uncertainties

# Studies of neutron-rich nuclei



- remarkable agreement between different many-body frameworks
- excellent agreement between theory and experiment for masses of oxygen and calcium isotopes based on specific chiral interactions
- need to quantify theoretical uncertainties

# Microscopic calculations of the equation of state



- microscopic framework to calculate equation of state for general proton fractions
- uncertainty bands determined
   by set of 7 Hamiltonians



 many-body framework allows treatment of general
 3N interaction

Drischler, KH, Schwenk, PRC 054314 (2016)