## Modern Theory of nuclear forces

Lectures 1+2: Foundations
Lecture 3: Foundations (cont.) + derivation of nuclear forces
Lecture 4: (i) Chiral nuclear forces: State of the art
(ii) Nuclear lattice simulations


## Intermediate summary: Nuclear chiral EFT a-la Weinberg

$$
[\left(\sum_{i=1}^{A} \frac{-\vec{\nabla}_{i}^{2}}{2 m_{N}}+\mathcal{O}\left(m_{N}^{-3}\right)\right)+\underbrace{V_{2 N}+V_{3 N}+V_{4 N}+\ldots}_{\text {derived within ChPT }}]|\Psi\rangle=E|\Psi\rangle
$$



## $+$

- unified description of $\pi \pi$, $\pi N$ and $N N$
- consistent many-body forces and currents
- systematically improvable
- bridging different reactions (electroweak, $\pi$-prod., ...)
- precision physics with/from light nuclei


## Chiral expansion of nuclear forces

Two-nucleon force


LO (Q ${ }^{0}$ )

NLO (Q2)


$\mathrm{N}^{2} \mathrm{LO}\left(\mathrm{Q}^{3}\right)$

$\left\langle V_{2 \mathrm{~N}}\right\rangle \sim 20 \mathrm{MeV} /$ pair

Three-nucleon force

$\qquad$





## Nucleon-nucleon force up to N3LO

Ordonez et al. '94; Friar \& Coon '94; Kaiser et al. '97; E.E. et al. '98, '03; Kaiser '99-'01; Higa, Robilotta '03; ...

- LO ( $\mathrm{Q}^{0}$ ):

- NLO ( $\mathbf{Q}^{2}$ ):



leading $2 \pi$-exchange
- N2LO ( $\mathbf{Q}^{3}$ ):

- $\mathrm{N}^{3} \mathrm{LO}\left(\mathbf{Q}^{4}\right)$ :


$x$.
15 LECs renormalization of contact terms

sub-subleading $2 \pi$-exchange

$3 \pi-e x c h a n g e$ (small)
+ isospin-breaking corrections...
van Kolck et al. '93, '96; Friar et al. '99,
'03, '04; Niskanen '02; Kaiser '06;
E.E. et al. '04,'05,'07; .


## Nucleon-nucleon force up to N3LO

Ordonez et al. '94; Friar \& Coon '94; Kaiser et al. '97; E.E. et al. '98, '03; Kaiser '99-'01; Higa, Robilotta '03; ...

- LO ( $\mathrm{Q}^{0}$ ):
- NLO ( $\mathbf{Q}^{2}$ ):

- ${ }^{3}$ LO ( $\mathbf{Q}^{4}$ ):

24 LECs fit to np data

leading $2 \pi$-exchange

- N2LO (Q ${ }^{3}$ ):

sub-subleading $2 \pi$-exchange
- $\{\leftarrow$ renormalization of $1 \pi$-exchange



15 LECs renormalization of contact terms


+ isospin-breaking corrections..
van Kolck et al. '93, '96; Friar et al. '99,
'03, '04; Niskanen '02; Kaiser '06;
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## Nucleon-nucleon force up to N3LO

Ordonez et al. '94; Friar \& Coon '94; Kaiser et al. '97; E.E. et al. '98, '03; Kaiser '99-'01; Higa, Robilotta '03; ...

- LO (Q ${ }^{0}$ ):
- NLO (Q2):
- $\mathrm{N}^{2} \mathrm{LO}\left(\mathrm{Q}^{3}\right)$ :
 24 LECs fit to np data
- $\mathrm{N}^{3} \mathrm{LO}\left(\mathrm{Q}^{4}\right):$



## LECs fixed from $\pi N$

$\rightarrow$ long-range tail of the nuclear force fixed by chiral symmetry and exp. information on the $\pi \mathrm{N}$ system

$3 \pi-e x c h a n g e$ (small)

+ isospin-breaking corrections...
van Kolck et al. '93, '96; Friar et al. '99,
'03, '04; Niskanen '02; Kaiser '06;
E.E. et al. '04,'05,'07; .


## Chiral $2 \pi$ exchange (upto N2LO)

$$
\begin{aligned}
\mathcal{V}_{N N} & =V_{C}(r)+\vec{\tau}_{1} \cdot \vec{\tau}_{2} W_{C}(r)+\left[V_{S}(r)+\vec{\tau}_{1} \cdot \vec{\tau}_{2} W_{S}(r)\right] \vec{\sigma}_{1} \cdot \vec{\sigma}_{2} \\
& +\left[V_{T}(r)+\vec{\tau}_{1} \cdot \vec{\tau}_{2} W_{T}(r)\right]\left(3 \vec{\sigma}_{1} \cdot \hat{r} \vec{\sigma}_{2} \cdot \hat{r}-\vec{\sigma}_{1} \cdot \vec{\sigma}_{2}\right)+\left[V_{L S}(r)+\vec{\tau}_{1} \cdot \vec{\tau}_{2} W_{L S}(r)\right] \vec{L} \cdot \vec{S},
\end{aligned}
$$

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\end{aligned}
$$

The profile functions (in Dimensional Regularization)

$$
\begin{aligned}
V_{C}^{T P E}(r) & =\frac{3 g^{2} m^{6}}{32 \pi^{2} f^{4}} \frac{e^{-2 x}}{x^{6}}\left\{\left(2 c_{1}+\frac{3 g^{2}}{16 M}\right) x^{2}(1+x)^{2}+\frac{g^{5} x^{5}}{32 M}+\left(c_{3}+\frac{3 g^{2}}{16 M}\right)\left(6+12 x+10 x^{2}+4 x^{3}+x^{4}\right)\right\} \\
W_{T}^{T P E}(r) & =\frac{g^{2} m^{6}}{48 \pi^{2} f^{4}} \frac{e^{-2 x}}{x^{6}}\left\{-\left(c_{4}+\frac{1}{4 M}\right)(1+x)\left(3+3 x+x^{2}\right)+\frac{g^{2}}{32 M}\left(36+72 x+52 x^{2}+17 x^{3}+2 x^{4}\right)\right\}, \\
V_{T}^{T P E}(r) & =\frac{g^{4} m^{5}}{128 \pi^{3} f^{4} x^{4}}\left\{-12 K_{0}(2 x)-\left(15+4 x^{2}\right) K_{1}(2 x)+\frac{3 \pi m e^{-2 x}}{8 M x}\left(12 x^{-1}+24+20 x+9 x^{2}+2 x^{3}\right)\right\}, \\
W_{C}^{T P E}(r) & =\frac{g^{4} m^{5}}{128 \pi^{3} f^{4} x^{4}}\left\{\left[1+2 g^{2}\left(5+2 x^{2}\right)-g^{4}\left(23+12 x^{2}\right)\right] K_{1}(2 x)+x\left[1+10 g^{2}-g^{4}\left(23+4 x^{2}\right)\right] K_{0}(2 x),\right. \\
& \left.+\frac{g^{2} m \pi e^{-2 x}}{4 M x}\left[2\left(3 g^{2}-2\right)\left(6 x^{-1}+12+10 x+4 x^{2}+x^{3}\right)\right]+g^{2} x\left(2+4 x+2 x^{2}+3 x^{2}\right)\right\}, \\
V_{S}^{T P E}(r) & =\frac{g^{4} m^{5}}{32 \pi^{3} f^{4}}\left\{3 x K_{0}(2 x)+\left(3+2 x^{2}\right) K_{1}(2 x)-\frac{3 \pi m e^{-2 x}}{16 M x}\left(6 x^{-1}+12+11 x+6 x^{2}+2 x^{3}\right)\right\}, \\
W_{S}^{T P E}(r) & =\frac{g^{2} m^{6}}{48 \pi^{2} f^{4}} \frac{e^{-2 x}}{x^{6}}\left\{\left(c_{4}+\frac{1}{4 M}\right)(1+x)\left(3+3 x+2 x^{2}\right)-\frac{g^{2}}{16 M}\left(18+36 x+31 x^{2}+14 x^{3}+2 x^{4}\right)\right\}, \\
V_{L S}^{T P E}(r) & =-\frac{3 g^{4} m^{6}}{64 \pi^{2} M f^{4}} \frac{e^{-2 x}}{x^{6}}(1+x)\left(2+2 x+x^{2}\right), \\
W_{L S}^{T P E}(r) & =\frac{g^{2}\left(g^{2}-1\right) m^{6}}{32 \pi^{2} M f^{4}} \frac{e^{-2 x}}{x^{6}}(1+x)^{2},
\end{aligned}
$$

## Chiral $2 \pi$ exchange (upto N2LO)

$$
\begin{aligned}
\mathcal{V}_{N N} & =V_{C}(r)+\vec{\tau}_{1} \cdot \vec{\tau}_{2} W_{C}(r)+\left[V_{S}(r)+\vec{\tau}_{1} \cdot \vec{\tau}_{2} W_{S}(r)\right] \vec{\sigma}_{1} \cdot \vec{\sigma}_{2} \\
& +\left[V_{T}(r)+\vec{\tau}_{1} \cdot \vec{\tau}_{2} W_{T}(r)\right]\left(3 \vec{\sigma}_{1} \cdot \hat{r} \vec{\sigma}_{2} \cdot \hat{r}-\vec{\sigma}_{1} \cdot \vec{\sigma}_{2}\right)+\left[V_{L S}(r)+\vec{\tau}_{1} \cdot \vec{\tau}_{2} W_{L S}(r)\right] \vec{L} \cdot \vec{S},
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\end{aligned}
$$



Is there any evidence from NN data?

## Chiral two-pion exchange and NN data

## Nijmegen Partial Wave Analysis

Rentmeester et al.'99, '03
Number of BC parameters needed to achieve $\chi^{2}$ datum $\sim 1$ for a given long-range part (input)
$31(1 \pi) \rightarrow 28(1 \pi+2 \pi[\mathrm{NLO}]) \rightarrow 23\left(1 \pi+2 \pi\left[\mathrm{~N}^{2} \mathrm{LO}\right]\right)$


## „Deconstructing" neutron-proton phase shufts Birse, McGovern '06

Idea: Subtract effects of the long-range intersction from phase shufts (DWBA) and look at the residual energy dependence



## Neution-protion phase shifits at N3LO

## Entem, Machleidt '04; E.E., Glöckle, Meißner '05








## The challenge: Understanding the 3 N force

- Today‘s few- and many-body calculations have reached the level of accuracy at which it is necessary to include 3NFs
- Inspite of decades of efforts, the structure of the 3NF is still poorely understood
Kalantar-Nayestanaki, EE, Messchendorp, Nogga, Rev. Mod. Phys. 75 (2012) 016301



## Most general structure of a local 3NF

Krebs, Gasparyan, EE, arXiv:1302.2872 [nucl-th]

## 22 independent operators (coord. space)

$$
\begin{aligned}
\tilde{\mathcal{G}}_{1} & =1, \\
\tilde{\mathcal{G}}_{2} & =\boldsymbol{\tau}_{1} \cdot \boldsymbol{\tau}_{3}, \\
\tilde{\mathcal{G}}_{3} & =\vec{\sigma}_{1} \cdot \vec{\sigma}_{3}, \\
\tilde{\mathcal{G}}_{4} & =\boldsymbol{\tau}_{1} \cdot \boldsymbol{\tau}_{3} \vec{\sigma}_{1} \cdot \vec{\sigma}_{3}, \\
\tilde{\mathcal{G}}_{5} & =\boldsymbol{\tau}_{2} \cdot \boldsymbol{\tau}_{3} \vec{\sigma}_{1} \cdot \vec{\sigma}_{2}, \\
\tilde{\mathcal{G}}_{6} & =\boldsymbol{\tau}_{1} \cdot\left(\boldsymbol{\tau}_{2} \times \boldsymbol{\tau}_{3}\right) \vec{\sigma}_{1} \cdot\left(\vec{\sigma}_{2} \times \vec{\sigma}_{3}\right), \\
\tilde{\mathcal{G}}_{7} & =\boldsymbol{\tau}_{1} \cdot\left(\boldsymbol{\tau}_{2} \times \boldsymbol{\tau}_{3}\right) \vec{\sigma}_{2} \cdot\left(\hat{r}_{12} \times \hat{r}_{23}\right), \\
\tilde{\mathcal{G}}_{8} & =\hat{r}_{23} \cdot \vec{\sigma}_{1} \hat{r}_{23} \cdot \vec{\sigma}_{3}, \\
\tilde{\mathcal{G}}_{9} & =\hat{r}_{23} \cdot \vec{\sigma}_{3} \hat{r}_{12} \cdot \vec{\sigma}_{1}, \\
\tilde{\mathcal{G}}_{10} & =\hat{r}_{23} \cdot \vec{\sigma}_{1} \hat{r}_{12} \cdot \vec{\sigma}_{3}, \\
\tilde{\mathcal{G}}_{11} & =\boldsymbol{\tau}_{2} \cdot \boldsymbol{\tau}_{3} \hat{r}_{23} \cdot \vec{\sigma}_{1} \hat{r}_{23} \cdot \vec{\sigma}_{2}, \\
\mathcal{G}_{12} & =\boldsymbol{\tau}_{2} \cdot \boldsymbol{\tau}_{3} \hat{r}_{23} \cdot \vec{\sigma}_{1} \hat{r}_{12} \cdot \vec{\sigma}_{2}, \\
\tilde{\mathcal{G}}_{13} & =\boldsymbol{\tau}_{2} \cdot \boldsymbol{\tau}_{3} \hat{r}_{12} \cdot \vec{\sigma}_{1} \hat{r}_{23} \cdot \vec{\sigma}_{2}, \\
\tilde{\mathcal{G}}_{14} & =\boldsymbol{\tau}_{2} \cdot \boldsymbol{\tau}_{3} \hat{r}_{12} \cdot \vec{\sigma}_{1} \hat{r}_{12} \cdot \vec{\sigma}_{2}, \\
\tilde{\mathcal{G}}_{15} & =\boldsymbol{\tau}_{1} \cdot \boldsymbol{\tau}_{3} \hat{r}_{13} \cdot \vec{\sigma}_{1} \hat{r}_{13} \cdot \vec{\sigma}_{3}, \\
\tilde{\mathcal{G}}_{16} & =\boldsymbol{\tau}_{2} \cdot \boldsymbol{\tau}_{3} \hat{r}_{12} \cdot \vec{\sigma}_{2} \hat{r}_{12} \cdot \vec{\sigma}_{3}, \\
\tilde{\mathcal{G}}_{17} & =\boldsymbol{\tau}_{1} \cdot \boldsymbol{\tau}_{3} \hat{r}_{23} \cdot \vec{\sigma}_{1} \hat{r}_{12} \cdot \vec{\sigma}_{3}, \\
\tilde{\mathcal{G}}_{18} & =\boldsymbol{\tau}_{1} \cdot\left(\boldsymbol{\tau}_{2} \times \boldsymbol{\tau}_{3}\right) \vec{\sigma}_{1} \cdot \vec{\sigma}_{3} \vec{\sigma}_{2} \cdot\left(\hat{r}_{12} \times \hat{r}_{23}\right), \\
\tilde{\mathcal{G}}_{19} & =\boldsymbol{\tau}_{1} \cdot\left(\boldsymbol{\tau}_{2} \times \boldsymbol{\tau}_{3}\right) \vec{\sigma}_{3} \cdot \hat{r}_{23} \hat{r}_{23} \cdot\left(\vec{\sigma}_{1} \times \vec{\sigma}_{2}\right), \\
\tilde{\mathcal{G}}_{20} & =\boldsymbol{\tau}_{1} \cdot\left(\boldsymbol{\tau}_{2} \times \boldsymbol{\tau}_{3}\right) \vec{\sigma}_{1} \cdot \hat{r}_{23} \vec{\sigma}_{2} \cdot \hat{r}_{23} \vec{\sigma}_{3} \cdot\left(\hat{r}_{12} \times \hat{r}_{23}\right), \\
\tilde{\mathcal{G}}_{21} & =\boldsymbol{\tau}_{1} \cdot\left(\boldsymbol{\tau}_{2} \times \boldsymbol{\tau}_{3}\right) \vec{\sigma}_{1} \cdot \hat{r}_{13} \vec{\sigma}_{3} \cdot \hat{r}_{13} \vec{\sigma}_{2} \cdot\left(\hat{r}_{12} \times \hat{r}_{23}\right), \\
\tilde{\mathcal{G}}_{22} & =\boldsymbol{\tau}_{1} \cdot\left(\boldsymbol{\tau}_{2} \times \boldsymbol{\tau}_{3}\right) \vec{\sigma}_{1} \cdot \hat{r}_{23} \vec{\sigma}_{3} \cdot \hat{r}_{12} \vec{\sigma}_{2} \cdot\left(\hat{r}_{12} \times \hat{r}_{23}\right),
\end{aligned}
$$



Building blocks:

$$
\boldsymbol{\tau}_{1}, \boldsymbol{\tau}_{2}, \boldsymbol{\tau}_{3}, \vec{\sigma}_{1}, \vec{\sigma}_{2}, \vec{\sigma}_{3}, \vec{r}_{12}, \vec{r}_{23}
$$

Constraints:

- locality,
- isospin symmetry,
- parity and time-reversal invariance


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\tilde{\mathcal{G}}_{19} & =\boldsymbol{\tau}_{1} \cdot\left(\boldsymbol{\tau}_{2} \times \boldsymbol{\tau}_{3}\right) \vec{\sigma}_{3} \cdot \hat{r}_{23} \hat{r}_{23} \cdot\left(\vec{\sigma}_{1} \times \vec{\sigma}_{2}\right), \\
\tilde{\mathcal{G}}_{20} & =\boldsymbol{\tau}_{1} \cdot\left(\boldsymbol{\tau}_{2} \times \boldsymbol{\tau}_{3}\right) \vec{\sigma}_{1} \cdot \hat{r}_{23} \vec{\sigma}_{2} \cdot \hat{r}_{23} \vec{\sigma}_{3} \cdot\left(\hat{r}_{12} \times \hat{r}_{23}\right), \\
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\end{aligned}
$$



Building blocks:

$$
\boldsymbol{\tau}_{1}, \boldsymbol{\tau}_{2}, \boldsymbol{\tau}_{3}, \vec{\sigma}_{1}, \vec{\sigma}_{2}, \vec{\sigma}_{3}, \vec{r}_{12}, \vec{r}_{23}
$$

Constraints:

- locality,
- isospin symmetry,
- parity and time-reversal invariance
$\longrightarrow V_{3 \mathrm{~N}}=\sum_{i=1}^{22} G\left(F_{i}\left(r_{12}, r_{23}, r_{31}\right)+5\right.$ perm.
derivable in ChPT; long-range
terms parameter-free predictions


## Leading chiral $3 N F$ and $3 N / 4 N$ continuum

- Nd scattering: accurate description at low energy except for $\mathrm{A}_{y}$-puzzle (fine tuned) and some breakup configurations
- Uncertainty grows rapidly with energy (higher orders ?)
- 4N continuum: an emerging field (lectures by Michele)


2 LECs tuned to few-N data (e.g. ${ }^{3} \mathrm{H},{ }^{4} \mathrm{He} \mathrm{BEs}$ )

Nd elastic cross sections at low energies


Nd breakup at $E_{d}=130 \mathrm{MeV}$
Stephan et al., PRC 82 (2010) 014003





## Leading chiral $3 N F$ and $3 N / 4 N$ continuum

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2 LECs tuned to few-N data
(e.g. ${ }^{3} \mathrm{H},{ }^{4} \mathrm{He}$ BEs)


Corrections to the leading 3NF beyond N2LO are being investigated

## Two-pion exchange BNF up to N4LO







## TWo-pion exchange BNF up to N4LO

Krebs, Gasparyan, EE '12


$$
\begin{aligned}
& +\mathrm{N}^{3} \mathrm{LO} \\
& \text { of }
\end{aligned}
$$







## TWo-pion exchange BNF up to N4LO

Krebs, Gasparyan, EE '12





## TWo-pion exchange BNF up to N4LO


$+\mathrm{N}^{3} \mathrm{LO}$

$+\mathrm{N}^{4} \mathrm{LO}$


## Pion-nucleon phase shifts in HB ChPT up to Q4 (KH PWA)



Values of low-energy constants extracted at $\mathbf{Q}^{4}$ (in powers of GeV )

|  | $c_{1}$ | $c_{2}$ | $c_{3}$ | $c_{4}$ | $\bar{d}_{1}+\bar{d}_{2}$ | $\bar{d}_{3}$ | $\bar{d}_{5}$ | $\bar{d}_{14}-\bar{d}_{15}$ | $\bar{e}_{14}$ | $\bar{e}_{15}$ | $\bar{e}_{16}$ | $\bar{e}_{17}$ | $\bar{e}_{18}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $Q^{4}$ fit to GW | -1.13 | 3.69 | -5.51 | 3.71 | 5.57 | -5.35 | 0.02 | -10.26 | 1.75 | -5.80 | 1.76 | -0.58 | 0.96 |
| $Q^{4}$ fit to KH | -0.75 | 3.49 | -4.77 | 3.34 | 6.21 | -6.83 | 0.78 | -12.02 | 1.52 | -10.41 | 6.08 | -0.37 | 3.26 |

## Summary: chiral nuclear forces

- Chiral NN potentials are available at N3LO and provide accurate description of NN scattering up to $\mathrm{E}_{\mathrm{lab}} \sim 200 \mathrm{MeV}$.
- 3NF: promising results at N2LO; corrections are under investigation
- 4NF: starts contributing at N3LO; probably small (expectation value for the a-particle about a few $100 \mathrm{keV} . .$. )


## Nuclear Lattice Effective Field Theory

The Collaboration: E.E., Hermann Krebs (Bochum), Timo Lähde (Jülich), Dean Lee (NC State), Ulf-G. Meißner (Bonn/Jülich), Gautam Rupak (Mississippi State)

Borasoy, E.E., Krebs, Lee, Meißner, Eur. Phys. J. A31 (07) 105,
Eur. Phys. J. A34 (07) 185,
Eur. Phys. J. A35 (08) 343,
Eur. Phys. J. A35 (08) 357,
E.E., Krebs, Lee, Meißner, Eur. Phys. J A40 (09) 199,

Eur. Phys. J A41 (09) 125,

|P $\operatorname{cg}_{5}^{6}$
E.E., Krebs, Lähde, Lee, Meißner

Phy
Phys. Rev. Lett. 110 (13) 112502, arXiv:1303.4856


HELMHOLTZ
| GEMEINSCHAFT
ر лӥисн
erc
European

## Nuclear lattice simulations

Discretized version of chiral EFT for nuclear dynamics

$$
[\left(\sum_{i=1}^{A} \frac{-\vec{\nabla}_{i}^{2}}{2 m_{N}}+\mathcal{O}\left(m_{N}^{-3}\right)\right)+\underbrace{V_{2 N}+V_{3 N}+V_{4 N}+\ldots}_{\text {derived within ChPT }}]|\Psi\rangle=E|\Psi\rangle
$$

## Lattice QCD


$\sim 0.1 \mathrm{fm}$

- fundamental, the only parameters are $m_{q}, a_{\text {strong }}$
- hard to go beyond 1 hadron...


## Chiral EFT on the lattice



- effective hadronic description, LECs to be determined from the data/LQCD
- much more efficient for atomic nuclei


## Leading-order action

- $\vec{n}$ refer to integer-valued spatial lattice vectors
- $\vec{l}=\{\hat{1}, \hat{2}, \hat{3}\}$ are unit lattice vectors in the spatial directions
- $\alpha_{t}=a_{t} / a$ is the ratio of the lattice spacings

- Derivatives (order- $a^{4}$ improved)

$$
\begin{aligned}
& \nabla_{l} f(\vec{n})=\frac{3}{4}[f(\vec{n}+\vec{l})-f(\vec{n}-\vec{l})]-\frac{3}{20}[f(\vec{n}+2 \vec{l})-f(\vec{n}-2 \vec{l})]+\frac{1}{60}[f(\vec{n}+3 \vec{l})-f(\vec{n}-3 \vec{l})] \\
& \nabla_{l}^{2} f(\vec{n})=-\frac{49}{18} f(\vec{n})+\frac{3}{2}[f(\vec{n}+\vec{l})+f(\vec{n}-\vec{l})]-\frac{3}{20}[f(\vec{n}+2 \vec{l})+f(\vec{n}-2 \vec{l})]+\frac{1}{90}[f(\vec{n}+3 \vec{l})+f(\vec{n}-3 \vec{l})]
\end{aligned}
$$

- Free Hamiltonian for non-relativistic nucleons: $H_{\text {free }}=\frac{1}{2 m} \sum_{\vec{n}, i, j} a_{i j}^{\dagger}(\vec{n}) \sum_{l} \nabla_{l}^{2} a_{i j}(\vec{n})$
- Nucleon local density operators $\rho(\vec{n})=\sum_{i, j} a_{i, j}^{\dagger}(\vec{n}) a_{i, j}(\vec{n}), \quad \rho_{S}(\vec{n})=\sum_{i, j, k} a_{i, j}^{\dagger}(\vec{n})\left[\sigma_{S}\right]_{i k} a_{k, j}(\vec{n})$

$$
\left.\rho_{I}(\vec{n})=\sum_{i, j, k} a_{i, j}^{\dagger}(\vec{n})\left[\tau_{I}\right]_{j k} a_{i, k}(\vec{n}), \quad \rho_{S, I}(\vec{n})=\sum_{i, j, k, l} a_{i, j}^{\dagger}(\vec{n})\left[\sigma_{S}\right]_{i l}\left[\tau_{I}\right]\right]_{j k} a_{l, k}(\vec{n})
$$

## Leading-order action

In the continuum (momentum space):

$$
\begin{aligned}
V_{\mathrm{LO}_{3}} & =C_{0,1} f(\vec{q})\left(\frac{1}{4}-\frac{1}{4} \vec{\sigma}_{1} \cdot \vec{\sigma}_{2}\right)\left(\frac{3}{4}+\frac{1}{4} \boldsymbol{\tau}_{1} \cdot \boldsymbol{\tau}_{2}\right) \\
& +C_{1,0} f(\vec{q})\left(\frac{3}{4}+\frac{1}{4} \vec{\sigma}_{1} \cdot \vec{\sigma}_{2}\right)\left(\frac{1}{4}-\frac{1}{4} \boldsymbol{\tau}_{1} \cdot \boldsymbol{\tau}_{2}\right) \\
& -\left(\frac{g_{A}}{2 F_{\pi}}\right)^{2} \boldsymbol{\tau}_{1} \cdot \boldsymbol{\tau}_{2} \frac{\vec{\sigma}_{1} \cdot \vec{q} \vec{\sigma}_{2} \cdot \vec{q}}{q^{2}+M_{\pi}^{2}}
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On the lattice:

$$
\begin{aligned}
& V_{\mathrm{LO}_{3}}=\frac{1}{L^{3}} \sum_{\vec{q}} f(\vec{q}):\left\{C_{0,1}\left[\frac{3}{32} \rho(\vec{q}) \rho(-\vec{q})-\frac{3}{32} \sum_{S} \rho_{S}(\vec{q}) \rho_{S}(-\vec{q})+\frac{1}{32} \sum_{I} \rho_{I}(\vec{q}) \rho_{I}(-\vec{q})-\frac{1}{32} \sum_{S, I} \rho_{S, I}(\vec{q}) \rho_{S, I}(-\vec{q})\right]\right. \\
&\left.+C_{1,0}[\cdots]\right\}:-\frac{g_{A}^{2} \alpha_{t}}{8 F_{\pi}^{2}} \sum_{S_{1,2}, I, \vec{n}_{1,2}}: \rho_{S_{1}, I}\left(\vec{n}_{1}\right) G_{S_{1} S_{2}} \rho_{S_{2}, I}\left(\vec{n}_{2}\right):
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$$

where the two-derivative pion correlator is defined as $G_{S_{1} S_{2}}(\vec{n}) \equiv\left\langle\nabla_{S_{1}} \pi_{I}\left(\vec{n}, n_{t}\right) \nabla_{S_{2}} \pi_{I}\left(\overrightarrow{0}, n_{t}\right)\right\rangle$

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Other LO lattice actions used in the simulations:

- $\mathrm{LO}_{1}$ : no smearing, $\mathrm{LO}_{2}$ : Gaussian smearing in all waves


## Two-particle phase shifts

Wave function in the asymptotic region (QM potential scattering):
$\Psi(\vec{r})=\left[\cos \delta_{L} j_{L}(k r)-\sin \delta_{L} y_{L}(k r)\right] Y_{L, m}(\theta, \phi)$

## Two-particle phase shifits

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Impose a spherical-wall boundary condition $\Psi\left(\vec{R}_{\text {Wall }}\right)=0$ (standing waves) and determine the energy spectrum

- interaction switched off: $\delta_{L}=0, j_{L}\left(k_{i}^{\text {free }} R_{\text {Wall }}\right)=0$
- interaction switched on: $\tan \left[\delta_{L}\left(k_{i}\right)\right]=\frac{j_{L}\left(k_{i} R_{\text {Wall }}\right)}{y_{L}\left(k_{i} R_{\text {Wall }}\right)}$


Generalization to coupled channels straightforward...

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Generalization to coupled channels straightforward...
Do the same thing on the lattice $\longrightarrow$ two-particle phase shifts from the energy spectrum!
Example: a toy-model potential $\quad V(\vec{r})=C\left\{1+\frac{r^{2}}{R_{0}^{2}}\left[3\left(\hat{r} \cdot \vec{\sigma}_{1}\right)\left(\hat{r} \cdot \vec{\sigma}_{2}\right)-\vec{\sigma}_{1} \cdot \vec{\sigma}_{2}\right]\right\} \exp \left(-\frac{1}{2} \frac{r^{2}}{R_{0}^{2}}\right)$




## Two-nucleon phase shifits $\left(\mathrm{LO}_{3}\right)$

E.E., Krebs, Lee, Meißner, EPJA 45 (10) 335

- 9 LECs fitted to S- and P-waves and the deuteron quadrupole moment
- Coulomb repulsion and isospin-breaking effects taken into account
- Accurate results, deviations consistent with the expected size of higher-order terms



## Calculation strategy

- Eucl.-time propagation of A nucleons $\rightarrow$ transition amplitude $Z_{A}(t)=\left\langle\Psi_{A}\right| \exp (-t H)\left|\Psi_{A}\right\rangle$
$\longrightarrow$ ground-state energies $E_{A}=-\lim _{t \rightarrow \infty} d\left(\ln Z_{A}\right) / d t$
- Excited state energies can be obtained from a large-t limit of a correlation matrix $Z_{A}^{i j}(t)=\left\langle\Psi_{A}^{i}\right| \exp (-t H)\left|\Psi_{A}^{j}\right\rangle$ between A-nucleon states $\Psi_{A}^{j}$ with the proper quantum numb.
- Use $H_{\mathrm{LO}}$ to run the simulation, higher-order terms (incl. Coulomb, 3NF, ...) taken into account perturvatively via $Z_{A}^{O}(t)=\left\langle\Psi_{A}\right| \exp (-t H / 2) O \exp (-t H / 2)\left|\Psi_{A}\right\rangle$


## AFQMC calculation of the ${ }^{4} \mathrm{He}$ BE



- We use temporal spacing $a_{t}=1.32 \mathrm{fm}$ and vary propagation time $L_{t}$ to carry out the $L_{t} \rightarrow \infty$ extrapolation via $E\left(N_{t}\right)=E(\infty)+c_{E} \exp \left(-N_{t} / \tau\right)$

Large-t extrapolated and exact results for ${ }^{2} \mathrm{H}\left(3^{3}, \mathrm{~L}=5.92 \mathrm{fm}\right)$

|  | ${ }^{2} \mathrm{H}$ (extr.) | ${ }^{2} \mathrm{H}$ (exact) |
| :--- | ---: | ---: |
| $E(\mathrm{LO})[\mathrm{MeV}]$ | $-9.070(12)$ | -9.078 |
| $\Delta E\left(\Delta \tilde{M}_{\pi}\right)[\mathrm{MeV}]$ | $-0.003548(12)$ | -0.003569 |
| $\Delta E\left(\Delta M_{\pi}^{\mathrm{IB}}\right)[\mathrm{MeV}]$ | $-0.002372(8)$ | -0.002379 |

## Auxillary Fleld QMC method

Transfer matrix with only nucleon fields (without smearing)

$$
M_{\mathrm{LO}}=: \exp \left(-H_{\text {free }} \alpha_{t}-\frac{1}{2} C \alpha_{t} \sum_{\vec{n}}[\rho(\vec{n})]^{2}-\frac{1}{2} C_{I} \alpha_{t} \sum_{\vec{n}, I}\left[\rho_{I}(\vec{n})\right]^{2}+\frac{g_{A}^{2} \alpha_{t}^{2}}{8 F_{\pi}^{2}} \sum_{S_{1,2}, I, \vec{n}_{1,2}} \rho_{S_{1}, I}\left(\vec{n}_{1}\right) G_{S_{1} S_{2}} \rho_{S_{2}, I}\left(\vec{n}_{2}\right)\right):
$$

## Auxillary Field QMC method

Transfer matrix with only nucleon fields (without smearing)

$$
M_{\mathrm{LO}}=: \exp \left(-H_{\text {free }} \alpha_{t}-\frac{1}{2} C \alpha_{t} \sum_{\vec{n}}[\rho(\vec{n})]^{2}-\frac{1}{2} C_{I} \alpha_{t} \sum_{\vec{n}, I}\left[\rho_{I}(\vec{n})\right]^{2}+\frac{g_{A}^{2} \alpha_{t}^{2}}{8 F_{\pi}^{2}} \sum_{S_{1,2}, I, \vec{n}_{1,2}} \rho_{S_{1}, I}\left(\vec{n}_{1}\right) G_{S_{1} S_{2}} \rho_{S_{2}, I}\left(\vec{n}_{2}\right)\right):
$$

Hubbard-Stratonovich transformation: $\exp \left(\rho^{2} / 2\right) \sim \int_{-\infty}^{\infty} d s \exp \left(-s^{2} / 2-s \rho\right)$

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$$

- Hubbard-Stratonovich transformation: $\exp \left(\rho^{2} / 2\right) \sim \int_{-\infty}^{\infty} d s \exp \left(-s^{2} / 2-s \rho\right)$

with $M_{\mathrm{LO}}^{\left(n_{t}\right)}\left(\pi_{i}, s, s_{I}\right)=: \exp \left(-H_{\mathrm{free}} \alpha_{t}+\sqrt{-C \alpha_{t}} \sum_{\vec{n}} s\left(\vec{n}, n_{t}\right) \rho(\vec{n})+i \sqrt{C_{I} \alpha_{t}} \sum_{\vec{n}, I} s_{I}\left(\vec{n}, n_{t}\right) \rho_{I}(\vec{n})\right.$

$$
\left.-\frac{g_{A} \alpha_{t}}{2 F_{\pi}} \sum_{S, I, \vec{n}}\left(\nabla_{S} \pi_{I}\left(\vec{n}, n_{t}\right)\right) \rho_{S, I}(\vec{n})\right):
$$

and $\quad S_{s s}^{\left(n_{t}\right)}=\frac{1}{2} \sum_{\vec{n}}\left(s\left(\vec{n}, n_{t}\right)\right)^{2}+\frac{1}{2} \sum_{\vec{n}, I}\left(s_{I}\left(\vec{n}, n_{t}\right)\right)^{2}, \quad S_{\pi \pi}^{\left(n_{t}\right)}=\frac{\alpha_{t}}{2} \sum_{\vec{n}, I} \pi_{I}\left(\vec{n}, n_{t}\right)\left[-\Delta+M_{\pi}^{2}\right] \pi_{I}\left(\vec{n}, n_{t}\right)$

## Auxillary Field QMC method



For a given configuration of the auxilliary \& pion fields:

$$
\left\langle\Psi^{\mathrm{init}}\right| e^{-H\left(s, s_{I}, \pi_{I}\right) t}\left|\Psi^{\mathrm{init}}\right\rangle=\operatorname{det} \boldsymbol{G}_{i j}\left(s, s_{I}, \pi_{I}\right) \text { with } \boldsymbol{G}_{i j}\left(s, s_{I}, \pi_{I}\right)=\langle i| e^{-H\left(s, s_{I}, \pi_{I}\right) t}|j\rangle
$$

Simulations for ${ }^{8} \mathrm{Be}$ and ${ }^{12} \mathrm{C}, \mathrm{L}=11.8 \mathrm{fm}$



Ground state energies ( $\mathrm{L}=11.8 \mathrm{fm}$ ) of ${ }^{4} \mathrm{He},{ }^{8} \mathrm{Be},{ }^{12} \mathrm{C}$ \& ${ }^{16} \mathrm{O}$

|  | ${ }^{4} \mathrm{He}$ | ${ }^{8} \mathrm{Be}$ | ${ }^{12} \mathrm{C}$ | ${ }^{16} \mathrm{O}$ |
| :---: | :---: | :---: | :---: | :---: |
| LO $\left[Q^{0}\right]$, in MeV | $-28.0(3)$ | $-57(2)$ | $-96(2)$ | $-144(4)$ |
| NLO $\left[Q^{2}\right]$, in MeV | $-24.9(5)$ | $-47(2)$ | $-77(3)$ | $-116(6)$ |
| NNLO $\left[Q^{3}\right]$, in MeV | $-28.3(6)$ | $-55(2)$ | $-92(3)$ | $-135(6)$ |
| Experiment, in MeV | $\frac{-28.30}{-56.5}$ | $\frac{-92.2}{-127.6}$ |  |  |

## The Hoyle state

EE, Krebs, Lähde, Lee, Meißner, PRL 106 (2011) 192501; PRL 109 (2012) 252501
Lattice results for low-lying even-parity states of ${ }^{12} \mathrm{C}$

|  | $0_{1}^{+}$ | $2_{1}^{+}\left(E^{+}\right)$ | $0_{2}^{+}$ | $2_{2}^{+}\left(E^{+}\right)$ |
| :---: | :---: | :---: | :---: | :---: |
| LO | $-96(2)$ | $-94(2)$ | $-89(2)$ | $-88(2)$ |
| NLO | $-77(3)$ | $-74(3)$ | $-72(3)$ | $-70(3)$ |
| NNLO | $-92(3)$ | $-89(3)$ | $-85(3)$ | $-83(3)$ |
| Exp | -92.16 | -87.72 | -84.51 | $-82(1)$ |

Probing (a-cluster) structure of the $\mathbf{0 1}^{\mathbf{+}}, \mathbf{0}_{\mathbf{2}}{ }^{+}$states


RMS radii and quadrupole moments

|  | LO | Experiment |
| :--- | :---: | :---: |
| $r\left(0_{1}^{+}\right)[\mathrm{fm}]$ | $2.2(2)$ | $2.47(2)[26]$ |
| $r\left(2_{1}^{+}\right)[\mathrm{fm}]$ | $2.2(2)$ | - |
| $Q\left(2_{1}^{+}\right)\left[e \mathrm{fm}^{2}\right]$ | $6(2)$ | $6(3)[27]$ |
| $r\left(0_{2}^{+}\right)[\mathrm{fm}]$ | $2.4(2)$ | - |
| $r\left(2_{2}^{+}[\mathrm{fm}]\right.$ | $2.4(2)$ | - |
| $Q\left(2_{2}^{+}\right)\left[e \mathrm{fm}^{2}\right]$ | $-7(2)$ | - |

## Summary: nuclear lattice simulations

- combining EFT and lattice simulations $\longrightarrow$ access to (light) nuclei
- exciting results for the ${ }^{12} \mathrm{C}$ spectrum, first ab initio calculation of the Hoyle state
- Work in progress: spectrum of ${ }^{16} \mathrm{O}$, volume dependence, reactions ...

