



Evgeny Epelbaum, RUBNuclear Physics School 2013, Otranto, Italy, May 27-31, 2013

Modern Theory of nuclear forces

Lectures 1+2: Foundations

- <u>Lecture 3</u>: 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

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





- unified description of ππ, πN and NN
- consistent many-body forces and currents
- systematically improvable
- bridging different reactions (electroweak, π-prod., ...)
- precision physics with/from light nuclei

Chiral expansion of nuclear forces



(numbers from Pudliner et al. PRL 74 (95) 4396)

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; ...



'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; ...



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; ...



E.E. et al. '04,'05,'07; ...

by chiral symmetry and exp. information on the πN system

 $\mathcal{V}_{NN} \;=\; V_C(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_C(r) \;+\; \left[V_S(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_S(r) \right] \vec{\sigma}_1 \cdot \vec{\sigma}_2$

 $+ \left[V_T(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_T(r) \right] \left(3 \vec{\sigma}_1 \cdot \hat{r} \vec{\sigma}_2 \cdot \hat{r} - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) + \left[V_{LS}(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_{LS}(r) \right] \vec{L} \cdot \vec{S} \,,$

$$\begin{aligned} \mathcal{V}_{NN} &= V_C(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_C(r) + \left[V_S(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_S(r) \right] \vec{\sigma}_1 \cdot \vec{\sigma}_2 \\ &+ \left[V_T(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_T(r) \right] \left(3\vec{\sigma}_1 \cdot \hat{r}\vec{\sigma}_2 \cdot \hat{r} - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) + \left[V_{LS}(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_{LS}(r) \right] \vec{L} \cdot \vec{S} \,, \end{aligned}$$

The profile functions (in Dimensional Regularization)

$$\begin{split} V_C^{TPE}(r) &= \frac{3g^2m^6}{32\pi^2f^4} \frac{e^{-2x}}{x^6} \Big\{ \left(2c_1 + \frac{3g^2}{16M} \right) x^2 (1+x)^2 + \frac{g^5x^5}{32M} + \left(c_3 + \frac{3g^2}{16M} \right) \left(6 + 12x + 10x^2 + 4x^3 + x^4 \right) \\ W_T^{TPE}(r) &= \frac{g^2m^6}{48\pi^2f^4} \frac{e^{-2x}}{x^6} \Big\{ - \left(c_4 + \frac{1}{4M} \right) (1+x) (3+3x+x^2) + \frac{g^2}{32M} \left(36+72x+52x^2+17x^3+2x^4 \right) \Big\}, \\ V_T^{TPE}(r) &= \frac{g^4m^5}{128\pi^3f^4x^4} \Big\{ - 12K_0(2x) - (15+4x^2)K_1(2x) + \frac{3\pi m e^{-2x}}{8Mx} \left(12x^{-1} + 24 + 20x + 9x^2 + 2x^3 \right) \Big\}, \\ W_C^{TPE}(r) &= \frac{g^4m^5}{128\pi^3f^4x^4} \Big\{ \left[1+2g^2(5+2x^2) - g^4(23+12x^2) \right] K_1(2x) + x \left[1+10g^2 - g^4(23+4x^2) \right] K_0(2x) + \frac{g^2m\pi e^{-2x}}{4Mx} \left[2(3g^2-2) \left(6x^{-1} + 12 + 10x + 4x^2 + x^3 \right) \right] + g^2x \left(2+4x+2x^2+3x^2 \right) \Big\}, \\ V_S^{TPE}(r) &= \frac{g^4m^5}{32\pi^3f^4} \Big\{ 3xK_0(2x) + (3+2x^2)K_1(2x) - \frac{3\pi m e^{-2x}}{16Mx} \left(6x^{-1} + 12 + 11x + 6x^2 + 2x^3 \right) \Big\}, \\ W_S^{TPE}(r) &= \frac{g^2m^6}{48\pi^2f^4} \frac{e^{-2x}}{x^6} \Big\{ \left(c_4 + \frac{1}{4M} \right) (1+x) (3+3x+2x^2) - \frac{g^2}{16M} \left(18+36x+31x^2+14x^3+2x^4 \right) \Big\}, \\ V_{LS}^{TPE}(r) &= -\frac{3g^4m^6}{64\pi^2Mf^4} \frac{e^{-2x}}{x^6} (1+x) \left(2+2x+x^2 \right), \\ W_{LS}^{TPE}(r) &= \frac{g^2(g^2-1)m^6}{32\pi^2Mf^4} \frac{e^{-2x}}{x^6} (1+x)^2, \end{split}$$

 $\mathcal{V}_{NN} = V_C(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_C(r) + \left[V_S(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_S(r) \right] \vec{\sigma}_1 \cdot \vec{\sigma}_2$

 $+ \left[V_T(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_T(r) \right] \left(3\vec{\sigma}_1 \cdot \hat{r}\vec{\sigma}_2 \cdot \hat{r} - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) + \left[V_{LS}(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_{LS}(r) \right] \vec{L} \cdot \vec{S} \,,$



 $\mathcal{V}_{NN} = V_C(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_C(r) + \left[V_S(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_S(r) \right] \vec{\sigma}_1 \cdot \vec{\sigma}_2$

 $+ \left[V_T(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_T(r) \right] \left(3 \vec{\sigma}_1 \cdot \hat{r} \vec{\sigma}_2 \cdot \hat{r} - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) + \left[V_{LS}(r) + \vec{\tau}_1 \cdot \vec{\tau}_2 W_{LS}(r) \right] \vec{L} \cdot \vec{S} \,,$



Is there any evidence from NN data?

Chiral two-pion exchange and NN data



"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



Neutron-proton phase shifts at N³LO

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



The challenge: Understanding the 3N 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)

 $\tilde{\mathcal{G}}_1 = 1$. $\tilde{\mathcal{G}}_2 = \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_3,$ $\tilde{\mathcal{G}}_3 = \vec{\sigma}_1 \cdot \vec{\sigma}_3$ $\tilde{\mathcal{G}}_4 = \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_3 \, \vec{\sigma}_1 \cdot \vec{\sigma}_3 \, .$ $\tilde{\mathcal{G}}_5 = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \vec{\sigma}_1 \cdot \vec{\sigma}_2 \, .$ $\tilde{\mathcal{G}}_6 = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3) \,,$ $ilde{\mathcal{G}}_7 = \boldsymbol{ au}_1 \cdot (\boldsymbol{ au}_2 imes \boldsymbol{ au}_3) \, ec{\sigma}_2 \cdot (\hat{r}_{12} imes \hat{r}_{23}) \, ,$ $\tilde{\mathcal{G}}_{8} = \hat{r}_{23} \cdot \vec{\sigma}_{1} \, \hat{r}_{23} \cdot \vec{\sigma}_{3} \, ,$ $\tilde{\mathcal{G}}_{9} = \hat{r}_{23} \cdot \vec{\sigma}_{3} \hat{r}_{12} \cdot \vec{\sigma}_{1},$ $\mathcal{G}_{10} = \hat{r}_{23} \cdot \vec{\sigma}_1 \, \hat{r}_{12} \cdot \vec{\sigma}_3$ $\tilde{\mathcal{G}}_{11} = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{23} \cdot \vec{\sigma}_1 \, \hat{r}_{23} \cdot \vec{\sigma}_2 \, .$ $\tilde{\mathcal{G}}_{12} = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{23} \cdot \vec{\sigma}_1 \, \hat{r}_{12} \cdot \vec{\sigma}_2 \, .$ $\tilde{\mathcal{G}}_{13} = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{12} \cdot \vec{\sigma}_1 \, \hat{r}_{23} \cdot \vec{\sigma}_2 \,,$ $\tilde{\mathcal{G}}_{14} = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{12} \cdot \vec{\sigma}_1 \, \hat{r}_{12} \cdot \vec{\sigma}_2 \, ,$ $\tilde{\mathcal{G}}_{15} = \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{13} \cdot \vec{\sigma}_1 \, \hat{r}_{13} \cdot \vec{\sigma}_3 \, ,$ $\tilde{\mathcal{G}}_{16} = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{12} \cdot \vec{\sigma}_2 \, \hat{r}_{12} \cdot \vec{\sigma}_3 \,,$ $\tilde{\mathcal{G}}_{17} = \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{23} \cdot \vec{\sigma}_1 \, \hat{r}_{12} \cdot \vec{\sigma}_3 \, ,$ $\mathcal{G}_{18} = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_1 \cdot \vec{\sigma}_3 \, \vec{\sigma}_2 \cdot (\hat{r}_{12} \times \hat{r}_{23}),$ $\tilde{\mathcal{G}}_{19} = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_3 \cdot \hat{r}_{23} \, \hat{r}_{23} \cdot (\vec{\sigma}_1 \times \vec{\sigma}_2) \, .$ $\tilde{\mathcal{G}}_{20} = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_1 \cdot \hat{r}_{23} \, \vec{\sigma}_2 \cdot \hat{r}_{23} \, \vec{\sigma}_3 \cdot (\hat{r}_{12} \times \hat{r}_{23}),$ $\hat{\mathcal{G}}_{21} = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_1 \cdot \hat{r}_{13} \, \vec{\sigma}_3 \cdot \hat{r}_{13} \, \vec{\sigma}_2 \cdot (\hat{r}_{12} \times \hat{r}_{23}),$ $\tilde{\mathcal{G}}_{22} = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_1 \cdot \hat{r}_{23} \, \vec{\sigma}_3 \cdot \hat{r}_{12} \, \vec{\sigma}_2 \cdot (\hat{r}_{12} \times \hat{r}_{23}),$



Building blocks:

 $\boldsymbol{ au}_1, \ \boldsymbol{ au}_2, \ \boldsymbol{ au}_3, \ ec{\sigma}_1, \ ec{\sigma}_2, \ ec{\sigma}_3, \ ec{r}_{12}, \ ec{r}_{23}$

Constraints:

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

$$\longrightarrow V_{3N} = \sum_{i=1}^{22} \mathcal{G}_i F_i(r_{12}, r_{23}, r_{31}) + 5 \text{ perm.}$$

Most general structure of a local 3NF

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

22 independent operators (coord. space)

 $\tilde{\mathcal{G}}_1 = 1$, $\tilde{\mathcal{G}}_2 = \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_3,$ $\tilde{\mathcal{G}}_3 = \vec{\sigma}_1 \cdot \vec{\sigma}_3$ $\tilde{\mathcal{G}}_4 = \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_3 \, \vec{\sigma}_1 \cdot \vec{\sigma}_3 \, .$ $\tilde{\mathcal{G}}_5 = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \vec{\sigma}_1 \cdot \vec{\sigma}_2 \, .$ $\tilde{\mathcal{G}}_6 = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3) \,,$ $ilde{\mathcal{G}}_7 = \boldsymbol{ au}_1 \cdot (\boldsymbol{ au}_2 imes \boldsymbol{ au}_3) \, ec{\sigma}_2 \cdot (\hat{r}_{12} imes \hat{r}_{23}) \, ,$ $\tilde{\mathcal{G}}_{8} = \hat{r}_{23} \cdot \vec{\sigma}_{1} \, \hat{r}_{23} \cdot \vec{\sigma}_{3} \, ,$ $\tilde{\mathcal{G}}_{9} = \hat{r}_{23} \cdot \vec{\sigma}_{3} \hat{r}_{12} \cdot \vec{\sigma}_{1},$ $\mathcal{G}_{10} = \hat{r}_{23} \cdot \vec{\sigma}_1 \, \hat{r}_{12} \cdot \vec{\sigma}_3$ $\tilde{\mathcal{G}}_{11} = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{23} \cdot \vec{\sigma}_1 \, \hat{r}_{23} \cdot \vec{\sigma}_2 \, .$ $\tilde{\mathcal{G}}_{12} = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{23} \cdot \vec{\sigma}_1 \, \hat{r}_{12} \cdot \vec{\sigma}_2 \, .$ $\tilde{\mathcal{G}}_{13} = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{12} \cdot \vec{\sigma}_1 \, \hat{r}_{23} \cdot \vec{\sigma}_2 \,,$ $\tilde{\mathcal{G}}_{14} = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{12} \cdot \vec{\sigma}_1 \, \hat{r}_{12} \cdot \vec{\sigma}_2 \, ,$ $\tilde{\mathcal{G}}_{15} = \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{13} \cdot \vec{\sigma}_1 \, \hat{r}_{13} \cdot \vec{\sigma}_3 \, ,$ $\tilde{\mathcal{G}}_{16} = \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{12} \cdot \vec{\sigma}_2 \, \hat{r}_{12} \cdot \vec{\sigma}_3 \,,$ $\tilde{\mathcal{G}}_{17} = \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_3 \, \hat{r}_{23} \cdot \vec{\sigma}_1 \, \hat{r}_{12} \cdot \vec{\sigma}_3 \, ,$ $\mathcal{G}_{18} = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_1 \cdot \vec{\sigma}_3 \, \vec{\sigma}_2 \cdot (\hat{r}_{12} \times \hat{r}_{23}),$ $\tilde{\mathcal{G}}_{19} = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_3 \cdot \hat{r}_{23} \, \hat{r}_{23} \cdot (\vec{\sigma}_1 \times \vec{\sigma}_2) \, .$ $\tilde{\mathcal{G}}_{20} = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_1 \cdot \hat{r}_{23} \, \vec{\sigma}_2 \cdot \hat{r}_{23} \, \vec{\sigma}_3 \cdot (\hat{r}_{12} \times \hat{r}_{23}),$ $\hat{\mathcal{G}}_{21} = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_1 \cdot \hat{r}_{13} \, \vec{\sigma}_3 \cdot \hat{r}_{13} \, \vec{\sigma}_2 \cdot (\hat{r}_{12} \times \hat{r}_{23}),$ $\tilde{\mathcal{G}}_{22} = \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) \, \vec{\sigma}_1 \cdot \hat{r}_{23} \, \vec{\sigma}_3 \cdot \hat{r}_{12} \, \vec{\sigma}_2 \cdot (\hat{r}_{12} \times \hat{r}_{23}),$



Building blocks:

 $\boldsymbol{ au}_1, \ \boldsymbol{ au}_2, \ \boldsymbol{ au}_3, \ ec{\sigma}_1, \ ec{\sigma}_2, \ ec{\sigma}_3, \ ec{r}_{12}, \ ec{r}_{23}$

Constraints:

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

$$\longrightarrow V_{3N} = \sum_{i=1}^{22} \mathcal{G}(F_i(r_{12}, r_{23}, r_{31})) + 5$$
 perm.

derivable in ChPT; long-range terms parameter-free predictions

Leading chiral 3NF and 3N/4N continuum

- Nd scattering: accurate description at low energy except for Ay-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. ³H, ⁴He BEs)

Nd elastic cross sections at low energies

Nd breakup at E_d=130 MeV Stephan et al., PRC 82 (2010) 014003





Leading chiral 3NF and 3N/4N continuum

- Nd scattering: accurate description at low energy except for Ay-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. ³H, ⁴He BEs)



Corrections to the leading 3NF beyond N²LO are being investigated

Krebs, Gasparyan, EE '12





Krebs, Gasparyan, EE '12



Krebs, Gasparyan, EE '12



Krebs, Gasparyan, EE '12







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



Values of low-energy constants extracted at Q⁴ (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}	$ar{e}_{15}$	\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 E_{lab} ~ 200 MeV.
- 3NF: promising results at N²LO; corrections are under investigation
- 4NF: starts contributing at N³LO; probably small (expectation value for the α-particle about a few 100 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,

Eur. Phys. J A41 (09) 125,

E.E., Krebs, Lee, Meißner, Eur. Phys. J A40 (09) 199,



Phys. Rev. Lett 104 (10) 142501, Eur. Phys. J. 45 (10) 335, Phys. Rev. Lett. 106 (11) 192501, E.E., Krebs, Lähde, Lee, Meißner Phys. Rev. Lett. 109 (12) 252501, Phys. Rev. Lett. 110 (13) 112502, arXiv:1303.4856





Deutsche Forschungsgemeinschaft DFG

HELMHOLTZ **GEMEINSCHAFT**





European Research Council

Nuclear lattice simulations

Discretized version of chiral EFT for nuclear dynamics

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



 fundamental, the only parameters are m_q, α_{strong}

hard to go beyond 1 hadron...



 effective hadronic description, LECs to be determined from the data/LQCD

Chiral EFT on the lattice

much more efficient for atomic nuclei

- \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)



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

• Free Hamiltonian for non-relativistic nucleons: $H_{\text{free}} = \frac{1}{2m} \sum_{\vec{n},i,j} a_{ij}^{\dagger}(\vec{n}) \sum_{l} \nabla_{l}^{2} a_{ij}(\vec{n})$

• Nucleon local density operators $\rho(\vec{n}) = \sum_{i,j} a_{i,j}^{\dagger}(\vec{n}) a_{i,j}(\vec{n}), \quad \rho_S(\vec{n}) = \sum_{i,j,k} a_{i,j}^{\dagger}(\vec{n}) [\sigma_S]_{ik} a_{k,j}(\vec{n})$ $\rho_I(\vec{n}) = \sum_{i,j,k} a_{i,j}^{\dagger}(\vec{n}) [\tau_I]_{jk} a_{i,k}(\vec{n}), \quad \rho_{S,I}(\vec{n}) = \sum_{i,j,k,l} a_{i,j}^{\dagger}(\vec{n}) [\sigma_S]_{il} [\tau_I]_{jk} a_{l,k}(\vec{n})$

In the continuum (momentum space):

$$\begin{split} V_{\rm LO_3} &= C_{0,1} f(\vec{q}) \left(\frac{1}{4} - \frac{1}{4} \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) \left(\frac{3}{4} + \frac{1}{4} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \right) \\ &+ C_{1,0} f(\vec{q}) \left(\frac{3}{4} + \frac{1}{4} \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) \left(\frac{1}{4} - \frac{1}{4} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \right) \\ &- \left(\frac{g_A}{2F_{\pi}} \right)^2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \frac{\vec{\sigma}_1 \cdot \vec{q} \, \vec{\sigma}_2 \cdot \vec{q}}{q^2 + M_{\pi}^2} \end{split}$$



In the continuum (momentum space):

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



On the lattice:

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

where the two-derivative pion correlator is defined as $G_{S_1S_2}(\vec{n}) \equiv \langle \nabla_{S_1} \pi_I(\vec{n}, n_t) \nabla_{S_2} \pi_I(\vec{0}, n_t) \rangle$

In the continuum (momentum space):

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



On the lattice:

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

where the two-derivative pion correlator is defined as $G_{S_1S_2}(\vec{n}) \equiv \langle \nabla_{S_1}\pi_I(\vec{n}, n_t) \nabla_{S_2}\pi_I(\vec{0}, n_t) \rangle$

Other LO lattice actions used in the simulations:

LO1: no smearing, LO2: Gaussian smearing in all waves

Borasoy, E.E., Krebs, Lee, Meißner, EPJA 34 (2007) 185

Wave function in the asymptotic region (QM potential scattering):





$$C = -2 \operatorname{MeV}, R_0 = 2 \times 10^{-2} \operatorname{MeV}^{-1}$$
$$\frac{r^2}{R_0^2} [3(\hat{r} \cdot \vec{\sigma}_1)(\hat{r} \cdot \vec{\sigma}_2) - \vec{\sigma}_1 \cdot \vec{\sigma}_2] \right\} \exp\left(-\frac{1}{2} \frac{r^2}{R_0^2}\right)$$
$$^3 S(D)_1 \qquad -0.155 \operatorname{MeV}$$

Borasoy, E.E., Krebs, Lee, Meißner, EPJA 34 (2007) 185



Generalization to coupled channels straightforward...

$$C = -2 \operatorname{MeV}, R_{0} = 2 \times 10^{-2} \operatorname{MeV}^{-1}$$

$$C = -2 \operatorname{MeV}, R_{0} = 2 \times 10^{-2} \operatorname{MeV}^{-1}$$

$$r^{2} \frac{V(\vec{r}) = C}{R_{0}^{2}} \left\{ 1 + \frac{r^{2}}{R_{0}^{2}} \frac{[3(\hat{r} \cdot \vec{\sigma}_{1})(\hat{r} \cdot \vec{\sigma}_{2}) + \vec{r}^{2}\vec{\sigma}_{1} \cdot \vec{\sigma}_{2}]}{[3(\hat{r} \cdot \vec{\sigma}_{1})(\hat{r} \cdot \vec{\sigma}_{2}) + R_{0}^{2}]} \right\} \exp\left(-\frac{1}{2} \frac{r^{2}}{R_{0}^{2}}\right)$$

$$\frac{^{3}S(D)_{1}}{^{-0.155} \operatorname{MeV}} -0.155 \operatorname{MeV}$$

Borasoy, E.E., Krebs, Lee, Meißner, EPJA 34 (2007) 185



Generalization to coupled channels straightforward...

Do the same thing on the lattice 2 MeV, $R_0 = 2 \times 10^{-2} \text{ MeV}$ for the energy spectrum! $C = -2 \text{ MeV}, R_0 = 2 \times 10^{-2} \text{ MeV}$ $\frac{r^2}{MeV} \left[V(\vec{r}) = C \left\{ 1 + \frac{r^2}{R_0^2} [3(\hat{r} \cdot \vec{\sigma}_1)(\hat{r} \cdot \vec{\sigma}_2) + R_0^2] \right\} \exp\left(-\frac{1}{2} \frac{r^2}{R_0^2}\right) \cdot \vec{\sigma}_2 \right] \exp\left(-\frac{1}{2} \frac{r^2}{R_0^2}\right)$ $\frac{^3S(D)_1}{^{-0.155} \text{ MeV}} = -0.155 \text{ MeV}$

Borasoy, E.E., Krebs, Lee, Meißner, EPJA 34 (2007) 185



Generalization to coupled channels straightforward...



Two-nucleon phase shifts (LO₃)

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 $Z_A(t) = \langle \Psi_A | \exp(-tH) | \Psi_A \rangle$

 \rightarrow ground-state energies $E_A = -\lim_{t \to \infty} d(\ln Z_A)/dt$

Excited state energies can be obtained from a large-t limit of a correlation matrix $Z_A^{ij}(t) = \langle \Psi_A^i | \exp(-tH) | \Psi_A^j \rangle$ between A-nucleon states Ψ_A^j with the proper quantum numb.

Use H_{LO} to run the simulation, higher-order terms (incl. Coulomb, 3NF, ...) taken into account perturvatively via $Z_A^O(t) = \langle \Psi_A | \exp(-tH/2) O \exp(-tH/2) | \Psi_A \rangle$



AFQMC calculation of the ⁴He BE

We use temporal spacing $a_t = 1.32 \text{ fm}$ and vary propagation time L_t to carry out the $L_t \to \infty$ extrapolation via $E(N_t) = E(\infty) + c_E \exp(-N_t/\tau)$

Large-t extrapolated and exact results for ²H (3³, L=5.92 fm)

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

Transfer matrix with only nucleon fields (without smearing)

$$M_{\rm LO} =: \exp\left(-H_{\rm free}\alpha_t - \frac{1}{2}C\alpha_t\sum_{\vec{n}}\left[\rho(\vec{n}\,)\right]^2 - \frac{1}{2}C_I\alpha_t\sum_{\vec{n},I}\left[\rho_I(\vec{n}\,)\right]^2 + \frac{g_A^2\alpha_t^2}{8F_\pi^2}\sum_{S_{1,2},I,\vec{n}_{1,2}}\rho_{S_1,I}(\vec{n}_1\,)\,G_{S_1S_2}\,\rho_{S_2,I}(\vec{n}_2\,)\right):$$

Transfer matrix with only nucleon fields (without smearing)

$$M_{\rm LO} =: \exp\left(-H_{\rm free}\alpha_t - \frac{1}{2}C\alpha_t\sum_{\vec{n}}\left[\rho(\vec{n}\,)\right]^2 - \frac{1}{2}C_I\alpha_t\sum_{\vec{n},I}\left[\rho_I(\vec{n}\,)\right]^2 + \frac{g_A^2\alpha_t^2}{8F_\pi^2}\sum_{S_{1,2},I,\vec{n}_{1,2}}\rho_{S_1,I}(\vec{n}_1\,)\,G_{S_1S_2}\,\rho_{S_2,I}(\vec{n}_2\,)\right):$$

Hubbard-Stratonovich transformation:



$$Z_A(t) \propto \int_{-\infty}^{\infty} \mathcal{D}s \prod_{I=1,2,3} \mathcal{D}s_I \mathcal{D}\pi_I \exp(-S_{\pi\pi} - S_{ss}) \det \mathcal{M}(\pi)$$

 L_t $\mathcal{M}_{i,j}(\pi_I, s, s_I) = \langle \psi_{i,X} | M_X^{(L_t-1)} \cdots M_X^{(0)} | \psi_{j,X}
angle$

Transfer matrix with only nucleon fields (without smearing)

$$M_{\rm LO} =: \exp\left(-H_{\rm free}\alpha_t - \frac{1}{2}C\alpha_t\sum_{\vec{n}}\left[\rho(\vec{n}\,)\right]^2 - \frac{1}{2}C_I\alpha_t\sum_{\vec{n},I}\left[\rho_I(\vec{n}\,)\right]^2 + \frac{g_A^2\alpha_t^2}{8F_\pi^2}\sum_{S_{1,2},I,\vec{n}_{1,2}}\rho_{S_1,I}(\vec{n}_1\,)\,G_{S_1S_2}\,\rho_{S_2,I}(\vec{n}_2\,)\right):$$

Hubbard-Stratonovich transformation:



Transfer matrix with (instantaneous) $Z_A(t_L) = \int_{-\infty}^{\infty} D_{T_I} D_{S_I} D_{T_I} D_{S_I} D_{T_I} \frac{D_{T_I} D_{S_I} D_{S_I} \frac{D_{T_I} D_{S_I} \frac{D_{T_I} D_{S_I} D_{S_I} \frac{D_{T_I} D_{S_I} \frac{D_{T_I} D_{S_I} D_{S_I} \frac{D_{T_I} D_{S_I} D_{S_I} \frac{D_{T_I} D_{S_I} D_{S_I} \frac{D_{T_I} D_{S_I} \frac{D_{T_I}$

with
$$M_{\text{LO}}^{(n_t)}(\pi_i, s, s_I) = : \exp\left(-H_{\text{free}}\alpha_t + \sqrt{-C\alpha_t}\sum_{\vec{n}} s(\vec{n}, n_t) \rho(\vec{n}\,) + i\sqrt{C_I\alpha_t}\sum_{\vec{n},I} s_{\vec{h}}(\vec{n}, n_t) \rho_I(\vec{n}\,) - \frac{g_A\alpha_t}{2F_{\pi}}\sum_{S,I,\vec{n}} \left(\nabla_S \pi_I(\vec{n}, n_t)\right) \rho_{\mathcal{M}_{\vec{h}}}(\vec{n}, \vec{n}) = \langle \psi_{i,X} | M_X^{(L_t-1)} \cdots M_X^{(0)} | \psi_{j,X} \rangle$$

and
$$S_{ss}^{(n_t)} = \frac{1}{2} \sum_{\vec{n}} \left(s(\vec{n}, n_t) \right)^2 + \frac{1}{2} \sum_{\vec{n}, I} \left(s_I(\vec{n}, n_t) \right)^2$$
, $S_{\pi\pi}^{(n_t)} = \frac{\alpha_t}{2} \sum_{\vec{n}, I} \pi_I(\vec{n}, n_t) \left[-\Delta + M_{\pi}^2 \right] \pi_I(\vec{n}, n_t)$



For a given configuration of the auxilliary & pion fields:

 $\langle \Psi^{\text{init}} | e^{-H(s,s_I,\pi_I)t} | \Psi^{\text{init}} \rangle = \det \boldsymbol{G}_{ij}(s,s_I,\pi_I) \text{ with } \boldsymbol{G}_{ij}(s,s_I,\pi_I) = \langle i | e^{-H(s,s_I,\pi_I)t} | j \rangle$

Ground states of ⁸Be and ¹²C

E.E., Krebs, Lee, Meißner, PRL 106 (11) 192501

Simulations for ⁸Be and ¹²C, L=11.8 fm



Ground state energies (L=11.8 fm) of ⁴He, ⁸Be, ¹²C & ¹⁶O

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

	0^+_1	$2^+_1(E^+)$	0_{2}^{+}	$2^+_2(E^+)$
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 0₁+, 0₂+ states



RMS radii and quadrupole moments

	LO	Experiment
$r(0_1^+)$ [fm]	2.2(2)	2.47(2) [26]
$r(2_1^+)$ [fm]	2.2(2)	_
$Q(2_1^+) \ [e \ {\rm fm}^2]$	6(2)	6(3) [27]
$r(0_2^+)$ [fm]	2.4(2)	—
$r(2_2^+)$ [fm]	2.4(2)	_
$Q(2_2^+) \ [e \ {\rm fm}^2]$	-7(2)	_

Summary: nuclear lattice simulations

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