Nuclei on the Lattice: Chiral Effective Field Theory Approach

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Nuclear Lattice Effective Field Theory collaboration

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Outline

- ChPT and low energy QCD
- Nuclear forces in chiral EFT
- Lattice EFT as an access to many-body physics
- Nucleon-Nucleon scattering within Lattice EFT
- Application to light nuclei
- Summary & Outlook

Nucleon-Nucleon forces

Phenomenological description by Meson-exchange



QCD Interpretation of NN forces

NN force as residual strong interaction between hadrons



Boson-Exchange Models as basis for NN-force
Highly sophisticated phen. NN potentials
Excellent description of many experimental data
Connection to QCD is unclear

Chiral EFT Interpretation of NN forces

- Model independent treatment
- At low energies NN force dominated by Goldstone Boson dynamics + short range int.
- Systematic perturbative description of few nucleon potentials
- Underlying QCD symmetries implemented by construction

Weinberg's scheme for NN

Weinberg, Nucl. Phys. B 363: 3 (1991)

No perturbative description for bound states



Construct effective potential perturbatively



Solve Lippmann-Schwinger equation nonperturbatively



Nucleon-nucleon force up to N³LO

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



+ 1/m and isospin-breaking corrections...

Neutron-proton phase shifts up to N³LO

np scattering at 50 MeV



Deuteron binding energy & asymptotic normalizations A_s and n_d

	NLO	$N^{2}LO$	$N^{3}LO$	Exp
$E_{d} [MeV]$ $A_{S} [fm^{-1/2}]$ n_{d}	$-2.171 \dots - 2.186$	-2.1892.202	-2.2162.223	-2.224575(9)
	$0.868 \dots 0.873$	0.8740.879	0.8820.883	0.8846(9)
	$0.0256 \dots 0.0257$	0.02550.0256	0.02540.0255	0.0256(4)

Entem & Machleidt '03; Epelbaum, Glöckle & Meißner '05

Three-nucleon forces

Three-nucleon forces in chiral EFT start to contribute at NNLO

(U. van Kolck ´94; Epelbaum et al. ´02; Nogga et al. ´05; Navratil et al. ´07)



 $c_{1,3,4}$ from the fit to πN -scattering data

D, *E* from ${}^{3}H, {}^{4}He, {}^{10}B$ binding energy + coherent *nd* - scattering length

LECs D and E incorporate short-range contr.



Resonance saturation interpretation of LECs



Delta contributions encoded in LECs (Bernard, Kaiser & Meißner '97)

$$c_3 = -2c_4 = c_3(\cancel{A}) - \boxed{\frac{4h_A^2}{9\Delta}}$$

Enlargement due to
Delta contribution



polarization transfer: $E_p^{\text{Lab}} = 22.7 \text{ MeV}$





For references see recent reviews:

Epelbaum, Prog. Part Nucl. Phys. 57 (06) 654 Epelbaum, Hammer, Meißner, Rev. Mod. Phys. 81 (09) 1773 Entem, Machleidt, Phys. Rept. 503 (11) 1 Epelbaum, Meißner, arXiv:1201.2136, to appear in Ann. Rev. Nucl. Part. Sci. Kalantar et al. Rep. Prog. Phys. 75 (12) 016301

- Generally good description of data.
 But some discrepancies arise. E.g.
 break-up observables for SCRE/SST
 configuration at low energy
- Hope for improvement at N³LO

Proton-³He elastic scattering

Viviani, Girlanda, Kievsky, Marcucci, Rosati arXiv: 1004.1306

p-³He differential cross section at low energies

proton vector analyzing power Ay-puzzle



As in n-d scattering case N^2LO 3NF's are not enough to resolve underprediction of A_y



Hope for improvement at higher orders

Three-nucleon forces

Three-nucleon forces at N³LO

Long range contributions Bernard, Epelbaum, H.K., Meißner ´08; Ishikawa, Robilotta ´07

- No additional free parameters
- \checkmark Expressed in terms of g_A, F_π, M_π
- Rich isospin-spin-orbit structure
- $\Delta(1232)$ -contr. are important



Shorter range contributions

Bernard, Epelbaum, H.K., Meißner ´11

- LECs needed for shorter range contr. $g_A, F_{\pi}, M_{\pi}, C_T$
- Central NN contact interaction does not contribute
- Unique expressions in the static limit for a renormalizable 3NF





Nuclear lattice simulations

Borasoy, H.K., Lee, Meißner, Nucl. Phys. A768 (2006) 179



Transfer matrix method

- Correlator function for A nucleons $Z_A(t) = \langle \Psi_A | \exp(-tH) | \Psi_A \rangle$ Slater Determinants for A free Nucleons
 - Ground state energy by time derivative of the correlator

$$E(t) = -\frac{d}{dt} \ln Z_A(t)$$

At large time only ground states survive

 $E_A^0 = \lim_{t \to \infty} E_A(t)$

Expectation value of normal ordered operator ():

$$Z_A^{\mathcal{O}}(t) = \langle \Psi_A | \exp(-tH/2)\mathcal{O}\exp(-tH/2) | \Psi_A \rangle$$
$$\lim_{t \to \infty} \frac{Z_A^{\mathcal{O}}(t)}{Z_A(t)} = \langle \Psi_A^0 | \mathcal{O} | \Psi_A^0 \rangle$$

Monte Carlo with auxiliary fields



Correlation function as path-integral over pions and auxiliary fields

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

Slater-determinant of single nucleon matrix elements

Single-nucleon matrix elements L_t -th temporal lattice step $\mathcal{M}_{i,j}(\pi_I, s, s_I) = \langle \psi_{i,X} | M_X^{(L_t-1)} \cdots M_X^{(0)} | \psi_{j,X} \rangle$

Free nucleons and pions

Positive definite free action:
$$\alpha_t = a_t/a$$

$$S_{ss}(s,s_I) = \frac{1}{2} \sum_{\vec{n}} s(\vec{n})^2 + \frac{1}{2} \sum_{I=1,2,3} \sum_{\vec{n}} s_I(\vec{n})^2 \quad \text{Auxiliary field contributions}$$

$$S_{\pi\pi}(\pi_I) = \frac{\alpha_t}{2} \sum_{I=1,2,3} \sum_{\vec{n}} \pi_I(\vec{n})(-\Delta + M_{\pi}^2)\pi_I(\vec{n}) \quad \text{Free instantaneous pions}$$

$$O(a^4) \text{-improved free nucleon lattice Hamiltonian} \quad f_{0,1,2,3} = \frac{49}{2}, -\frac{3}{4}, \frac{3}{40}, -\frac{1}{180}$$

$$H_{\text{free}} = \frac{1}{m} \sum_{k=0}^{3} \sum_{\vec{n}_s, l_s, i, j} f_k \left[a_{i,j}^{\dagger}(\vec{n}_s) \left[a_{i,j}(\vec{n}_s + k \, \hat{l}_s) + a_{i,j}(\vec{n}_s - k \, \hat{l}_s) \right] \right]$$

Nucleon density operators with different spin-isospin polarizations

$$\rho^{a^{\dagger},a}(\vec{n}_{s}) = \sum_{i,j} a^{\dagger}_{i,j}(\vec{n}_{s}) a_{i,j}(\vec{n}_{s}) \qquad \rho^{a^{\dagger},a}_{I}(\vec{n}_{s}) = \sum_{i,j,j'} a^{\dagger}_{i,j}(\vec{n}_{s})[\tau_{I}]_{j,j'} a_{i,j'}(\vec{n}_{s})$$

$$\rho^{a^{\dagger},a}_{S,I}(\vec{n}_{s}) = \sum_{i,i',j,j'} a^{\dagger}_{i,j}(\vec{n}_{s})[\sigma_{S}]_{i,i'}[\tau_{I}]_{j,j'} a_{i',j'}(\vec{n}_{s})$$

Leading order interactions

Transfer matrix from n_t - th step in temporal direction $C < 0, C_I > 0$ Small sign oscillation from pion-nucleon vertex $M^{(n_t)} = : \exp \left[-H_{\text{free}} \alpha_t - \frac{g_A \alpha_t}{2F_{\pi}} \sum_{S,I} \nabla_S \pi_I(\vec{n}_s, n_t) \rho_{S,I}^{a^{\dagger},a}(\vec{n}_s) + \sqrt{-C\alpha_t} \sum_{\vec{n}_s} s(\vec{n}_s, n_t) \rho_I^{a^{\dagger},a}(\vec{n}_s) + i \sqrt{C_I \alpha_t} \sum_I \sum_{\vec{n}_s} s_I(\vec{n}_s, n_t) \rho_I^{a^{\dagger},a}(\vec{n}_s) \right] :$ No sign oscillation for contact interactions if the number of protons and neutrons are equal

Real determinant in the pion-less case $\tau_2 \mathcal{M} \tau_2 = \mathcal{M}^* \longrightarrow \det \mathcal{M}^* = \det \mathcal{M}$ Lee, Phys. Rev. C70: 064002 (2004)

Antisymmetry of $\tau_2 \longrightarrow$ real eigenvalues of \mathcal{M} are doubly degenerate



Approximate SU(4) symmetry

Wigner spin-isospin SU(4) symmetry transformation:

Wigner, Phys. Rev. 51 (1937) 106

 $\delta N = \alpha_{\mu\nu}\sigma^{\mu}\tau^{\nu}N$ with $\sigma^{\mu} = (1, \vec{\sigma}), \tau^{\mu} = (1, \vec{\tau})$

SU(4) invariance in the limit of infinite $a({}^{1}S_{0})$ and $a({}^{3}S_{1})$ scattering length SU(4)-breaking terms $\sim 1/a({}^{3}S_{1}) - 1/a({}^{1}S_{0}), q/\Lambda_{\chi}$

Mehen, Stewart, Wise, Phys. Rev. Lett. 83 (1999) 931

Large NN scattering length approximate SU(4) symmetry

$$M_{\mathrm{SU}(4)}^{(n_t)} = : \exp\left[-H_{\mathrm{free}}\alpha_t + \sqrt{-C\alpha_t}\sum_{\vec{n}_s} [s(\vec{n}_s, n_t)\rho^{a^{\dagger}, a}(\vec{n}_s)] :\right]$$



- Pionless SU(4)-symmetric simulations are cheaper
- Decrease computational effort by using SU(4)-filter

Hybrid Monte Carlo



$$H_{\rm HMC} = \frac{1}{2} \sum_{I,\vec{n}} (p_{\pi_I}^2(\vec{n}\,) + p_s^2(\vec{n}\,) + p_{s_I}^2(\vec{n}\,)) + V(\pi_I, s, s_I) \quad t$$

$$V(\pi_I, s, s_I) = S_{\pi\pi} + S_{ss} - \log\{|\det \mathcal{M}|\}$$





Scattering from finite volume

F	Rotation group $SO(3) \longrightarrow SO(3, Z)$				
	Representation	J_z	Example		
	A_1	$0 \operatorname{mod} 4$	$Y_{0,0}$		
	T_1	$0, 1, 3 \operatorname{mod} 4$	$\{Y_{1,0},Y_{1,1},Y_{1,-1}\}$		
	E	$0,2 \operatorname{mod} 4$	$\left\{Y_{2,0}, \frac{Y_{2,-2}+Y_{2,2}}{\sqrt{2}}\right\}$		
	T_2	$1,2,3 \operatorname{mod} 4$	$\left\{Y_{2,1}, \frac{Y_{2,-2}-Y_{2,2}}{\sqrt{2}}, Y_{2,-1}\right\}$		
	A_2	$2 \operatorname{mod} 4$	$\frac{Y_{3,2} - Y_{3,-2}}{\sqrt{2}}$		

Every irreducible repr. includes definite $J \mod 4$ quantum numbers

$$Z_{0,0}(s,q^2) = \sqrt{1/4\pi} \sum_{n \in \mathbb{Z}^3} \frac{1}{(n^2 - q^2)^s}$$

Scattering from finite volume



$$\exp(2\,i\,\delta_0) = \frac{Z_{0,0}(1;q^2) + i\,\pi^{3/2}q}{Z_{0,0}(1;q^2) - i\,\pi^{3/2}q}$$

Lüscher formula for phase-shifts

Note: No extension to mixing angles available

Spherical wall method

Borasoy, Epelbaum, H.K., Lee, Meißner, Eur. Phys. J.A34 (2007) 185

Spherical wall imposed in the center-of-mass frame



Spherical wall removes copies of interactions due to periodic boundaries

- Energy spectrum by solving Schrödinger Eq. on the lattice (Lanczos method)
- Illustration for a toy-model: $C = -2 \,\mathrm{MeV}, R_0 = 2 imes 10^{-2} \,\mathrm{MeV}^{-1}$

$$V(\vec{r}) = C\left\{1 + \frac{r^2}{R_0^2} \left[3(\hat{r} \cdot \vec{\sigma}_1)(\hat{r} \cdot \vec{\sigma}_2) - \vec{\sigma}_1 \cdot \vec{\sigma}_2\right]\right\} \exp\left(-\frac{1}{2}\frac{r^2}{R_0^2}\right)$$

Very shallow bound state in the ${}^{3}S(D)_{1}$ channel with energy $-0.155 \,\mathrm{MeV}$

Illustration for the toy model

Borasoy, Epelbaum, H.K., Lee, Meißner, Eur. Phys. J.A34 (2007) 185



Chiral EFT at NLO: Mixing angles

Borasoy, Epelbaum, H.K., Lee, Meißner, Eur. Phys. J. A35 (2008) 343



9 NLO LECs fitted to the various S(D) and P(F)-wave phase-shifts + Quadrupole moment of the deuteron

Two different LO contact interactions in momentum space $\mathcal{L}_{C}^{\text{LO}_{1,2}} \sim \sum_{\vec{q}} f_{1,2}(\vec{q}) \left[CN^{\dagger}(\vec{q})N(\vec{q})N^{\dagger}(-\vec{q})N(-\vec{q}) + C_{I}N^{\dagger}(\vec{q})\vec{\tau}N(\vec{q}) \cdot N^{\dagger}(-\vec{q})\vec{\tau}N(-\vec{q}) \right]$ $f_{1}(\vec{q}) = 1 \rightarrow \text{ original repr.} \quad f_{2}(\vec{q}) \sim \exp(-b\sum_{l=1,2,3} (1 - \cos q_{l})) \rightarrow \text{ Gaussian smearing}$



- Fairly accurate description for momenta $\leq M_{\pi}$
- Mixing angle changes sign by LO → NLO
- Deviations appear consistent with higher-order effects

S-wave phase shifts

Two different LO contact interactions in momentum space $\mathcal{L}_{C}^{\text{LO}_{1,2}} \sim \sum_{\vec{q}} f_{1,2}(\vec{q}) \left[CN^{\dagger}(\vec{q})N(\vec{q})N^{\dagger}(-\vec{q})N(-\vec{q}) + C_{I}N^{\dagger}(\vec{q})\vec{\tau}N(\vec{q}) \cdot N^{\dagger}(-\vec{q})\vec{\tau}N(-\vec{q}) \right]$ $f_{1}(\vec{q}) = 1 \implies \text{original repr.} \quad f_{2}(\vec{q}) \sim \exp(-b\sum_{l=1,2,3} (1 - \cos q_{l})) \implies \text{Gaussian smearing}$



Accurate NLO-description in both cases for momenta $\leq 80 \,\mathrm{MeV}$

Better convergence with smeared action

P-wave phase shifts



Better convergence with non-smeared action

Improving convergence

Project the smearing out of the P-waves

$$V_{\rm LO_3} = C_{^1S_0}f(\vec{q})\left(\frac{1}{4} - \frac{1}{4}\vec{\sigma}_1\cdot\vec{\sigma}_2\right)\left(\frac{3}{4} + \frac{1}{4}\vec{\tau}_1\cdot\vec{\tau}_2\right) + C_{^3S_1}f(\vec{q})\left(\frac{3}{4} + \frac{1}{4}\vec{\sigma}_1\cdot\vec{\sigma}_2\right)\left(\frac{1}{4} - \frac{1}{4}\vec{\tau}_1\cdot\vec{\tau}_2\right) + V_{\rm OPE}(\vec{q})\left(\frac{3}{4} + \frac{1}{4}\vec{\tau}_1\cdot\vec{\tau}_2\right)\left(\frac{3}{4} + \frac{1}{4}\vec{\tau}_1\cdot\vec{\tau}_2\right) + V_{\rm OPE}(\vec{q})\left(\frac{3}{4} + \frac{1}{4}\vec{\tau}_1\cdot\vec{\tau}_2\right) + V_{\rm OPE}(\vec{\tau}_1\cdot\vec{\tau}_2\right) + V_{\rm OPE}(\vec{\tau}_$$



Spin 1/Isospin 0 projector

Fast convergence in all partial waves
 NLO can be treated perturbatively
 Small systematic errors at NLO



Triton and Helium-3

Binding energy difference between Triton and Helium-3 is a testable prediction



Different asymptotic fits with different subsets of data points: Lüscher '86 $E(L) = E(\infty) - \frac{C}{L}e^{-L/L_0} + O\left(e^{-\sqrt{2}L/L_0}\right)$

Infinite volume	Experimental	
extrapolation	value	
$0.78(5){ m MeV}$	$0.76{ m MeV}$	

Results for Helium-4

Epelbaum, H.K. Lee, Meißner: Phys. Rev. Lett. 106 (2011) 192501, Phys. Rev. Lett 104 (2010) 142501, Eur. Phys. J. A45 (2010) 335

Ground state energy of Helium-4 in a box of length $L = 11.8 \, {
m fm}$



Accurate description of experimental value already at LO

Cancelations betw. NLO + IB + EM and NNLO

Results for Beryllium-8

Epelbaum, H.K. Lee, Meißner: Phys. Rev. Lett. 106 (2011) 192501, Phys. Rev. Lett 104 (2010) 142501, Eur. Phys. J. A45 (2010) 335

Ground state energy of Beryllium-8 in a box of length $L=11.8\,{
m fm}$



Cancelations betw. NLO + IB + EM and NNLO

Results for Carbon-12

Epelbaum, H.K. Lee, Meißner: Phys. Rev. Lett. 106 (2011) 192501, Phys. Rev. Lett 104 (2010) 142501, Eur. Phys. J. A45 (2010) 335

Ground state energy of Carbon-12 in a box of length $L = 11.8 \,\mathrm{fm}$



- Results for two different SU(4) couplings
- Finite volume corrections smaller than combined statistical and extrapolation error bars

Production of ¹²C in stellar environment



- Existence of the Hoyle state was experimentally confirmed: Cook et al. '57
- First principle calculations of the Hoyle state has been one of the biggest challenges in nuclear structure theory.

Hoyle state 0⁺₂

Epelbaum, H.K., Lähde, Lee, Meißner, Phys. Rev. Lett 109 (2012) 252501





No signal for 0^+_2 if initial/final states with all three alpha clusters at rest

Hoyle state is not a loosly-bound BEC of three alpha clusters

+ Strong signal for 0_2^+ if there is some relative motion excited betw. two alpha clusters

Hoyle state as bent-arm or obtuse triangular configuation

No visible relaxation to the ground state for Euclidean time probed

Carbon-12: summary

Low-lying even parity states of ¹²C in units of MeV

	LO	+ NLO + IB + EM	+ NNLO	Exp. Value
0_{1}^{+}	-96(2)	-77(3)	-92(3)	-92.16
2^{+}_{1}	-94(2)	-74(3)	-89(3)	-87.72
0_{2}^{+}	-89(2)	-72(3)	-85(3)	-84.51
2^{+}_{2}	-88(2)	-70(3)	-83(3)	-82.6(1)

Root-mean-square radii and quadrupole moments of ¹²C

	r(01+) [fm]	r(2 ₁ ⁺) [fm]	Q(2 ⁺ ₁) [e fm ²]	r(0 ⁺ ₂) [fm]	r(2 ⁺ ₂) [fm]	Q(2 ⁺ ₁) [e fm ²]
LO	2.2(2)	2.2(2)	6(2)	2.4(2)	2.4(2)	-7(2)
Exp.	2.47(2)	_	6(3)		3.07(13)	

 \mathbf{H} Interpretation of 2_2^+ -state as rotational excitation of alpha chain

Electromagnetic transitions of 12C

	B(E2, $2_1^+ \rightarrow 0_1^+$) [e ² fm ⁴]	B(E2, $2_1^+ \rightarrow 0_2^+$) [e^2 fm ⁴]	B(E2, $2_2^+ \rightarrow 0_1^+$) [e ² fm ⁴]	B(E2, $2_2^+ \rightarrow 0_2^+$) [e ² fm ⁴]	m(E0, 02+→01+) [e fm2]
LO	5(2)	1.5(7)	2(1)	6(2)	3(1)
Exp.	7.6(4)	2.6(4)	0.73(13)	—	5.5(1)

Summary

Lattice EFT is a promising tool for a quantitative description of light nuclei LECs are fitted to binding energies and to phase-shifts by spherical wall method First simulations of ground (and excited) states for light nuclei with A=4,8,12 Interpretation of the Hoyle state in Carbon-12 as bent-arm chain of alpha clusters Prediction of 2⁺₂ state in Carbon-12

Outlook



Spectrum of Oxygen-16

Ground states of Nitrogen-14 and Neon-20

Multi-channel projection Monte Carlo

Construct several Slater determinants for A single nucleons

 $|\Psi^1_A
angle, |\Psi^2_A
angle, \dots, |\Psi^K_A
angle$

• Correlator function matrix for A nucleons $Z_A^{ij}(t) = \langle \Psi_A^i | \exp(-tH) | \Psi_A^j \rangle$

Slater Determinants for A free Nucleons

- O Diagonalize $Z_A^{ij}(t)$ at large t to isolate the different energy eigenstates
- Use the eigenvectors of $Z_A^{ij}(t)$ to calculate expectation values of some operator O for each energy eigenstate