EFFECTIVE FIELD THEORY FOR LATTICE NUCLEI

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Collaboration

Jerusalem, Israel N. Barnea, D. Gazit J. Kirscher

האוניברסיטה העברית בירושלים The Hebrew University of Jerusalem

Trento, Italy
L. Contessi







Orsay, France U. van Kolck



ANL, USA A. Lovato



PUNCHLINES

- This talk is about nuclei that do not exist neither in the laboratory nor in the cosmos, but only in our minds (and possibly in our computers...).
- We want to understand if it is possible to infer some systematics and some general behaviors of "nuclear physics" in a regime where the pion mass is unphysical, but such that unquenched Lattice QCD simulations are possible.
- Extrapolation to the physical case is very tricky and is not the main aim of this work at the moment.



Image from M. Savage website (UW/INT)



LQCD - The Single Baryon Case

Lattice QCD

- QCD is the fundamental theory for nuclear physics.
- It is formulated in terms of quarks and gluons.
- At low energy QCD is non-perturbative → lattice simulations (LQCD).
- Neutron and proton masses are predictions.
- Same for pion masses.

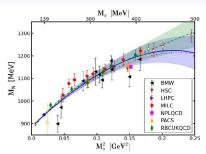
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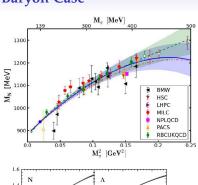


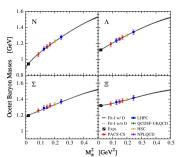
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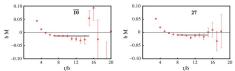




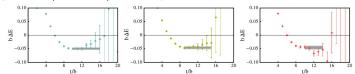


LQCD - Multi Baryon Configurations

Deuteron ($\overline{10}$) and dineutron (27) simulations



Triton simulations with different lattice sizes $(24^3 \times 48, 32^3 \times 48, 48^3 \times 64)$



- LQCD simulations with $SU_f(3)$ symmetry
- Large pion mass $m_{vi} = 800 \text{MeV}$
- Results with smaller m_{π} are already available.



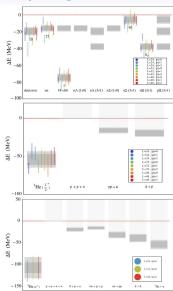
LQCD - Few-Body Baryon Spectra

2-body system - Deutron, dineutron,...

3-body system - ³He, triton

4-body system - ⁴He

NPLQCD Collaboration, PRD 87 034506 (2013)

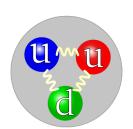




- At this point LQCD simulations for A ≥ 2 nuclei are still far away from the physical value of the pion mass.
- Currently no reliable and/or usable NN interactions can be derived from lattice simulations.
- Contemporary nuclear theory is based on Effective Field Theory → phenomenology.
- Quark and Gluon degrees of freedom are replaced by baryons and mesons.

$$\mathcal{L}_{QCD}(q,G) \longrightarrow \mathcal{L}_{Nucl}(N,\pi,\ldots)$$

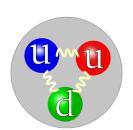
- The L_{Nucl}(N, π,...) is constructed to retain QCL symmetries.
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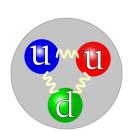
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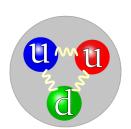
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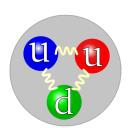
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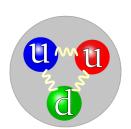
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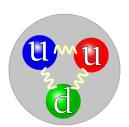
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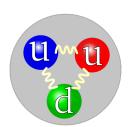
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Effective Field Theory potentials

Low Energy Constants

- There are 2 free parameters in LO, 7 at NLO, ...
- NNN and NNNN forces come in naturally at orders N2LO and N3LO.
- The NNN force contains 2 free parameters

 $\chi^2/{
m datum}$ for the reproduction of the 1999 np database

Bin (MeV)	# of data	$ m N^3LO$	NNLO	NLO	AV18
0-100	1058	1.06	1.71	5.20	0.95
100-190	501	1.08	12.9	49.3	1.10
190-290	843	1.15	19.2	68.3	1.11
0-290	2402	1.10	10.1	36.2	1.04

	Two-nucleon force	Three-nucleon force	Four-nucleon force
Qº	XH	_	—
	XHMMH	_	—
Q³	취석	HH HX X	
Q ⁴		work in progress	141 141 ·

$$V = -\left(\frac{g_A}{2f_\pi}\right)^2 \frac{(\sigma_1 \cdot q)(\sigma_2 \cdot q)}{q^2 + m_\pi^2} \tau_1 \cdot \tau_2$$

+ $C_S + C_T \sigma_1 \cdot \sigma_2$
+ $V_{NIO} + V_{N2IO} + \dots$

3 nucleon force >>

D. R. Entem and R. Machleidt, PRC **68**, 041001(R) (2003). Epelbaum *et al.*, EPJA **19**, 401 (2004), NPA **747**, 362 (2005).

4 nucleon force ...

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EFT for Lattice Nuclei

Energy Scales

- Nucleon mass M_n , and the difference with the mass of the Δ baryon $\delta M = M_{\Lambda} - M_n$
- The pion mass m_{π} , pion exchange momentum $q_{\pi} = m_{\pi}/\hbar c$, and energy

$$E_{\pi} = \frac{\hbar^2 q_{\pi}^2}{M_n} = \frac{m_{\pi}}{M_n} m_{\pi}$$

Nuclear binding energy B/A

Scale	Nature	LQCD@ m_{π} =500MeV	LQCD@ m_{π} =800MeV
M_n	940 MeV	1300 MeV	1600 MeV
δM	300 MeV	300 MeV	180 MeV
m_{π}	140 MeV	500 MeV	800 MeV
E_{π}	20 MeV	200 MeV	400 MeV
B/A	10 MeV	15 Mev	25 MeV

Conclusions

- For the nature case $\mathcal{L} \longrightarrow \mathcal{L}_{EFT}(N, \pi)$
- For lattice nuclei at $m_{\pi} > 400 \text{MeV}$, $E_{\pi} \gg B/A$
- In this case #EFT is the natural theory $\mathcal{L}\longrightarrow\mathcal{L}_{EFT}(N)$

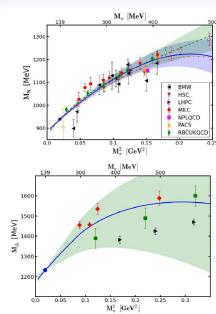


The nucleon Δ mass difference

Nucleon mass - n,p

 Δ mass

L. Alvarez-Ruso *et* al., ArXiv hep-ph: 1304.0483 (2013)





#EFT for Lattice Nuclei

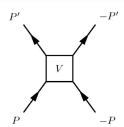
We write all possible terms in the Lagrangian L
ordered by the number of derivatives:

$$\mathcal{L} = N^{\dagger} \left(i \partial_{0} + \frac{\vec{\nabla}}{2M} \right) N - a_{1} N^{\dagger} N N^{\dagger} N - a_{2} N^{\dagger} \sigma N \cdot N^{\dagger} \sigma N$$
$$-a_{3} N^{\dagger} \tau N \cdot N^{\dagger} \tau N - a_{4} N^{\dagger} \sigma \tau N \cdot N^{\dagger} \sigma \tau N + \dots$$
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- Higher order terms include more derivatives.
- Naively, the order goes as the number of derivatives.
- The 3-body term appears at LO to avoid the Thomas collapse.
- Due to Fermi symmetry the number of terms can be cut by half.
- The coefficients depend on the cutoff Λ .

Some further wishes (to be explained later

- The potential needs to be local
- Avoid 3-body spin-isospin operators.



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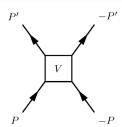
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#EFT Potential at NLO

• At LO the #EFT potential takes the form

$$V_{LO}^{2b} = a_1 + a_2 \, \sigma_1 \cdot \sigma_2 + a_3 \, \tau_1 \cdot \tau_2 + a_4 (\sigma_1 \cdot \sigma_2) (\tau_1 \cdot \tau_2)$$

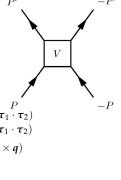
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J. Kirscher, H. W. Griesshammer, D. Shukla, H. M. Hofman, arXiv: 0903.5583 A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, PRL 111. 032501

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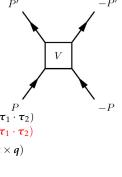
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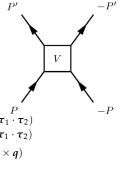
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(2013). ← I → ← I → Q ○

Due to antisymmetrization of the nuclear wave function

$$V_{LO}^{2b} = C_1^{LO} + C_2^{LO} \, \sigma_1 \cdot \sigma_2$$

The leading order also contains a 3-body term of the form

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• Using the freedom to choose these parameters we set

$$\begin{split} V_{NLO}^{2b} &= \ C_1^{NLO} q^2 + C_2^{NLO} q^2 \ \sigma_1 \cdot \sigma_2 + C_3^{NLO} q^2 \ \tau_1 \cdot \tau_2 + C_4^{NLO} q^2 (\sigma_1 \cdot \sigma_2) (\tau_1 \cdot \tau_2) \\ &+ C_5^{NLO} i \frac{1}{2} (\sigma_1 + \sigma_2) (k \times q) + C_6^{NLO} (\sigma_1 \cdot q) (\sigma_2 \cdot q) \\ &+ C_7^{NLO} \ \tau_1 \cdot \tau_2 (\sigma_1 \cdot q) (\sigma_2 \cdot q) \end{split}$$

- The antisymmetric potential V_{NLO} contains
 - 1. LO 2-body: 2 parameters.
 - 2. LO 3-body: 1 parameter.
 - 3. NLO: 7 parameters.
- · At the moment we consider only LO.



Coordinate space

• We introduce a Gaussian cutoff in q

$$F_{\Lambda}(q) = \left(\frac{\sqrt{4\pi}}{\Lambda}\right)^3 e^{-q^2/\Lambda^2} \Longrightarrow F_{\Lambda}(r) = e^{-\Lambda^2 r^2/4}$$

The potential matrix elements can be evaluated now

$$V(\mathbf{r}, \mathbf{r}') = N\langle \mathbf{r} | \int d\mathbf{k} d\mathbf{q} V(\mathbf{k}, \mathbf{q}) f_{\Lambda}(\mathbf{q}) | \mathbf{r}' \rangle$$

= N' V(-i\nabla_y, -i\nabla_x) e^{-\Lambda^2 x^2 / 4} \delta(y)

where

$$x = \frac{1}{2}(r + r')$$
 ; $y = \frac{1}{2}(r' - r)$

The LO potential contains no momentum dependence therefore

$$V_{LO}^{2b}(r) = \left(C_1^{LO} + C_2^{LO} \,\sigma_1 \cdot \sigma_2\right) e^{-\Lambda^2 r^2/4}$$

- With our choice of parameterization also V_{NLO} is local.
- The 3-body term takes the form

$$V_{LO}^{3b} = D_1^{LO} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 e^{-\Lambda^2 (r_{13}^2 + r_{23}^2)}$$



The Hamiltonian

At leading order the coordinate space Hamiltonian is

$$H = -\sum_{i} \frac{\hbar^{2}}{2M_{n}} \nabla_{i}^{2} + \sum_{i < j} \left(C_{1}^{LO}(\Lambda) + C_{2}^{LO}(\Lambda) \sigma_{i} \cdot \sigma_{j} \right) e^{-\Lambda^{2} r_{ij}^{2}}$$
$$+ \sum_{i < j < k} \sum_{C \neq c} D_{1}^{LO}(\Lambda) \left(\tau_{i} \cdot \tau_{j} \right) e^{-\Lambda^{2} (r_{ik}^{2} + r_{jk}^{2})}$$

In the 3-body term the notation \sum_{cyc} stands for cyclic permutation of particles (*ijk*).

We use four methods

- 1. Numerov, A = 2
- 2. The Effective Interaction Hypershperical Harmonics (EIHH) method, $6 \ge A \ge 3$
- 3. (Refined) Resonating Group Model (RRGM) for $N \le 12$
- 4. The Auxiliary Field Diffusion Monte-Carlo (AFDMC) method, $A \ge 2$

Auxiliary Field Diffusion Monte Carlo

- In order to extend the prediction to heavier mass nuclei we employ a QMC algorithm, namely AFDMC.
- The Fermion ground state of the Hamiltonian is computed by means of imaginary time projection with constraints to avoid the sign problem.

$$\langle R, S | 0_A \rangle \sim \lim_{\tau \to \infty} \langle R, S | e^{-(\tilde{H} - E_0)\tau} | R'S' \rangle \langle R'S' | \Psi \rangle$$

- A population of points |R,S| in the coordinate/spin space evolved in imaginary time.
- Ĥ is a modified Hamiltonian defined on a set of artificial boundary conditions imposed to obtain a finite overlap with an antisymmetric function.

Auxiliary Field Diffusion Monte Carlo

- The propagator contains operators that span a multicomponent wavefunction with order 4^A components.
- This is the approach used in GFMC calculations.
- In AFDMC we make use of a basis set in which the single particle wavefunctions take the form

$$\phi(\mathbf{r}_i, s_i) = \begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} \varphi_n(\mathbf{r}_i)$$

- Linearization of the operators is achieved through the Hubbard-Stratonovitch transform.
- As an example, the propagator corresponding to $\hat{V} = v_{\sigma \cdot \sigma}(r_{12})\sigma_1 \cdot \sigma_2$ is:

$$e^{-\hat{V}\Delta\tau} = \frac{1}{\sqrt{\pi}} \int dx_1 e^{-\frac{x_1^2}{2}} e^{-x_1} \sqrt{-\Delta\tau v_{\sigma,\sigma}(r_{12})} \sigma_1 \times \\ \times \int dx_2 e^{-\frac{x_2^2}{2}} e^{-x_2} \sqrt{-\Delta\tau v_{\sigma,\sigma}(r_{12})} \sigma_2$$

Auxiliary Field Diffusion Monte Carlo

PRO:

- Very favorable scaling (A^3 instead of 4^A)
- No problem in computing nuclei up to A = 90

CON:

- Limited freedom on the choice of the trial functions → some possible ambiguities in the results.
- No upper bound property
- No easy way to include spin-orbit and three body forces in the propagator for finite nuclei (no problems in pure neutron systems instead)

The "Experimental" data

There are 4 input parameters in our model:

- 1. The nucleon mass M_n
- 2. LECs: $C_1^{LO}(\Lambda)$, $C_2^{LO}(\Lambda)$, $D_1^{LO}(\Lambda)$

Table : Masses [MeV]

particle	LQCD	Nature
π	805.9 ± 8.9	135.0-139.6
n	1634.0 ± 18.0	939.6
p	1634.0 ± 18.0	938.3

Table: Binding energies [MeV]

nuclei	LQCD	Nature
D	-19.5 ± 4.8	-2.224
nn	-15.9 ± 3.8	-
^{3}H	-53.9 ± 10.7	-8.48
³ He	-53.9 ± 10.7	-7.72
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NPLQCD Collaboration, PRD 87 034506 (2013)



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The 2-body LECs

The 2-body potential is diagonal in the S, T basis.

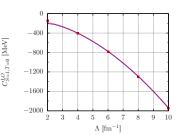
$$\begin{split} V_{S,T}^{LO}(r;\Lambda) &= \langle S,T|V^{LO}(r;\Lambda)|S,T\rangle \\ &= \left\{ C_1^{LO}(\Lambda) + [2S(S+1)-3]C_2^{LO}(\Lambda) \right\} F_{\Lambda}(r) \\ &\equiv C_{ST}^{LO}(\Lambda)F_{\Lambda}(r) \end{split}$$

- $C_{ST}^{LO}(\Lambda)$ are fitted to the D, nn B.E.
- We expect to ge

$$a_s \approx 1/\sqrt{m_N B}$$

• For LQCD@ $m_{\pi} = 800 MeV$

$$a_{{\rm S=0,T=1}}^{LO}=1.4\pm0.20~{\rm fm}$$
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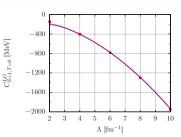
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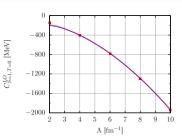
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Calibration of D_1

⁴He binding energy without NNN force

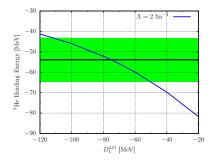
Λ	EIHH	AFDMC
$[fm^{-1}]$	[MeV]	[MeV]
2.0	-256.8	-256.9
4.0	-478.3	-478.2
6.0	-767.1	-766.4
8.0	-1122.9	-1120.8
LQCD	-107.0	0±24.2

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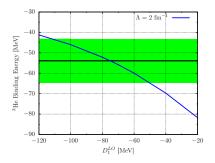


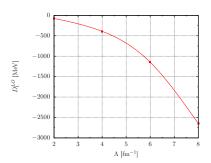
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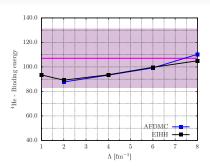
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Few Predictions

The binding energy of ⁴He

Λ	EIHH	AFDMC
$[fm^{-1}]$	[MeV]	[MeV]
2.0	-89.2(1)	-87.7(1)
4.0	-93.6(1)	-93.3(2)
6.0	-99.7(3)	-99.2(2)
8.0	-105.0(12)	-110.3(2)
LQCD	-107.0	± 24.2

- The computed ⁴He energy is within the LQCD simulations uncertainty.
- It has residual cutoff dependence.
- The radii of D, ³He, ⁴He exhibit strong cutoff dependence.
- These issues might be artifacts of our "local" formalism.

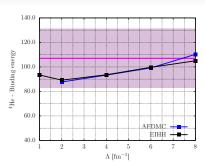


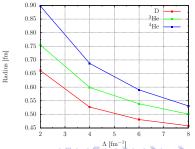
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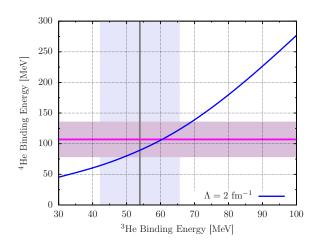
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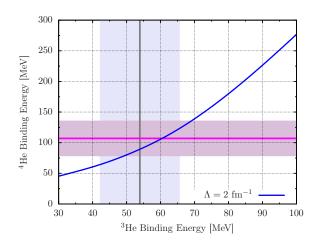


Conclusion

The EFT error due to uncertainty in the binding energy of ³He is roughly as large as the ⁴He measurment error.



The Tjon line(?)



Conclusion

The EFT error due to uncertainty in the binding energy of $^3\mathrm{He}$ is roughly as large as the $^4\mathrm{He}$ measurment error.

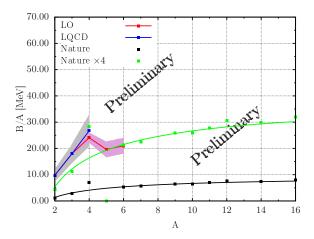


Few more predictions

Binding energies of the Light nuclei

LOCD	EET A 2.4 -1
~	EFT $\Lambda = 2 \text{ fm}^{-1}$
9.5 ± 4.8	-19.5
5.9 ± 3.8	-15.9
3.9 ± 10.7	-53.9
	unbound
7.0 ± 24.2	-89.2
	-66 (?)
	-98.2
	-121.(3)
	$\begin{array}{c} 2.5 \pm 4.8 \\ 5.9 \pm 3.8 \\ 3.9 \pm 10.7 \\ \hline 7.0 \pm 24.2 \end{array}$

Saturation Energy on the Lattice



Even more predictions...

We were able to perform calculations of $^{16}O.$ AFDMC calculations are non-trivial, especially at large Λ due to the large cancelations in the attractive (2-body) and repulsive (3-body) components in the potential.

Table: Binding energies of ¹⁶O from FDMC calculations (MeV)

	Λ (fm $^{-1}$)					
m_{π} (MeV)	2	4	6	8		
805	346.6(3)	334.9(6)	324(1)	305(1)		
510	115.5(4)	108.0(4)	105.8(8)	100(1)		
140	61.59(2)	56.9(6)	48(1)	45(2)		

Comments

- The three-body force used here has no isospin dependence (should be equivalent, but there might be some redundance).
- As it stands, ^{16}O is unbound with respect to breakup in $4(^{4}\text{He})$. However, at $m_{\pi} = 805\text{MeV}$ the difference $BE(^{4}\text{He}) BE(^{16}O)/4$ can be as small as 1.4MeV
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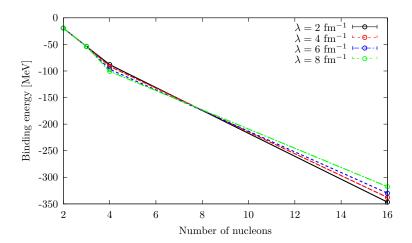
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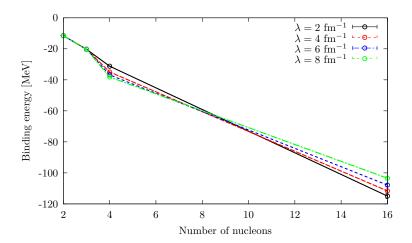
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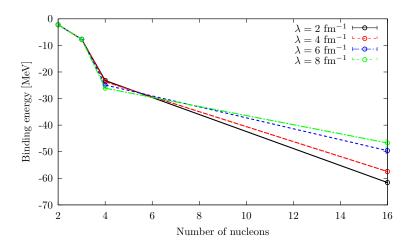
Summary of AFDMC results for m_{π} =805 MeV



Summary of AFDMC results for m_{π} =510 MeV



Summary of AFDMC results for m_{π} =140 MeV



Summary and Conclusions

- Lattice QCD simulations of few-nucleon systems open up a new front in nuclear physics.
- ÆFT is the appropriate theory to study these Lattice Nuclei, down to rather small pion masses.
- 3. Fitted to recent LQCD data we found that #EFT@LO reproduces the ^4He binding energy for $m_\pi = 805\text{MeV}$ and $m_\pi = 510\text{MeV}$ nucleons.
- The np, nn scattering lengths for this system are about a factor of 2 too small in comparison with recent NPLQCD calculations.
- 5. At LO we see probelms with the calculated nuclear radii.
- 6. More LQCD data are avilable to go behyond LO.

Ongoing work

- Begin the journey to include NLO in calculations.
- More LQCD data at different m_{π} to understand the systematics of some properties (e.g. evolution of the LEC's, BEs, saturation,...)
- Larger (A=40) calculations, and better wavefunctions in AFDMC (e.g. from RRG to check the cluster structyre in 16 O)
- Redo the calculations using a recently developed QMC algorithm in momentum space: systematic comparison of non-local and local formulation (effect of regulators?) as a function of the mass.