Status of matching nuclear many-body theory to LQCD

Going into the medium mass region

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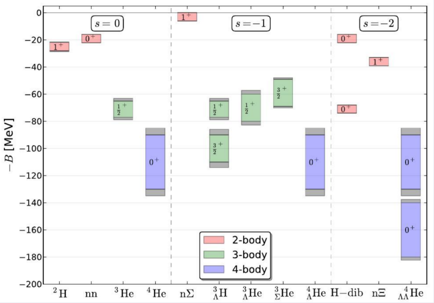
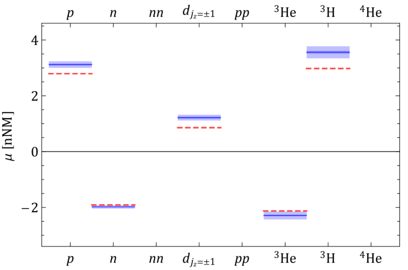
Lattice QCD Input for Neutrinoless Double-β Decay
INT Seattle - 07 July, 2017

Motivations

- tremendous progress in LQCD for light nuclei at large m_π





NPLQCD (2013),(2015)

- exponential increase in difficulty as we increase baryon number A

Need a reliable way to extend LQCD predictions to larger systems

potential model: extract potential directly from the lattice [HALQCD]

EFT matching: use observables at small A to fix coupling of a proper EFT

The plan for EFT matching

- Use a theory with only nucleons and contact interactions (EFT($\not\pi$))

Why we expect it's going to work:

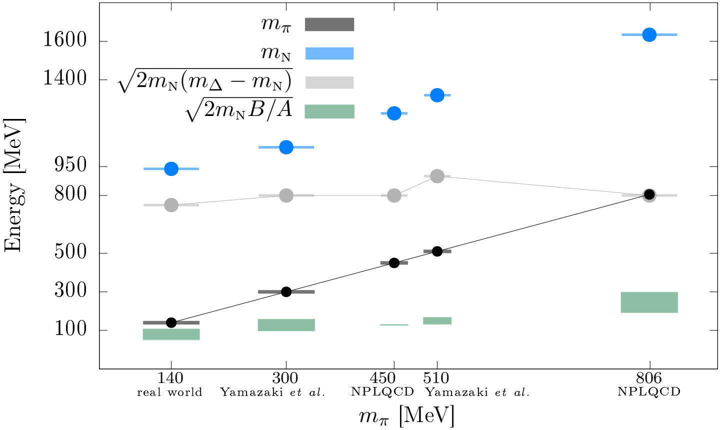


figure from: J. Kirscher, Int. J. Mod. Phys. E, 25, 1641001 (2016)

Pionless EFT

EFT($\not\pi$)

[Chen,Rupak,Savage(1999), Bedaque&vanKolck (2002), Epelbaum,Hammer,Meißner(2009)]

- describe NN scattering for $q < m_\pi$ with contact interactions
- LO is renormalizable (at least) up to $A = 6$ [Stetcu,Barret,vanKolck(2007)]
- works better than expected for $A = 4$ [Platter,Hammer,Meißner(2005)]

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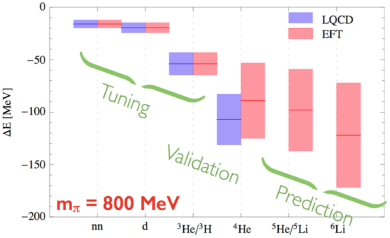
Applications of EFT($\not\pi$)to lattice nuclei

- binding energies with A up to 6
  Barnea,Contessi,Gazit,Pederiva,vanKolck(2015)
- n-d scattering
  Kirschner,Barnea,Gazit,Pederiva,vanKolck(2015)
- mag. moments & polarizabilities
  Kirscher,Pazy,Drachman,Barnea(2017)



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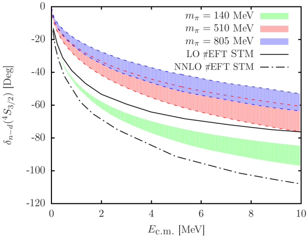

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	$\not\pi$EFT	$\not\pi$EFT	
m_π [MeV]	140	510	805
$^4a_{\text{nD}}$ [fm]	5.5 ± 1.3	2.3 ± 1.3	1.6 ± 1.3
$^2a_{\text{nD}}$ [fm]	0.61 ± 0.50	2.2 ± 2.1	0.62 ± 1.0
	experiment [79]	LQCD	
$^4a_{\text{nD}}$ [fm]	6.4 ± 0.020	?	?
$^2a_{\text{nD}}$ [fm]	0.65 ± 0.040	?	?

- “halo“ triton @ $m_\pi = 510$ MeV

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large m_π by NPLQCD, Chang et al. (2015)

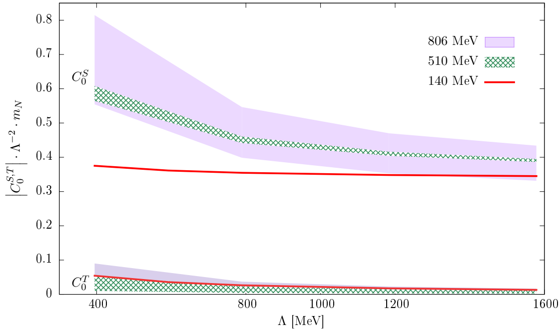
	m_π = 137 MeV			m_π = 806 MeV		
	deutron	triton	helion	deutron	triton	helion
shell model	0.879	2.793	-1.913	1.138	3.119	-1.981
LO	0.879	2.746	-1.862	1.138	3.118	-1.979
NLO	0.857	2.979	-2.130	1.220	3.405	-2.170
EXP/LQCD	0.857	2.979	-2.127	1.220(95)	3.56(19)	-2.29(12)

- polarizabilities not so good but strong regulator dependence

EFT($\not\pi$) Hamiltonian at LO

$$\hat{H}_{LO} = -\sum_i^A \frac{\hbar^2}{2M}\nabla_i^2 + \sum_{i<j}\left[C_0^S + C_0^T \vec{\sigma}_i \cdot \vec{\sigma}_j\right] f_\Lambda(r_{ij}) + D \sum_{i<j<k}\sum_{cyc} f_\Lambda(r_{ij}) f_\Lambda(r_{ik})$$

- $f_\Lambda(r) = exp(-r^2\Lambda^2/4)$ for $\Lambda = 2, 4, 6, 8$ fm^{-1}



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Many Body calculation

Problem: to ensure renormalizability we need $\Lambda = 2, 4, 6, 8$ fm^{-1}

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Auxiliary Field Diffusion Monte Carlo

[K.E.Schmidt & S.Fantoni (1999), J.Carlson et. al. (2015)]

Use projection operator on initial $|\Phi_T\rangle$ to get close to ground-state $|G\rangle$

$$e^{-\tau \hat{H}}|\Phi_T\rangle = |\Psi(\tau)\rangle \quad \xrightarrow{\tau\to\infty} \quad |G\rangle$$

- correlations explicitly built into "source" state $|\Phi_T\rangle$

pro: can deal efficiently with large Λ and moderate A

con: fundamentally limited by sign problem

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pro: can deal efficiently with large Λ and moderate A

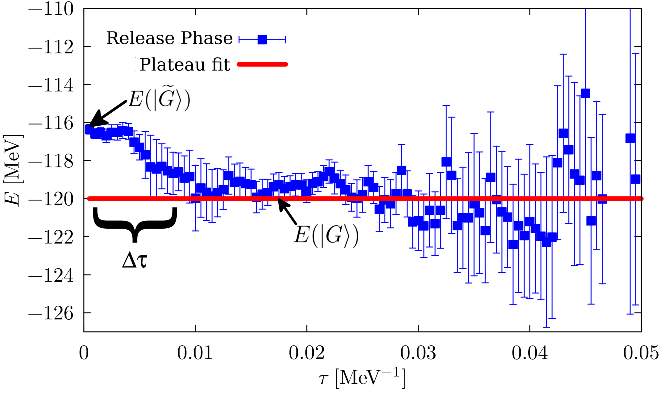
con: fundamentally limited by sign problem$\rightarrow$ fixed-phase

$$\widetilde{e^{-\tau\hat{H}}}|\Phi_T\rangle = |\widetilde{\Psi}(\tau)\rangle \quad \xrightarrow{\tau\to\infty} \quad |\widetilde{G}\rangle \approx |G\rangle$$

[Ortiz, Ceperley and Martin (1993)]

Going the last mile: release phase

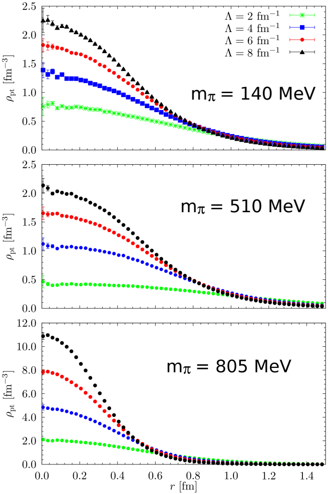
Release Phase: $e^{-\delta \hat{H}}|\widetilde{G}\rangle = |\Psi_{RP}(\delta)\rangle \rightarrow |G\rangle + e^{-\delta(E_A - E_G)}|A\rangle + \dots$



KEY: time scale $\Delta\tau$ controlled by the quality of $|\Phi_T\rangle$

Benchmark for ^{4}He

L.Contessi,A.Lovato,F.Pederiva,A.R.,J.Kirschner,U.vanKolck, arXiv:1701.06516

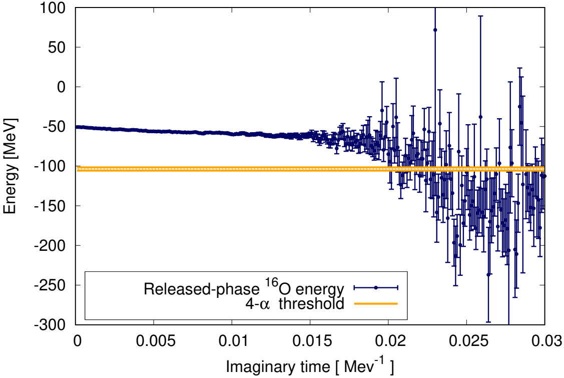


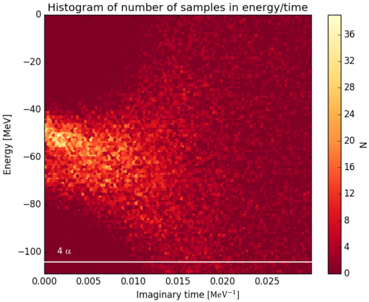
Λ	m_π = 140 MeV	m_π = 510 MeV	m_π = 805 MeV
2 fm^{-1}	-23.17 ± 0.02	-31.15 ± 0.02	-88.09 ± 0.01
4 fm^{-1}	-23.63 ± 0.03	-34.88 ± 0.03	-91.40 ± 0.03
6 fm^{-1}	-25.06 ± 0.02	-36.89 ± 0.02	-96.97 ± 0.01
8 fm^{-1}	-26.04 ± 0.05	-37.65 ± 0.03	-101.72 ± 0.03
$\rightarrow \infty$	$-30^{\pm 0.3\,\text{(sys)}}_{\pm 2\,\text{(stat)}}$	$-39^{\pm 1\,\text{(sys)}}_{\pm 2\,\text{(stat)}}$	$-124^{\pm 3\,\text{(sys)}}_{\pm 1\,\text{(stat)}}$
Exp.	-28.30	–	–
LQCD	–	-43.0 ± 14.4	-107.0 ± 24.2

- consistent with prev studies: no 4N needed!
- at physical m_π close to experiment
- at larger m_π match LQCD predictions for any cutoff Λ! Plateau identification seems consistent [vs. Iritani et al. (2016)]

Puzzles with ^{16}O

Release-Phase run at $m_\pi = 140$ MeV, $\Lambda = 8$ fm^{-1} [similar in ALL cases]



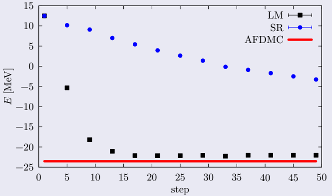


- seems to suggest ^{16}O is unstable for breakup BUT:
  - noise too strong to estimate $E(|G\rangle)$ reliably
  - poor constrained projection $E(|\widetilde{G}\rangle) \approx -50MeV \Rightarrow$ improve $|\Phi_T\rangle$

New results for ^{16}O with better optimizer

Wave-Function optimizer for AFDMC: find minimum of $\langle \Phi_T | \hat{H} | \Phi_T \rangle$

- based on Linear Method from quantum chemistry [Tolouse&Umrigar(2007)]
- flexible cubic spline representation
- reasonably robust with very noisy data



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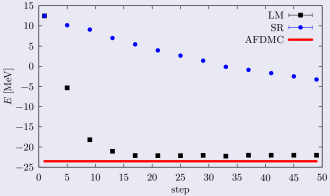
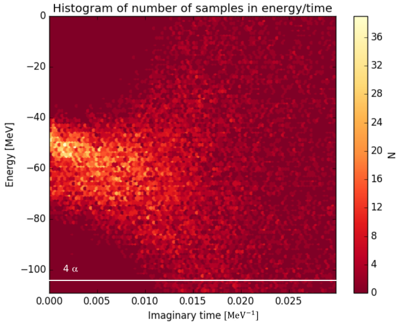
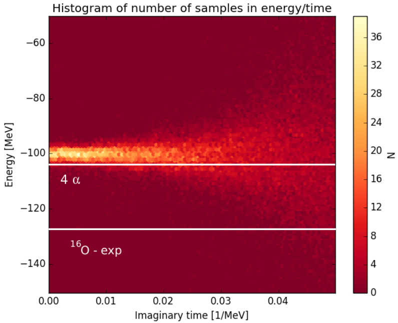
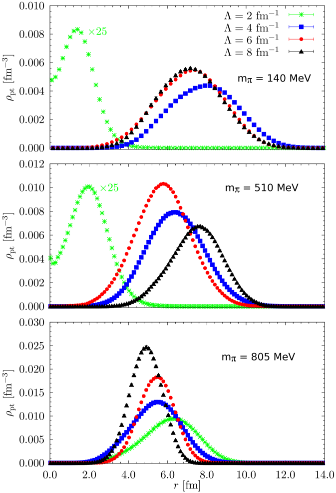






Clusterized state of ^{16}O

L.Contessi,A.Lovato,F.Pederiva,A.R.,J.Kirschner,U.vanKolck, arXiv:1701.06516

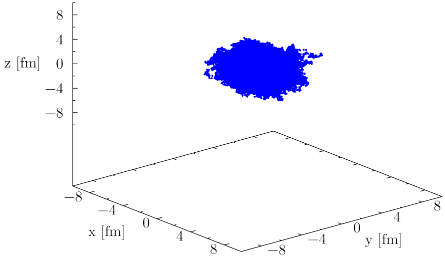


Λ	m_π = 140 MeV	m_π = 510 MeV	m_π = 805 MeV
2 fm^{-1}	-97.19 ± 0.06	-116.59 ± 0.08	-350.69 ± 0.05
4 fm^{-1}	-92.23 ± 0.14	-137.15 ± 0.15	-362.92 ± 0.07
6 fm^{-1}	-97.51 ± 0.14	-143.84 ± 0.17	-382.17 ± 0.25
8 fm^{-1}	-100.97 ± 0.20	-146.37 ± 0.27	-402.24 ± 0.39
$\to \infty$	$-115^{\pm 1 \text{ (sys)}}_{\pm 8 \text{ (stat)}}$	$-151^{\pm 2 \text{ (sys)}}_{\pm 10 \text{ (stat)}}$	$-504^{\pm 20 \text{ (sys)}}_{\pm 12 \text{ (stat)}}$
Exp.	-127.62	–	–
4-α thresh.	-120 ± 8	-156 ± 12	-496 ± 16

- extrapolated energies compatible with 4α $\to$ agrees with NN only calculation with HAL-QCD [Mc.Ilroy et al. arXiv:1701.02607]
- at large Λ the nucleon density doesn't look like a spherical nucleus at all! Are we actually producing separate clusters?

Clusterized state of ^{16}O

Trajectories for m_π=140 MeV and $\Lambda = 2$(left), 8(right) fm^{-1}:



- finite range interaction seems critical for stability of oxygen

Error estimates for nuclear many-body observables (my 2¢)

- EFT($\not{\pi}$)only renormalizable nuclear EFT we know (except maybe KSW-like)
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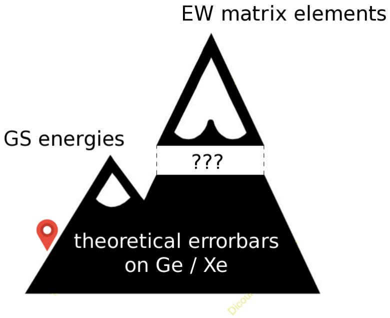

Factor of 2 spread in ME among "well motivated phenomenology" is already an amazing achievement!

Conclusions and future directions

What have we seen?

- confirm that α-particle described reasonably well at LO
  - indirect evidence of correct identification of plateau in LQCD
- LO EFT($\not\pi$) well behaved up to $A = 16$ [no need for A-body contact]
- unbound ^{16}O at LO for all values of m_π [maybe just barely at physical]

Future directions

- can NLO or NNLO calculations save ^{16}O?
- how about the stability of ^{8}Be, ^{12}C and ^{40}Ca?
- proper error propagation including errors in LEC (so far only cut-off and AFDMC), maybe with better LQCD data?

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Thanks for your attention

Wave-function optimization with Linear Method

- Slater-Jastrow wave function

$$\Phi_T(X) \equiv \langle X|\Phi_T\rangle = \langle X| \left(\prod_{i<j<k} U_{ijk}\right) \left(\prod_{i<j} F_{ij}\right) |D\rangle$$

- set of M parameters $\vec{\alpha}$ to be optimized using: $E(\vec{\alpha}) = \frac{\langle\Phi_T|\hat{H}|\Phi_T\rangle}{\langle\Phi_T|\Phi_T\rangle}$

Linear Method

J. Tolouse & C. Umrigar, J. Chem. Phys. 126(8), 084102 (2007)

- at each step expand: $\frac{|\Phi(\vec{\alpha})\rangle}{\sqrt{\langle\Phi(\vec{\alpha})|\Phi(\vec{\alpha})\rangle}} = |\Phi(\vec{\alpha}_k)\rangle + \sum_i^M \delta_i |\Phi_i(\vec{\alpha}_k)\rangle + \ldots$
- find optimal update solving for

$$\nabla_{\vec{\delta}} E^{lin}(\vec{\alpha}_k, \delta) = \nabla_{\vec{\delta}} \frac{\langle\Phi^{lin}(\vec{\alpha}_k, \delta)|\hat{H}|\Phi^{lin}(\vec{\alpha}_k, \delta)\rangle}{\langle\Phi^{lin}(\vec{\alpha}_k, \delta)|\Phi^{lin}(\vec{\alpha}_k, \delta)\rangle} = 0$$