

Bridging LQCD and Many-Body Nuclear Physics with a Pionless Effective Field Theory



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- A. Roggero (INT)
- U. van Kolck (Orsay)
- J. Kirscher (CCNY)
- N. Barnea (HUJ)

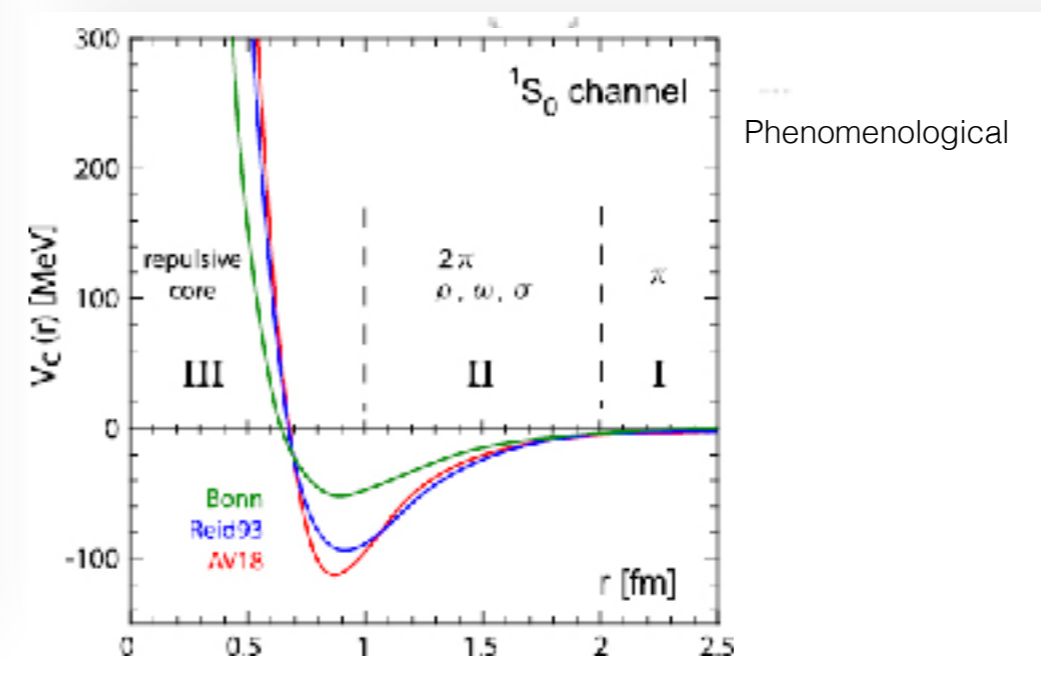
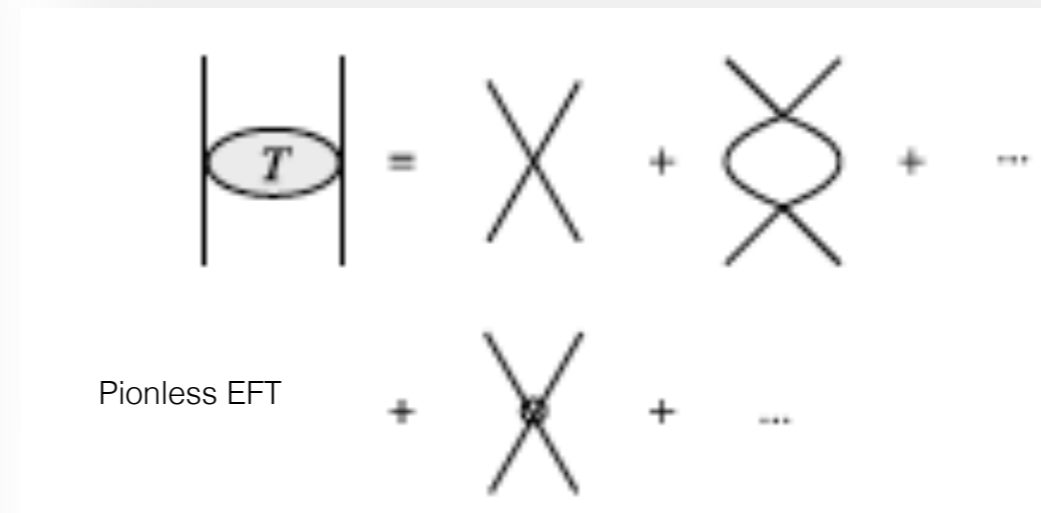
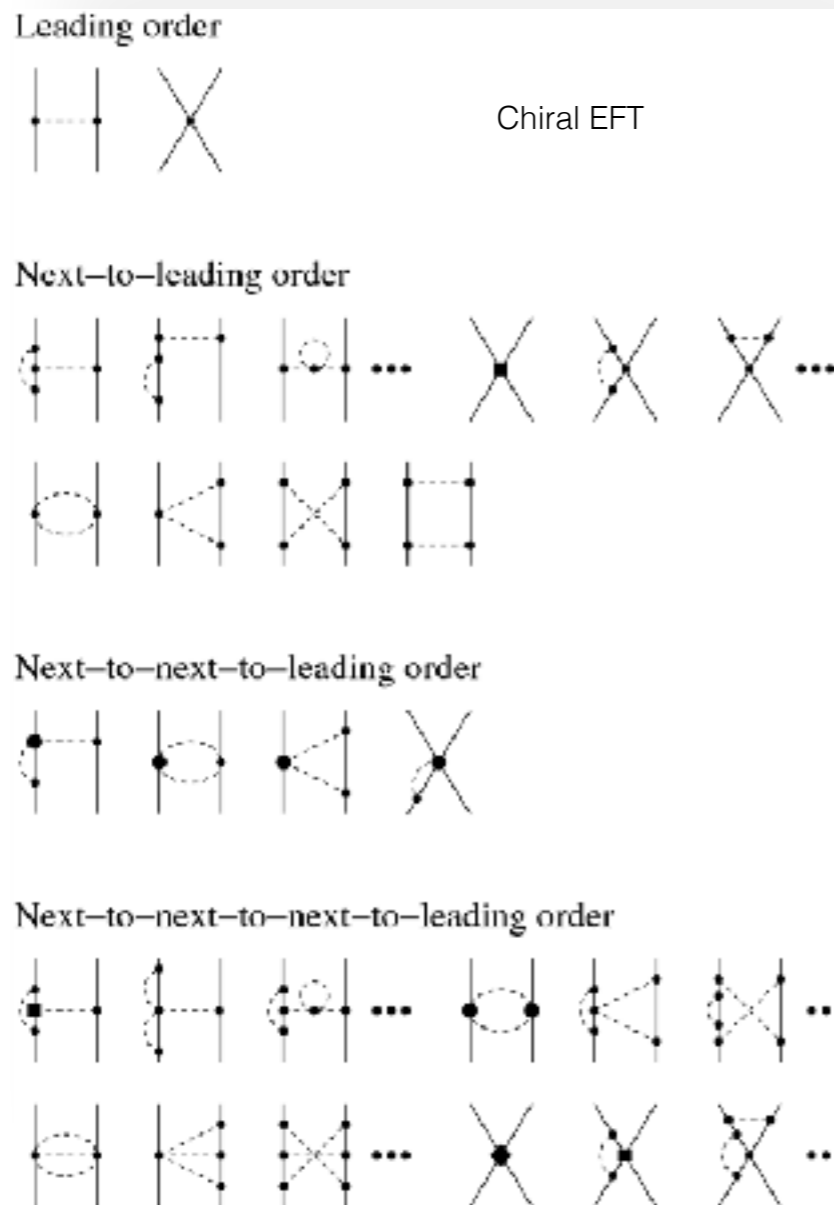
ν -less double- β decay, INT, Seattle 07/3/2017

OUTLINE

- Lattice nuclei
- Pionless EFT in local formulation
- Results for ${}^4\text{He}$ and ${}^{16}\text{O}$
- Conclusions

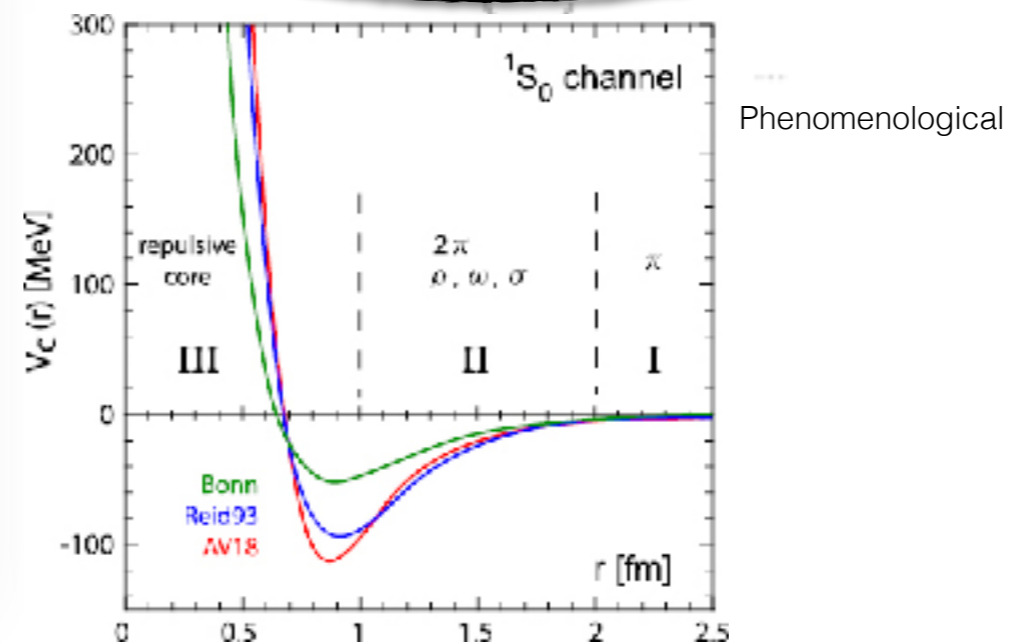
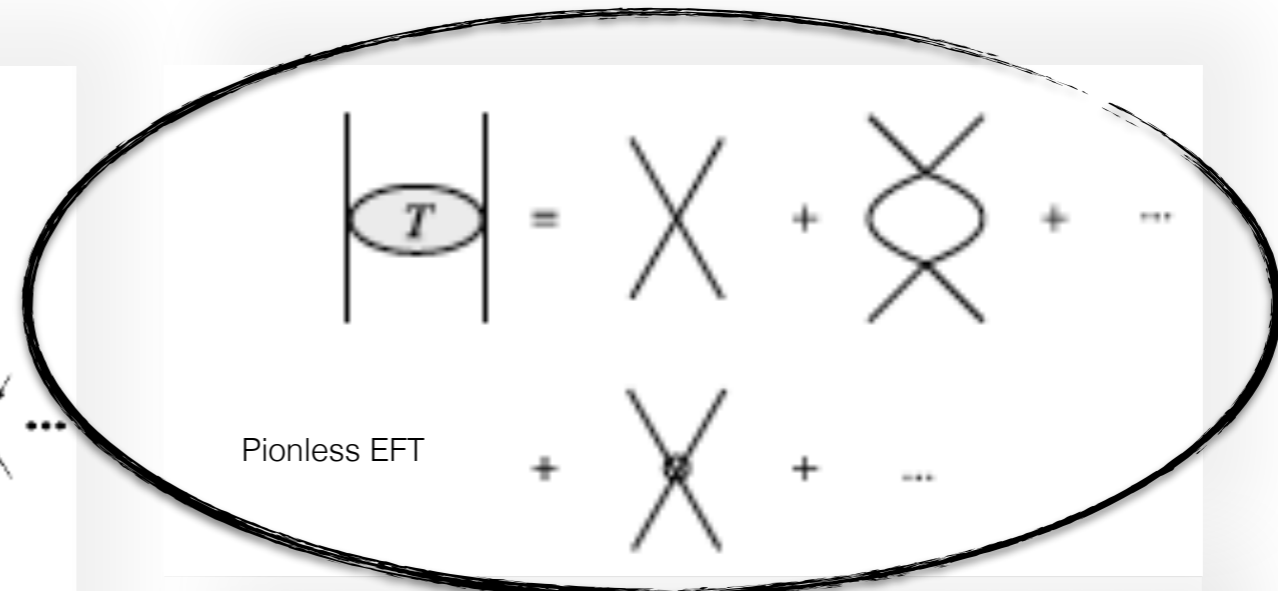
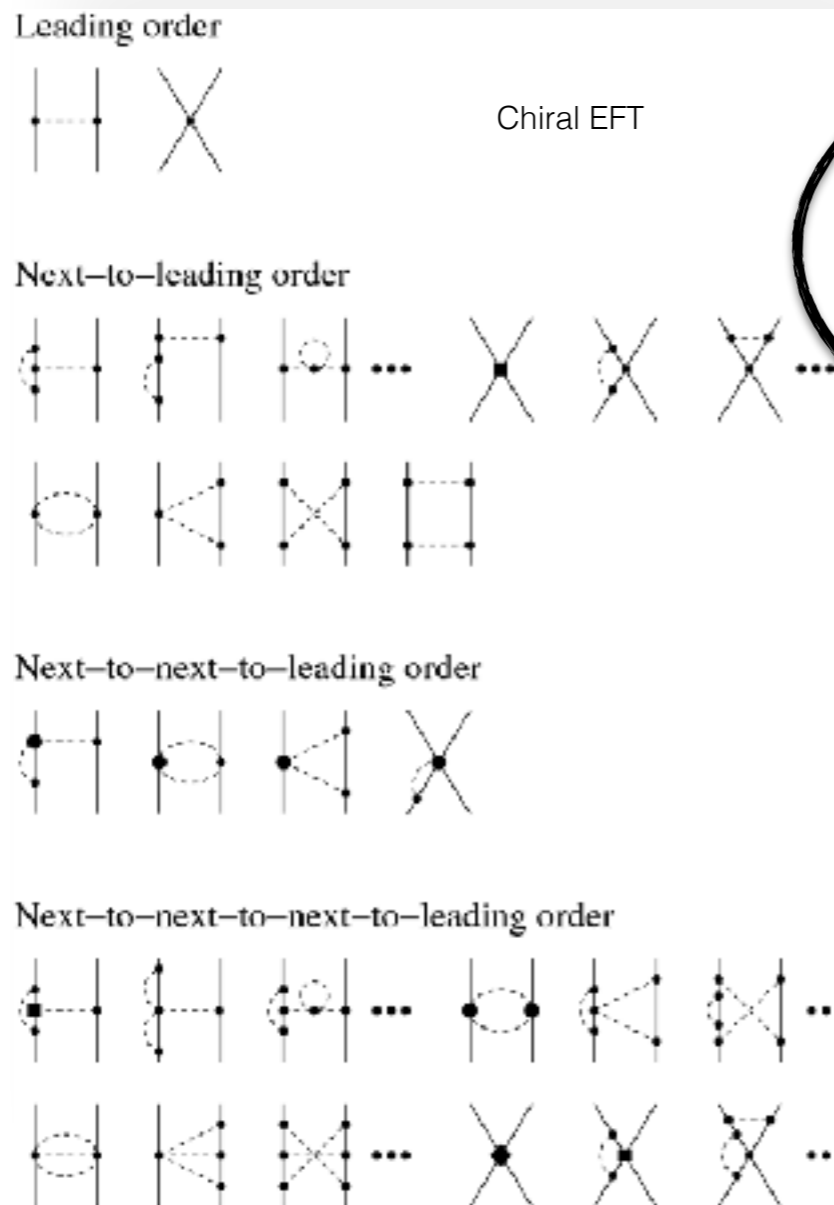
NUCLEAR HAMILTONIANS

The non-relativistic approach to nuclear physics is based on the use of a model nucleon-nucleon force.



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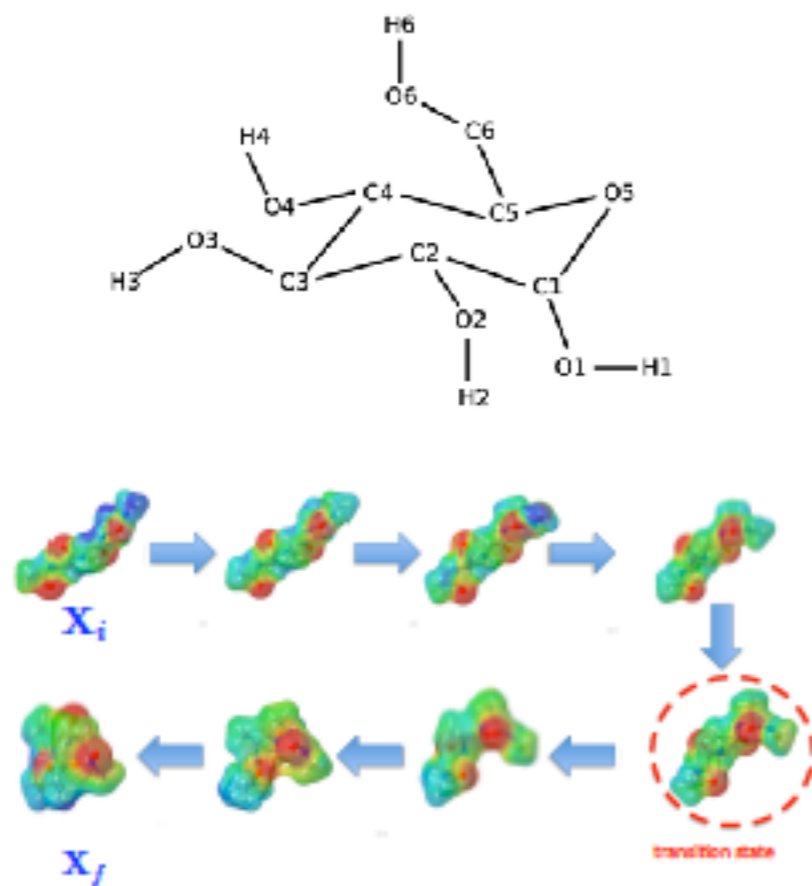
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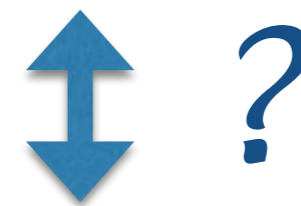
mc Ab initio calculations?

Ok, *strictly speaking we should solve QCD....*

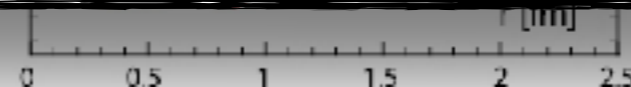
We are not alone! Cfr. chemistry:



“Effective” force fields
among atoms
(GROMOS, AMBER,..)



“Ab initio”: all electrons,
Coulomb force only



RELATION TO LQCD

Route 1: compute nn potentials on the lattice

S. Aoki et al.(HAL-QCD collaboration)

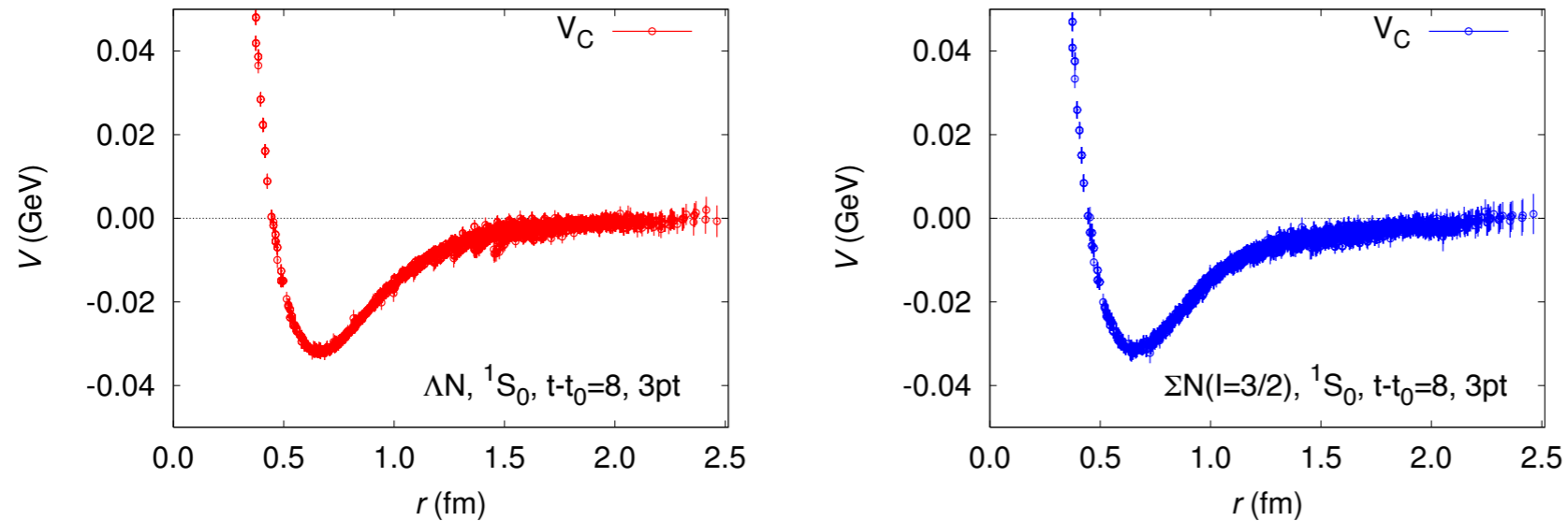


Fig. 10. Left: The central potential in the 1S_0 channel of the ΛN system in 2 + 1 flavor QCD as a function of r . Right: The central potential in the 1S_0 channel of the $\Sigma N(I = 3/2)$ system as a function of r .

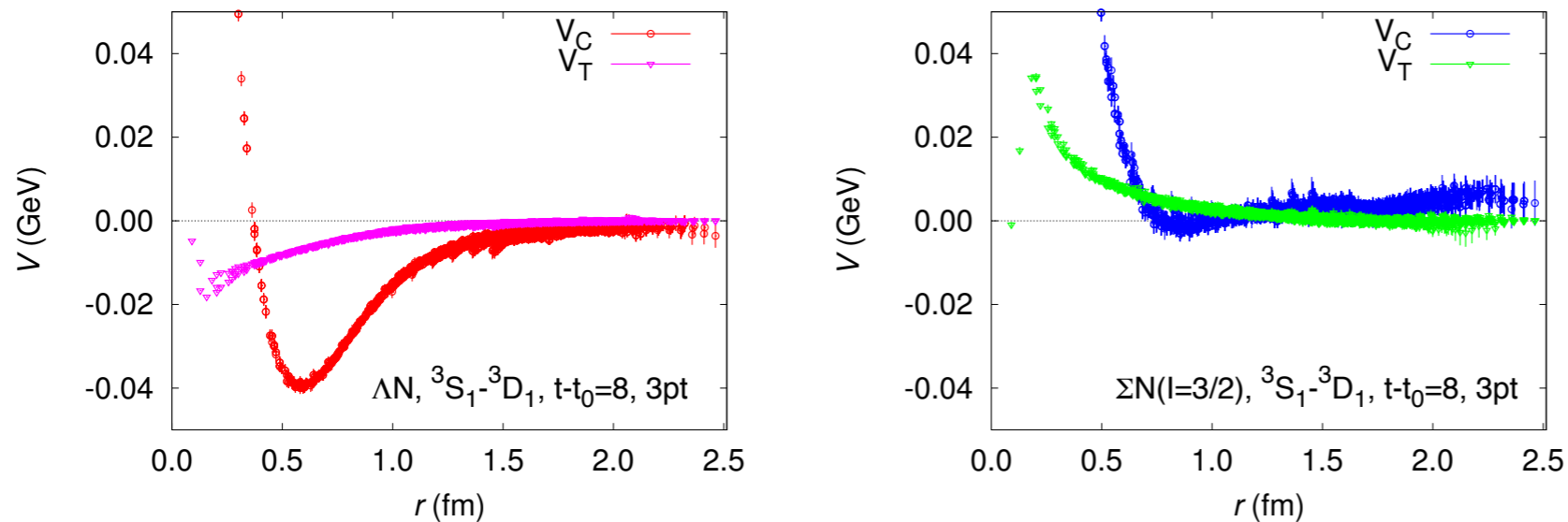


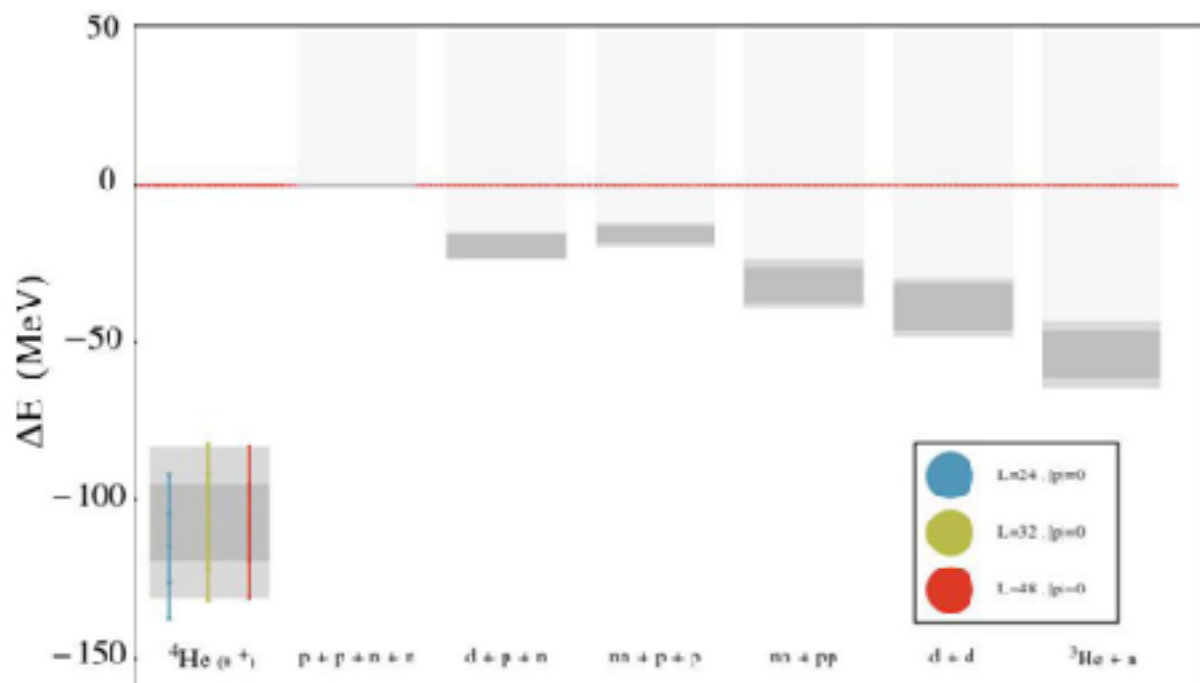
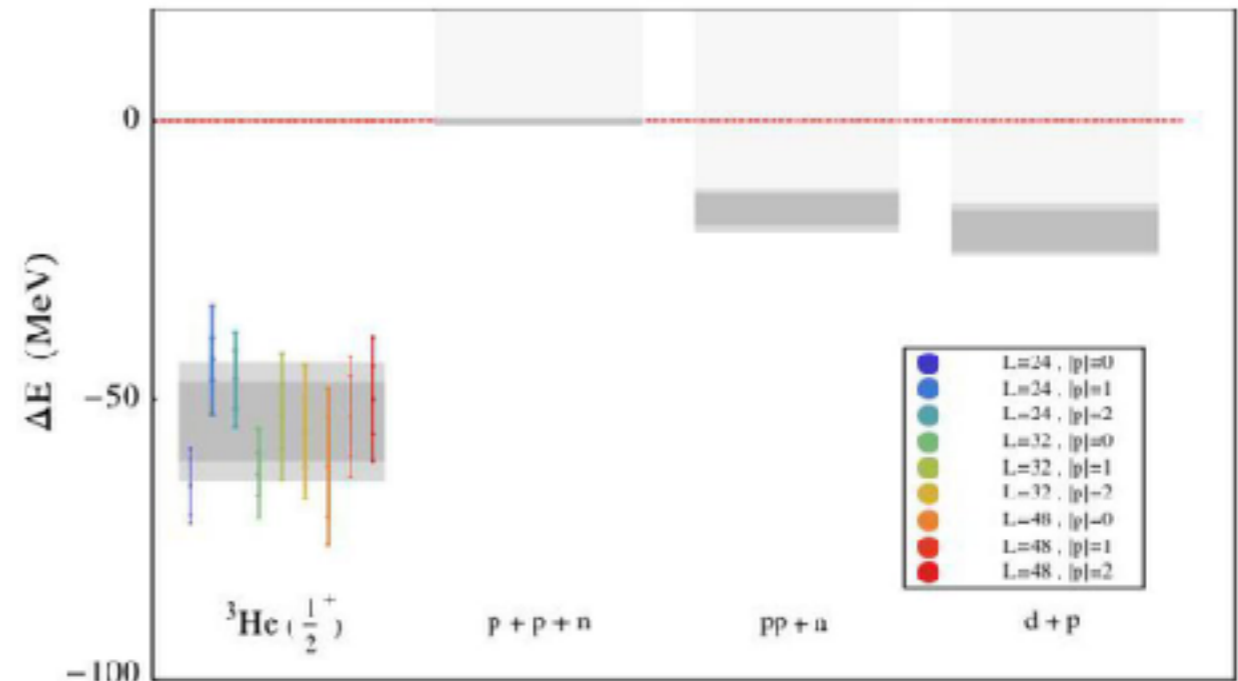
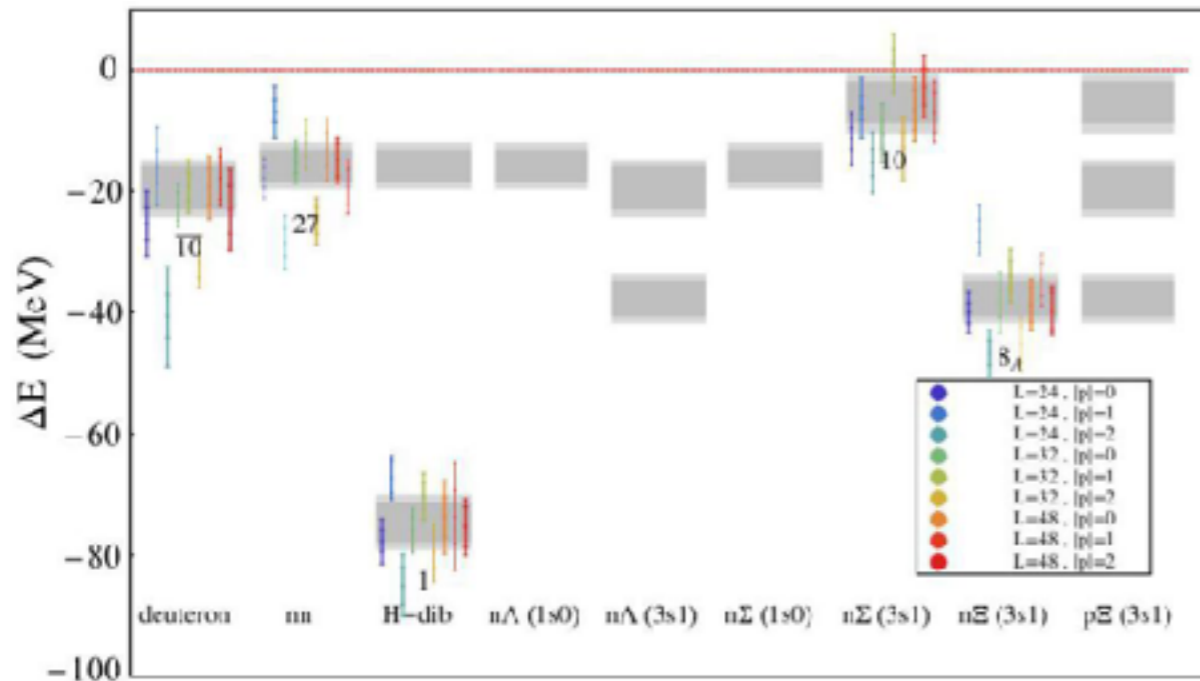
Fig. 11. Left: The central potential (circle) and the tensor potential (triangle) in the $^3S_1 - ^3D_1$ channel of the ΛN system as a function of r . Right: The central potential (circle) and the tensor potential (triangle) in the $^3S_1 - ^3D_1$ channel of the $\Sigma N(I = 3/2)$ system as a function of r .

Notice:

Potential energy is **not an observable**, and this determination is **not univocal!**

RELATION TO LQCD

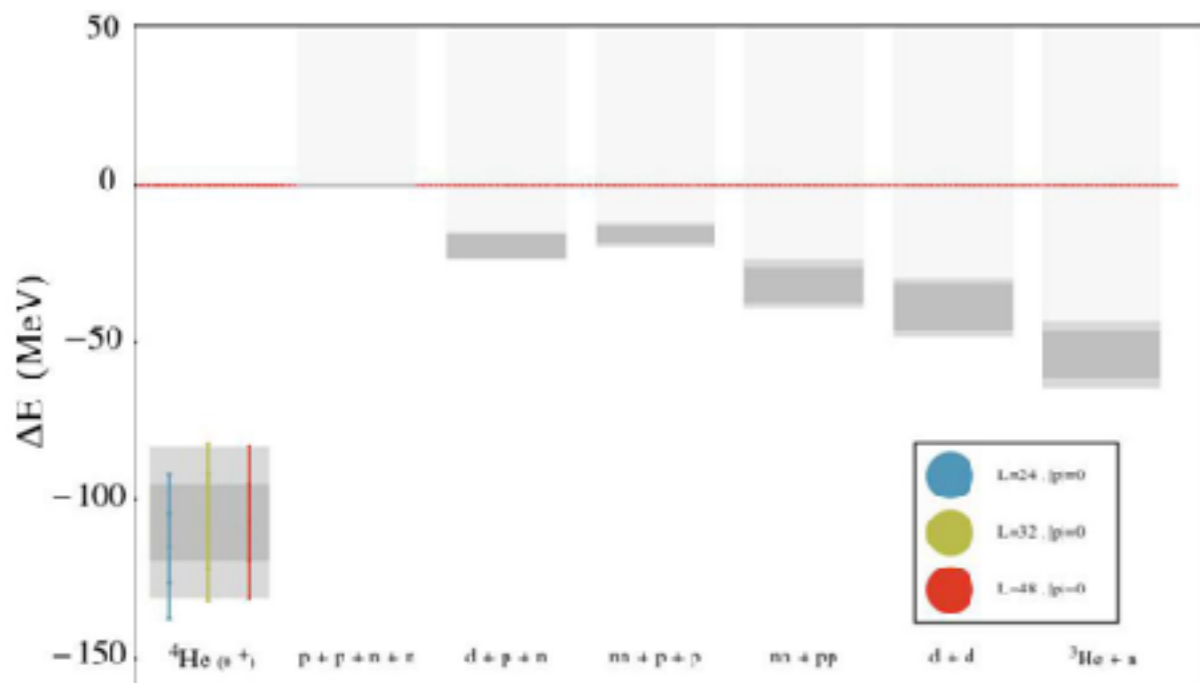
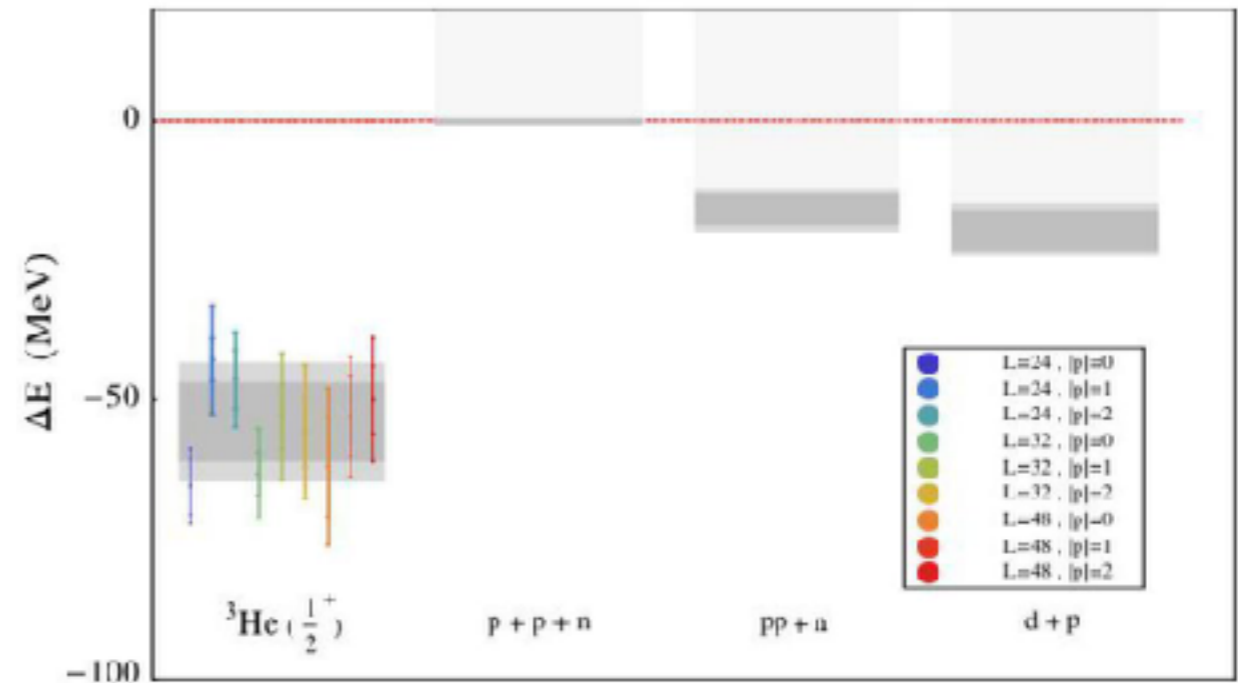
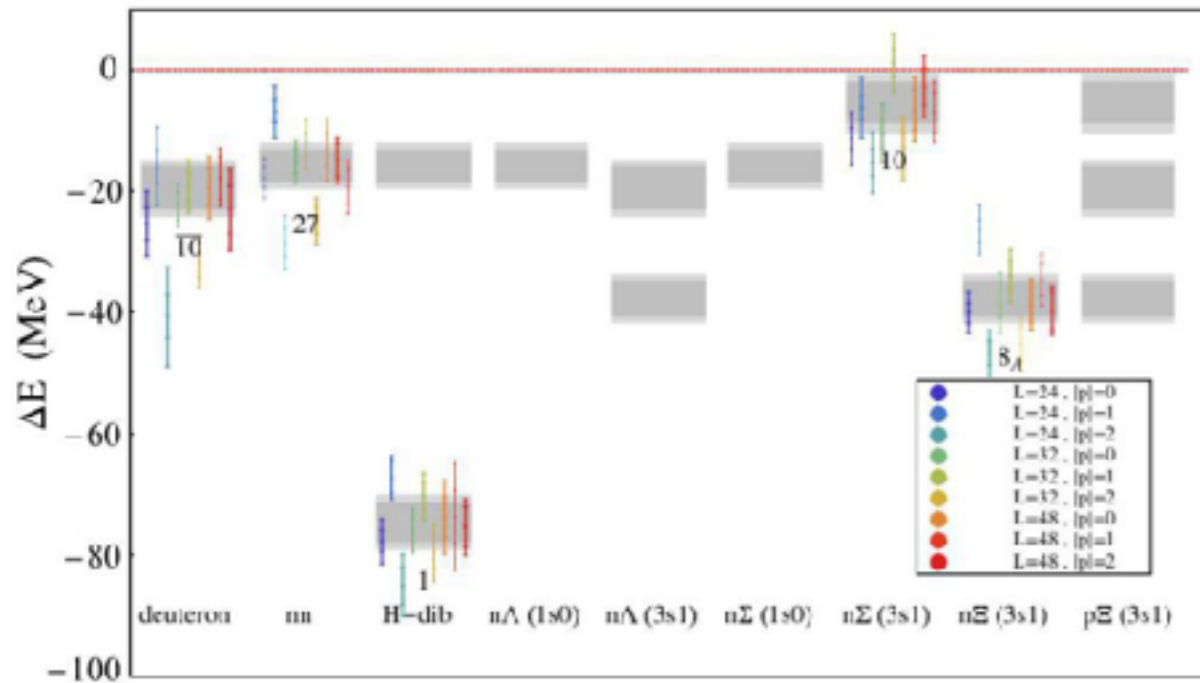
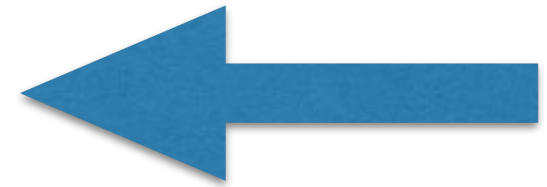
Route 2: direct use of LQCD observables



- LQCD simulations with $SU_f(3)$ symmetry
- Large pion mass $m_\pi = 800\text{MeV}$
- Results with $m_\pi \sim 450\text{ MeV}$ are available.

RELATION TO LQCD

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LQCD AND EFT (IN A NUTSHELL...)

- As of today LQCD simulations for $A \geq 2$ nuclei are **still away from the physical value of the pion mass**.
- The debate about whether reliable and/or usable NN interactions can be derived from **lattice simulations** is still open.

A REASONABLE PROCEDURE:

- Quark and gluon degrees of freedom are replaced by baryons and mesons.
 $\mathcal{L}_{QCD}(q, G) \rightarrow \mathcal{L}_{NucI}(N, \pi, \dots)$
- The $\mathcal{L}_{NucI}(N, \pi, \dots)$ is constructed **to retain QCD symmetries**.
- $\mathcal{L}_{NucI}(N, \pi, \dots)$ is an expansion in “low momentum” Q .
- Contains all terms compatible with QCD up to a “given order”.
- The low-energy coupling constants of the theory (LECs) are explicit function of a “momentum cutoff” Λ .

ENERGY SCALES

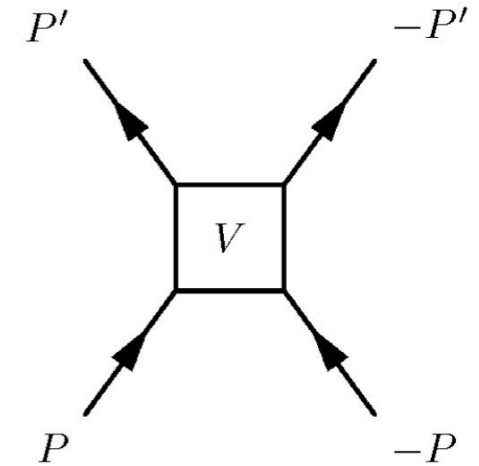
- The nucleon mass M_n , and the difference with the mass of the Δ baryon $\delta M = M_\Delta - M_n$
- The pion mass m_π , pion exchange momentum & energy
- Nuclear binding energy

Scale	Nature	LQCD@ $m_\pi=500\text{MeV}$	LQCD@ $m_\pi=800\text{MeV}$
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

For $m_\pi \sim 800$ MeV the natural effective theory is a pion-less theory, in which the only active degrees of freedom are nucleons

PIONLESS EFT LAGRANGIAN

$$\mathcal{L} = N^\dagger \left(i\partial_0 + \frac{\vec{\nabla}^2}{2M} \right) N - a_1 N^\dagger N N^\dagger N - a_2 N^\dagger \vec{\sigma} N \cdot N^\dagger \vec{\sigma} N \\ - a_3 N^\dagger \vec{\tau} N \cdot N^\dagger \vec{\tau} N - a_4 N^\dagger \vec{\sigma} \vec{\tau} N \cdot N^\dagger \vec{\sigma} \vec{\tau} N + \dots \\ - d_1 N^\dagger \vec{\tau} N \cdot N^\dagger \vec{\tau} N N^\dagger N$$



- Higher order terms include more derivatives.
- Very naively, the order goes as the number of derivatives (beware of $\mathcal{N} \dots$)
- The 3-body term appears at LO to avoid the Thomas collapse (theory must be renormalizable at all orders!)
- The coefficients depend on the cutoff Λ .

Some further wishes (mostly QMC related)

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

WHY PIONLESS?

For a 2 body system typical momentum related to the poles in the S matrix: $Q_2 = \sqrt{m_N B_2}$

Can we extend it to A nucleon systems?

This should be compared to m_π the breakdown scale of the theory.

$$Q_A = \sqrt{m_N \frac{B_A}{A}}$$

Hyp.: All nucleons contribute equally on average

	$m_\pi=140\text{MeV}$	$m_\pi=510\text{MeV}$	$m_\pi=805\text{MeV}$
m_N (MeV)	940	1300	1600
B_4 (MeV)	28	40*	120*
Q_4 (MeV)	115	161	310
B_{16} (MeV)	127	150*	500*
Q_{16} (MeV)	122	156	316

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Ok!

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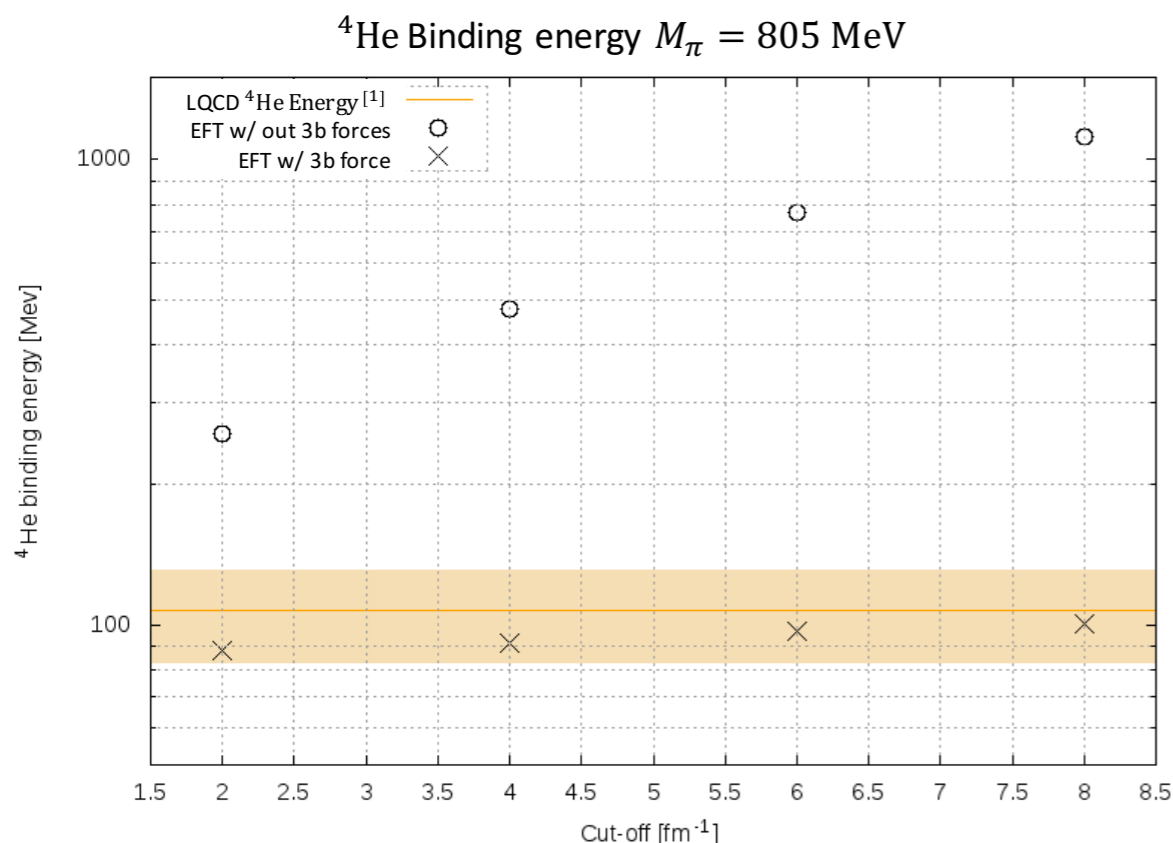
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COORDINATE SPACE FORMULATION

The leading order contains no momentum dependence, therefore:

$$V_{LO}^{2b}(r) = [C^{LO}(\Lambda)_1 + C^{LO}(\Lambda)_2 \vec{\sigma}_1 \cdot \vec{\sigma}_2] e^{-\Lambda^2 r^2 / 4}$$

“Thomas collapse”



[1] - S. R. Beane, E. Chang and al. [Phys. rev. D 87, 034506 (2013)]

All expectations will have in principle a residual dependence on Λ . We require the theory to be **renormalized at all orders**.

If we see a cutoff **dependence on observables**, this means that **we are not using the correct power counting**.

CONSEQUENCE

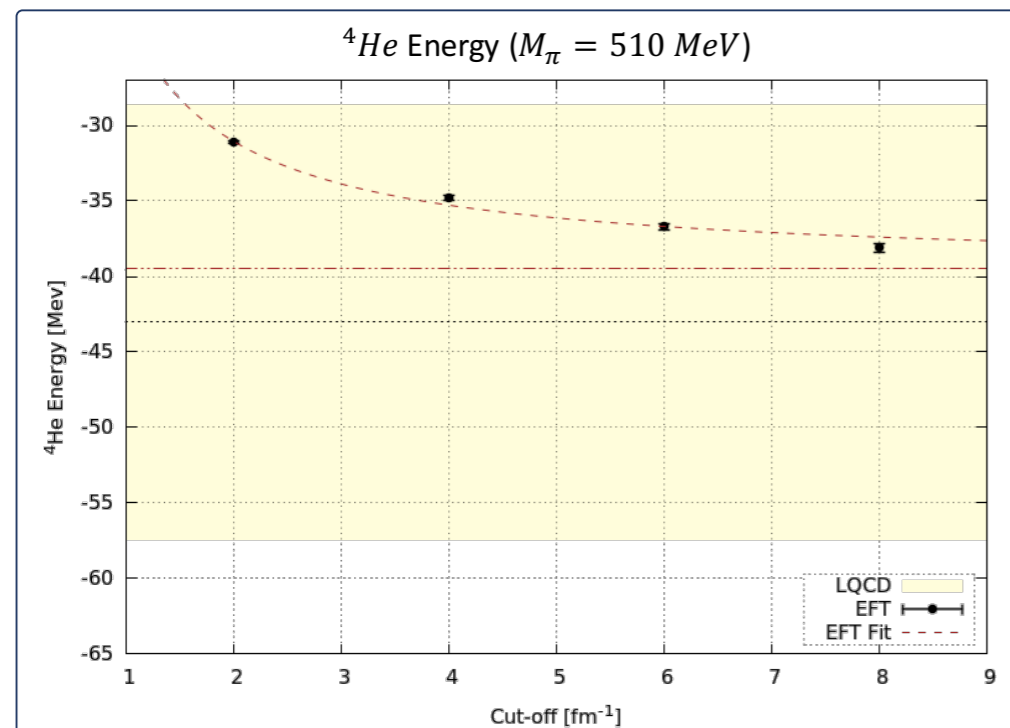
► **We need a three-body force at leading order**

► **No evidence of a 4-body interaction at leading order.**

COORDINATE SPACE FORMULATION

After regularization and renormalization the LO Hamiltonian becomes:

$$V^{LO} = \sum_{i<j} [C_0^\Lambda e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2} + C_1^\Lambda e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2} (\vec{\sigma}_i \cdot \vec{\sigma}_j)] + D_0^\Lambda \sum_{(i<j) \neq k} \left[e^{-\frac{\Lambda^2}{2}(|r_{ij}|^2 + |r_{ik}|^2)} + e^{-\frac{\Lambda^2}{2}(|r_{ij}|^2 + |r_{jk}|^2)} + e^{-\frac{\Lambda^2}{2}(|r_{jk}|^2 + |r_{ik}|^2)} \right]$$



PRL 114, 052501 (2015)

PHYSICAL REVIEW LETTERS

week ending
6 FEBRUARY 2015

Effective Field Theory for Lattice Nuclei

N. Barnea,¹ L. Contessi,² D. Gazit,¹ F. Pederiva,^{2,3} and U. van Kolck^{4,5}

PHYSICAL REVIEW C 92, 054002 (2015)

Spectra and scattering of light lattice nuclei from effective field theory

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(Received 30 June 2015; published 17 November 2015)

THE NON RELATIVISTIC NUCLEAR PROBLEM

We will focus on the treatment of the many-nucleon problem as a *non-relativistic quantum problem* for A interacting nucleons (baryons). This means that we assume that the system is well described by a Hamiltonian, and observables can be predicted from the solution of the time independent Schroedinger equation:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

where $|\Psi\rangle$ is a A nucleon state, and

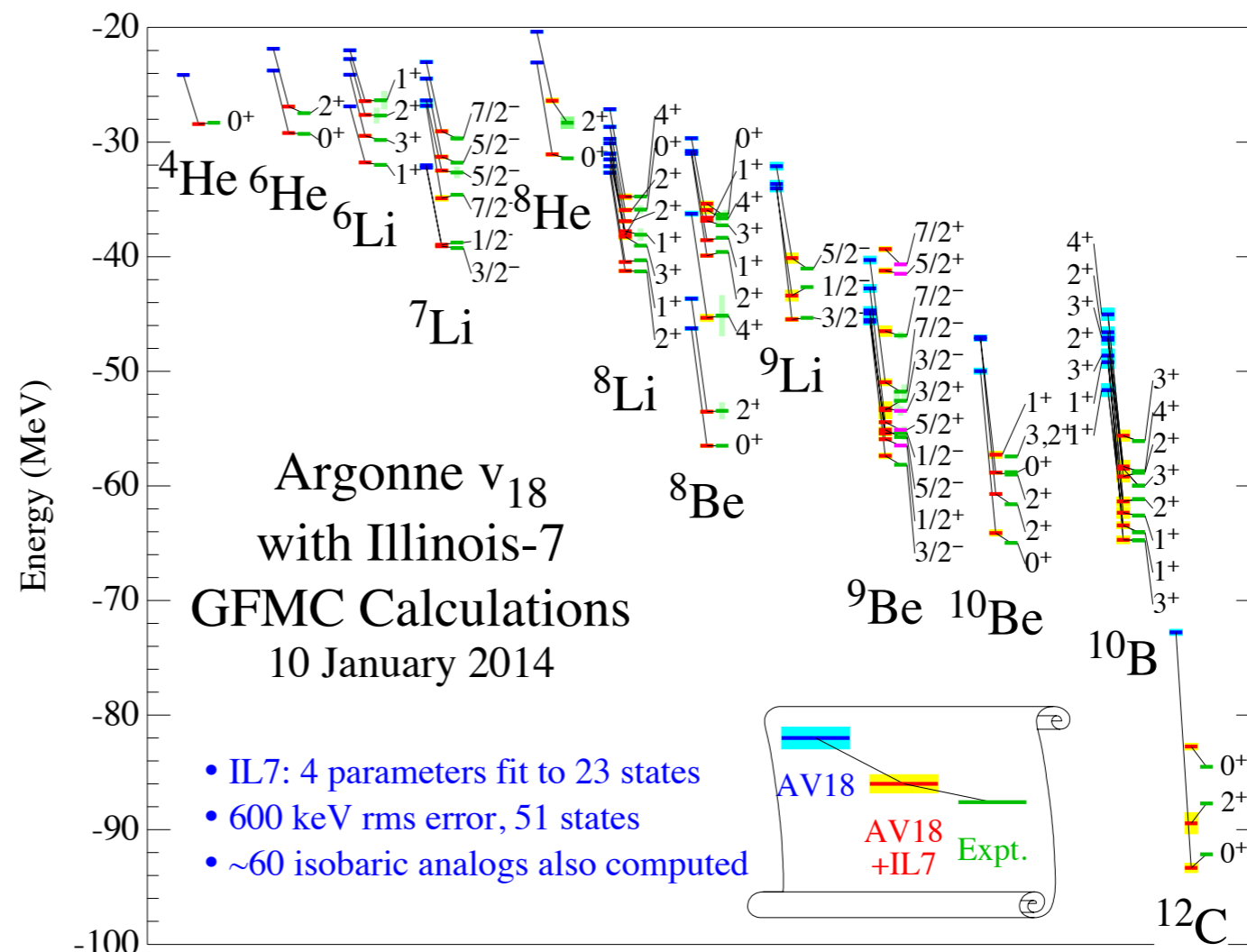
$$\hat{H} = \sum_{i=1}^A -\frac{\hat{p}_i^2}{2m_i} + \hat{V}(1, 2, 3, \dots, N)$$

Many-nucleon systems

PROBLEM

for realistic many-nucleon Hamiltonians, propagators must be evaluated on wave functions that have a number of components exponentially growing with A (spin/isospin singlet/triplet state for each pair of nucleons)

Very accurate results have been obtained in the years for the ground state and some excitation properties of nuclei with $A \leq 12$ by the Argonne based group (GFMC calculations by Pieper, Wiringa, Carlson, Schiavilla...). These calculations include two- and three-nucleon interactions.



Courtesy of R. Wiringa, ANL

Many-Body theory: projection Monte Carlo

We compute ground state energies of nuclei by means of projection Monte Carlo methods. The ground state of a many-body system is computed by applying an “imaginary time propagator” to an arbitrary state that has to be non-orthogonal to the ground state (power method):

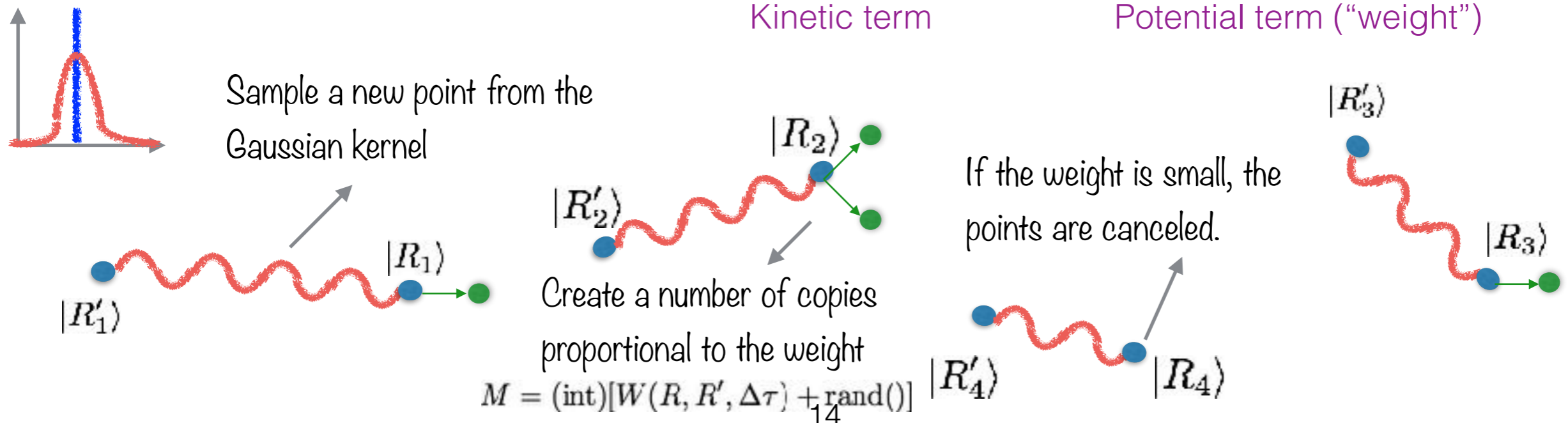
$$\langle R | \Psi(\tau) \rangle = \langle R | e^{-(\hat{H} - E_0)\tau} | R' \rangle \langle R' | \Psi(0) \rangle$$

In the limit of “short” τ (let us call it “ $\Delta\tau$ ”), the propagator can be broken up as follows (Trotter-Suzuki formula):

$$\langle R | e^{-(\hat{H} - E_0)\Delta\tau} | R' \rangle \sim e^{-\frac{(R - R')^2}{2 \frac{\hbar}{m} \Delta\tau}} e^{-\left(\frac{V(R) + V(R')}{2} - E_0\right)\Delta\tau}$$

Kinetic term

Potential term (“weight”)



Auxiliary Field Diffusion Monte Carlo (AFDMC)

K. E. Schmidt, S. Fantoni, A quantum Monte Carlo method for nucleon systems, Phys. Lett. B446 (1999)

The computational cost of GFMC can be reduced by introducing a way of **sampling over the space of states**, rather than summing explicitly over the full set.

For simplicity let us consider only one of the terms in the interaction. We start by observing that:

$$\sum_{i < j} v(r_{ij}) \vec{\sigma}_i \cdot \vec{\sigma}_j = \frac{1}{2} \sum_{i; \alpha, j; \beta} \sigma_{i; \alpha} A_{i; \alpha, j; \beta} \sigma_{j; \beta} = \sum_{n=1}^{3A} \lambda_n \hat{O}_n^2$$

Linear combination of spin operators for different particles

Then, we can linearize the operatorial dependence in the propagator by means of an integral transform:

$$e^{-\frac{1}{2} \lambda \hat{O}_n^2 \Delta \tau} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2}} e^{-x \sqrt{\lambda \Delta \tau} \hat{O}_n}$$

auxiliary fields → Auxiliary Field Diffusion Monte Carlo

Hubbard-Stratonovich transformation

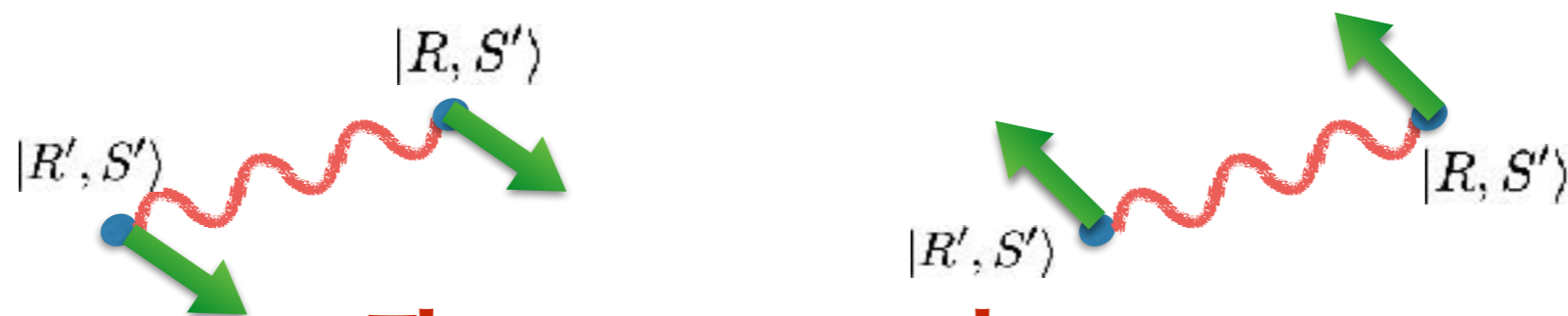
Auxiliary Field Diffusion Monte Carlo (AFDMC)

The operator dependence in the exponent has become **linear**.

In the Monte Carlo spirit, the integral can be performed by sampling values of x from the Gaussian $e^{-\frac{x^2}{2}}$. For a given x the action of the propagator will become:

$$e^{-x\sqrt{\lambda\Delta\tau}\hat{O}_n}|S\rangle = \prod_{k=1}^{3A} e^{-x\sqrt{\lambda\Delta\tau}\phi_n^k\sigma_k}|S\rangle$$

In a space of spinors, each factor corresponds to a rotation induced by the action of the Pauli matrices



**The sum over the states
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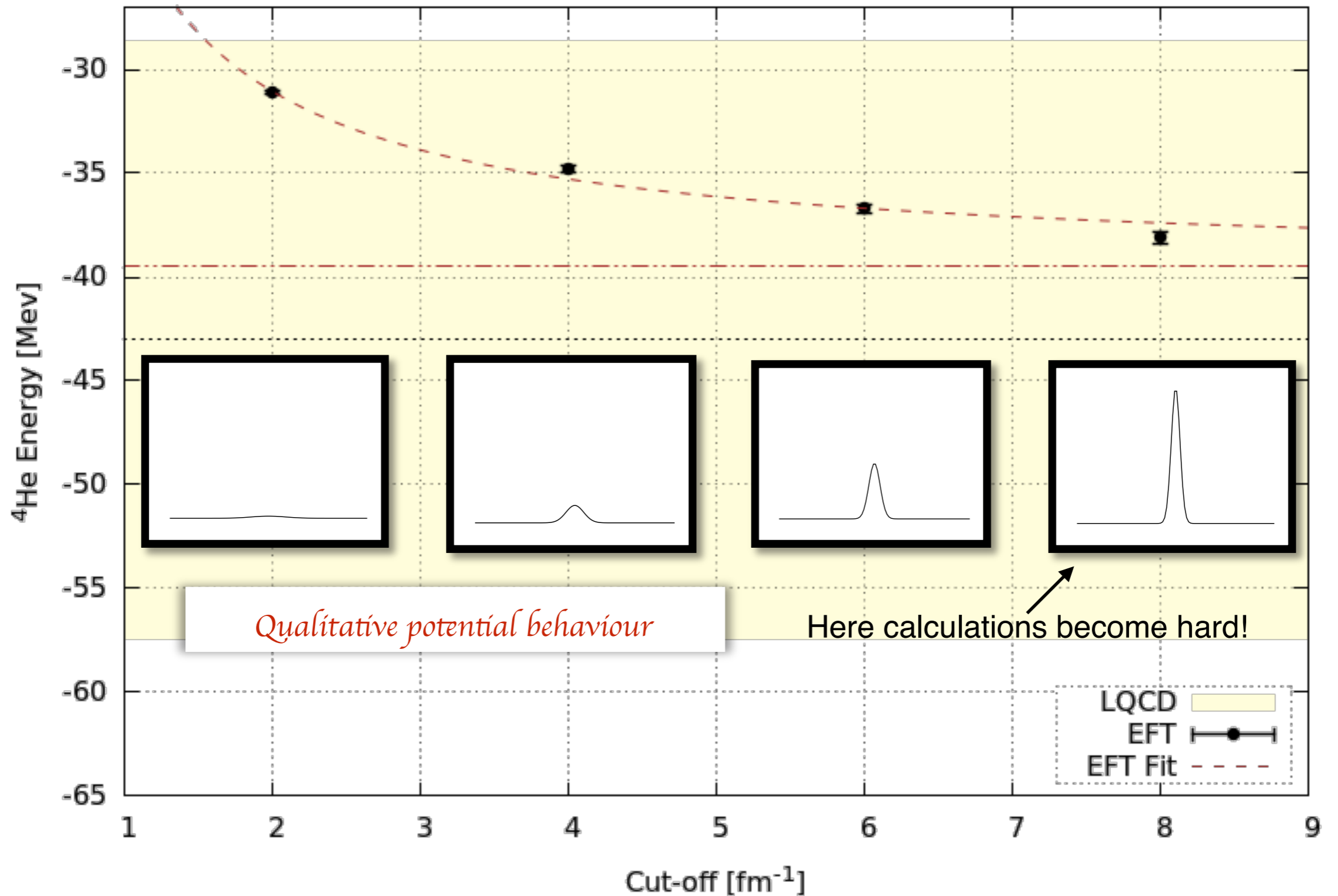
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CUTOFF DEPENDENCE OF THE POTENTIAL

${}^4\text{He}$ Energy ($M_\pi = 510 \text{ MeV}$)



^{16}O CALCULATIONS

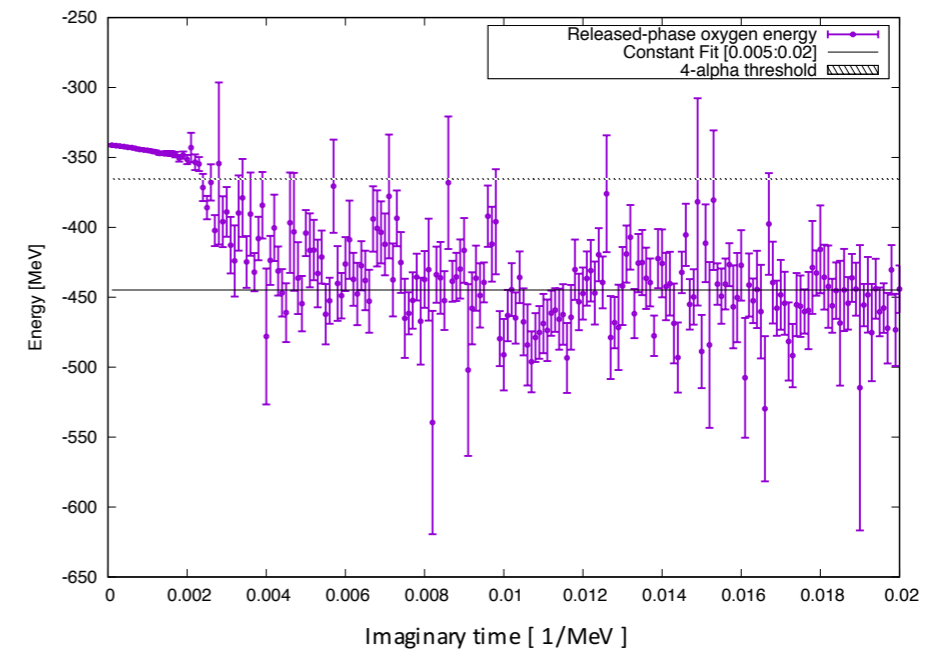
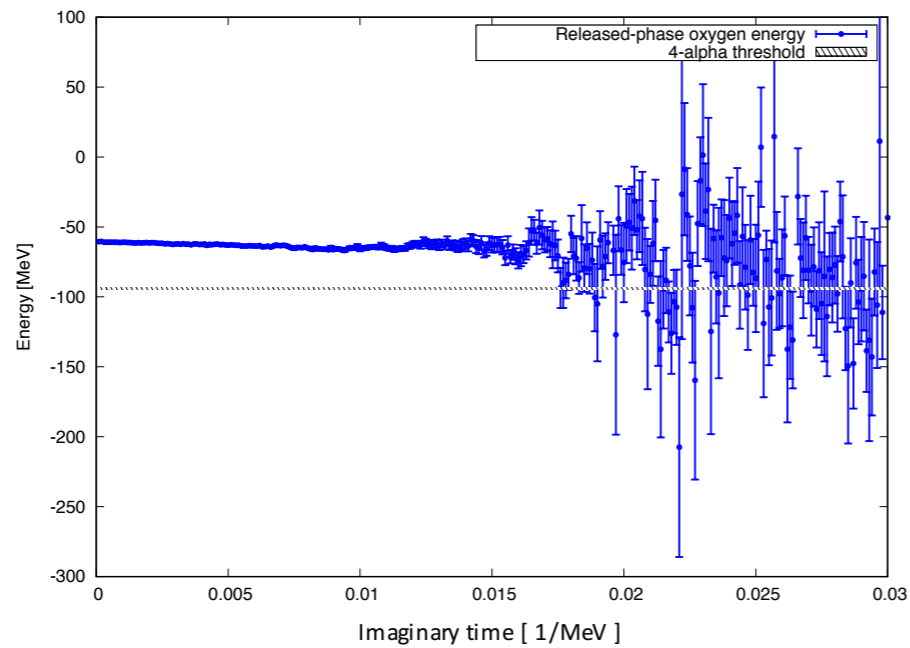
Released node calculations (L. Contessi, A. Lovato, unpublished)

M_π 140 MeV

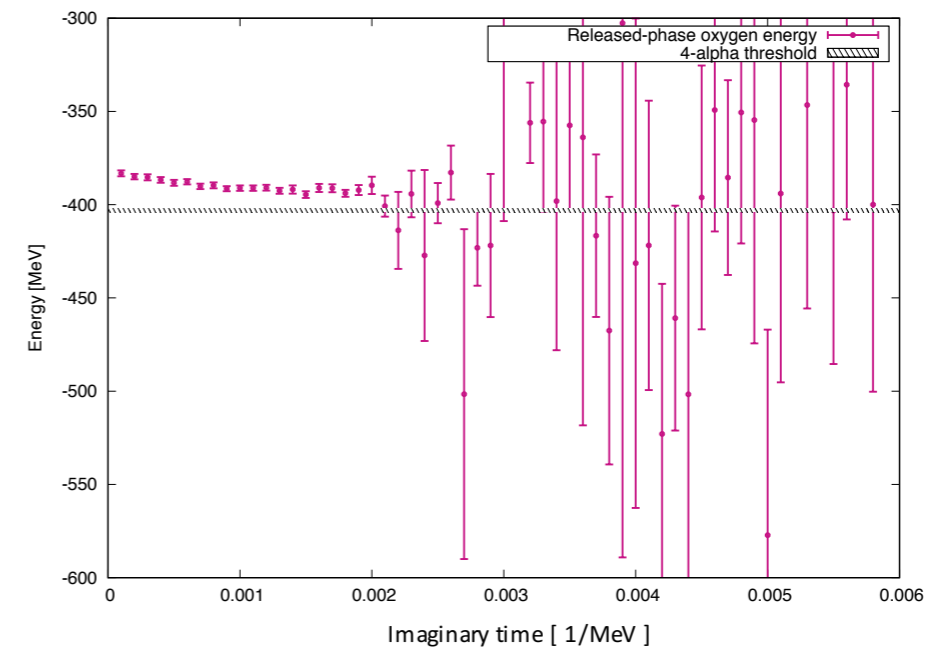
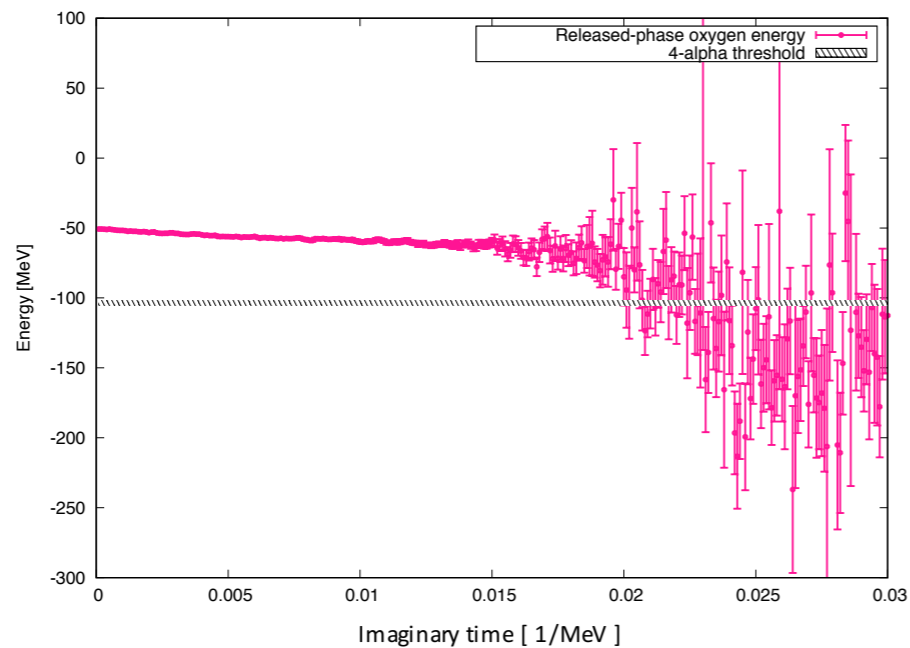
800 MeV

Cut-off

4 fm^{-1}



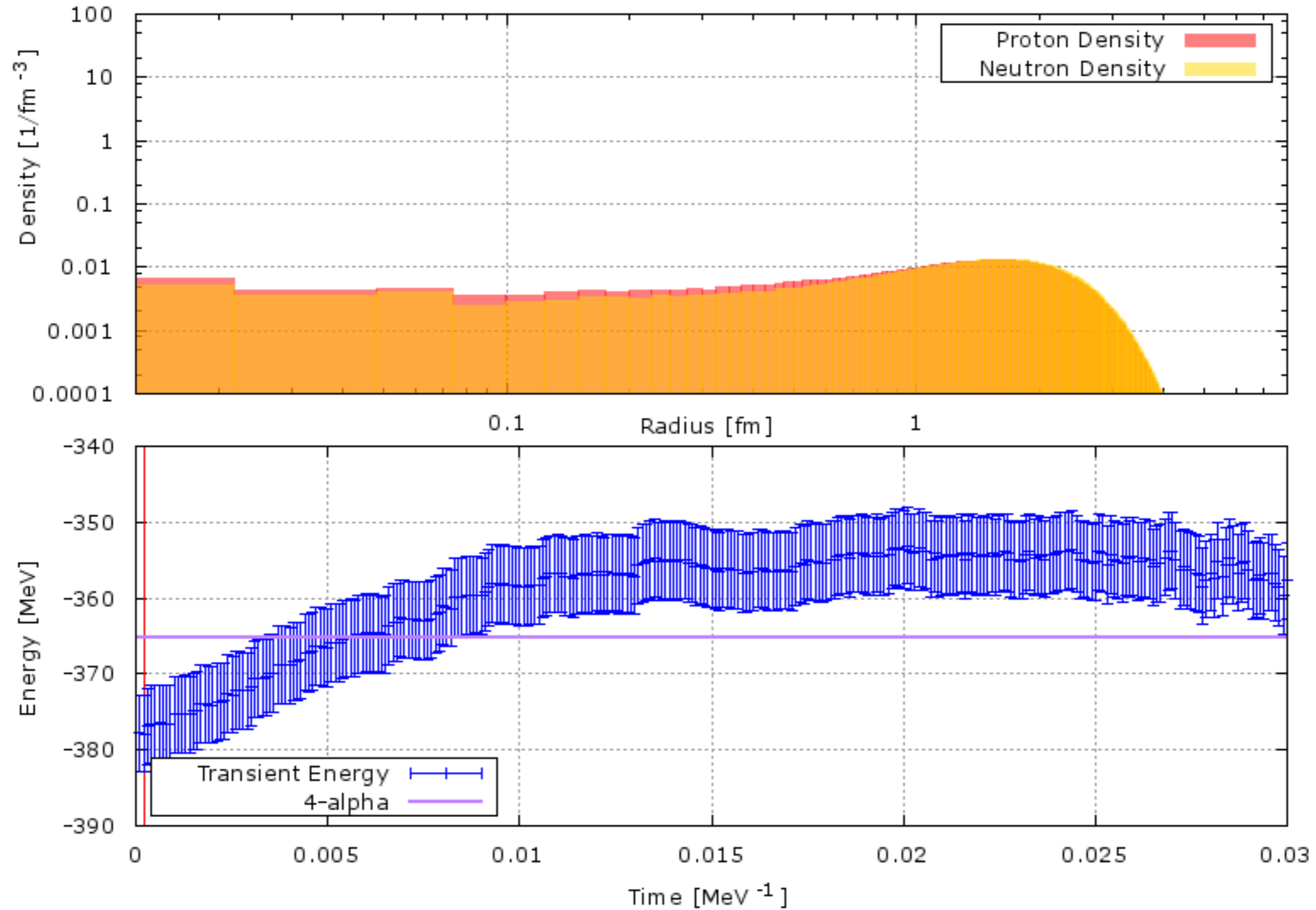
8 fm^{-1}



^{16}O CALCULATIONS

L. Contessi, unpublished

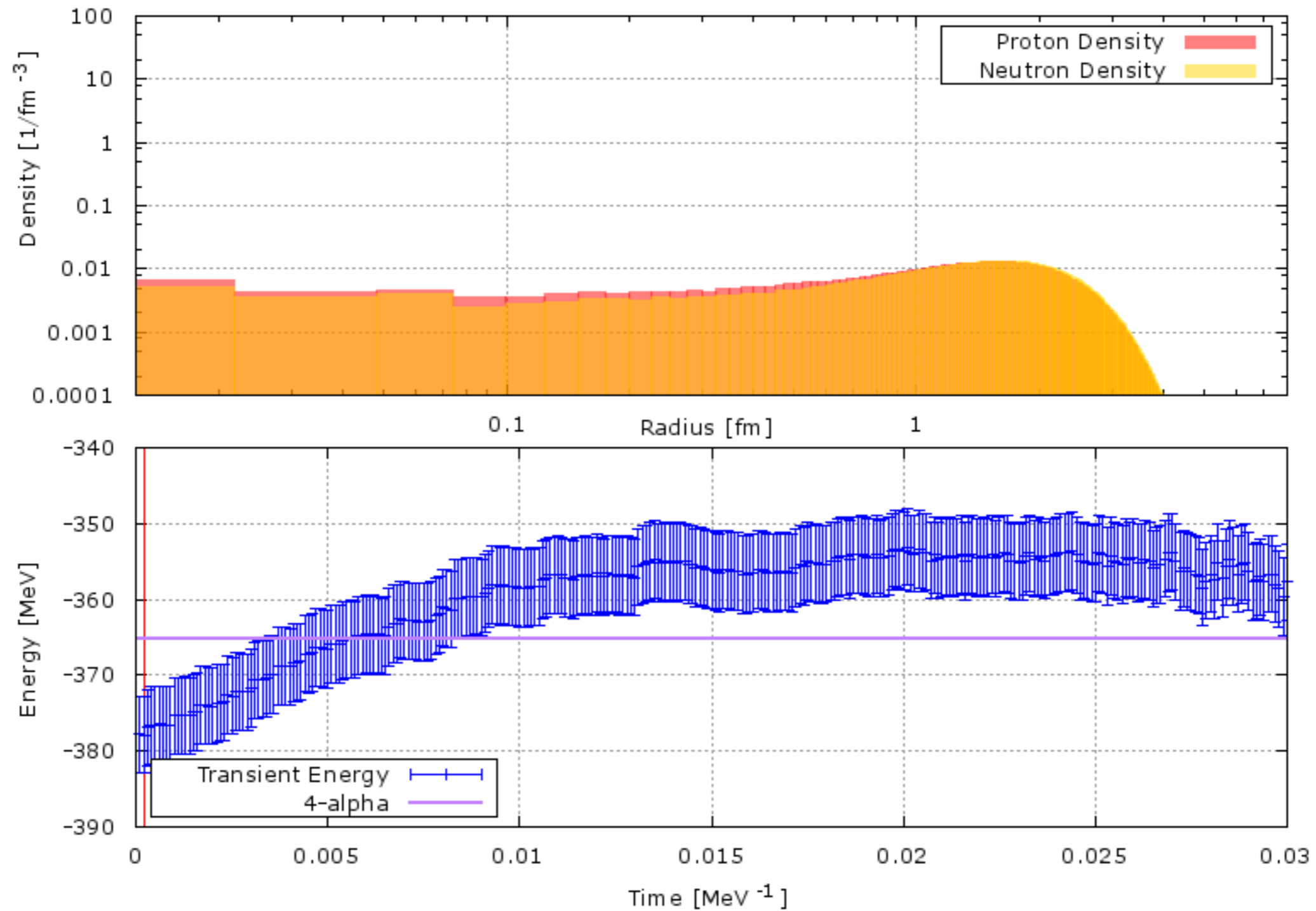
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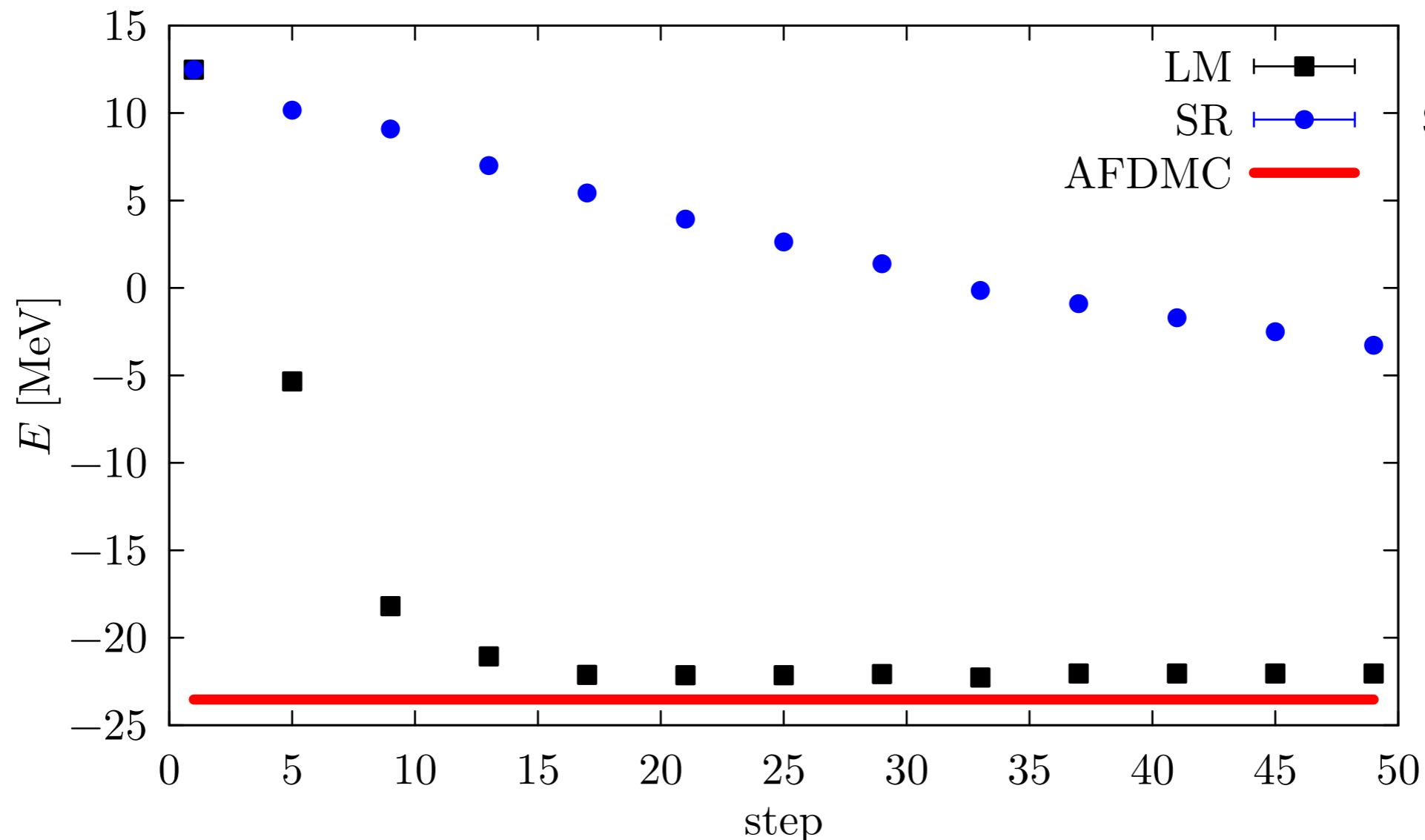
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LINEAR OPTIMIZATION OF THE WAVEFUNCTION



S. Sorella et al.

In order to improve the results it is necessary to **improve the importance/reference wavefunction**. This can be obtained by expanding the correlation and (even more important) the orbitals in order to have a **phase as close as possible to the exact one**. An improved version of the LM by Umrigar and Toulouse was used in this paper (A. Roggero and A. Lovato)

LINEAR OPTIMIZATION OF THE WAVEFUNCTION

J. Toulouse and C. J. Umrigar, J. Chem. Phys. **126**, 084102 (2007), A. Lovato and A. Roggero, *tbp*

We consider a trial state dependent on a set of parameters $\{p_1 \dots p_k\}$:

$$|\bar{\Psi}_T(\mathbf{p})\rangle = \frac{|\Psi_T(\mathbf{p})\rangle}{\sqrt{\langle \Psi_T(\mathbf{p}) | \Psi_T(\mathbf{p}) \rangle}}$$

Expanding the state in the parameters at first order we get:

$$|\bar{\Psi}_T^{\text{lin}}(\mathbf{p})\rangle = |\bar{\Psi}_T(\mathbf{p}^0)\rangle + \sum_{i=1}^{N_p} \Delta p_i |\bar{\Psi}_T^i(\mathbf{p}^0)\rangle$$

We then look for the variation of the parameters $\Delta \mathbf{p}$ that minimizes:

$$E_{\text{lin}}(\mathbf{p}) \equiv \frac{\langle \bar{\Psi}_T^{\text{lin}}(\mathbf{p}) | H | \bar{\Psi}_T^{\text{lin}}(\mathbf{p}) \rangle}{\langle \bar{\Psi}_T^{\text{lin}}(\mathbf{p}) | \bar{\Psi}_T^{\text{lin}}(\mathbf{p}) \rangle}$$

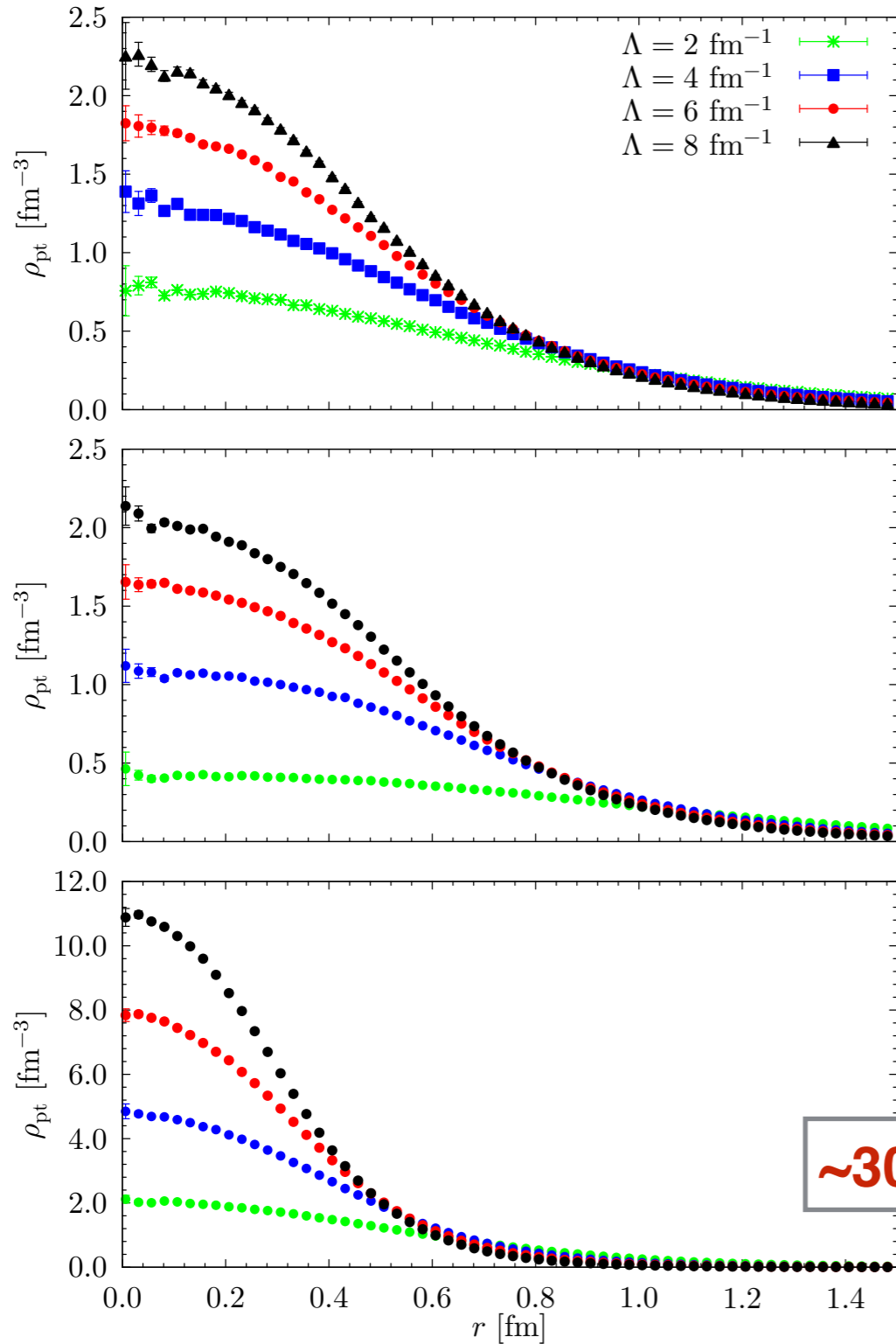
corresponding to solve the linear equation:

$$\bar{H} \Delta \mathbf{p} = \Delta E \bar{S} \Delta \mathbf{p}$$

where \bar{H} and \bar{S} are the matrix elements of the Hamiltonian and the overlaps of the basis

$$\{|\bar{\Psi}_T(\mathbf{p}^0)\rangle, |\bar{\Psi}_T^1(\mathbf{p}^0)\rangle, \dots, |\bar{\Psi}_T^{N_p}(\mathbf{p}^0)\rangle\} \quad \text{where} \quad |\bar{\Psi}_T^i(\mathbf{p}^0)\rangle = \left. \frac{\partial |\Psi_T(\mathbf{p})\rangle}{\partial p_i} \right|_{\mathbf{p}=\mathbf{p}^0}$$

RESULTS FOR ${}^4\text{He}$



Λ	$m_\pi = 140 \text{ MeV}$	$m_\pi = 510 \text{ MeV}$	$m_\pi = 805 \text{ MeV}$
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
$\rightarrow \infty$	$-30^{+0.3(\text{sys})}_{+2.6(\text{stat})}$	$-39^{+1(\text{sys})}_{+2(\text{stat})}$	$-124^{+2(\text{sys})}_{+1(\text{stat})}$
Exp.	-28.30	-	-
LQCD	-	-43.0 ± 14.4	-107.0 ± 24.2

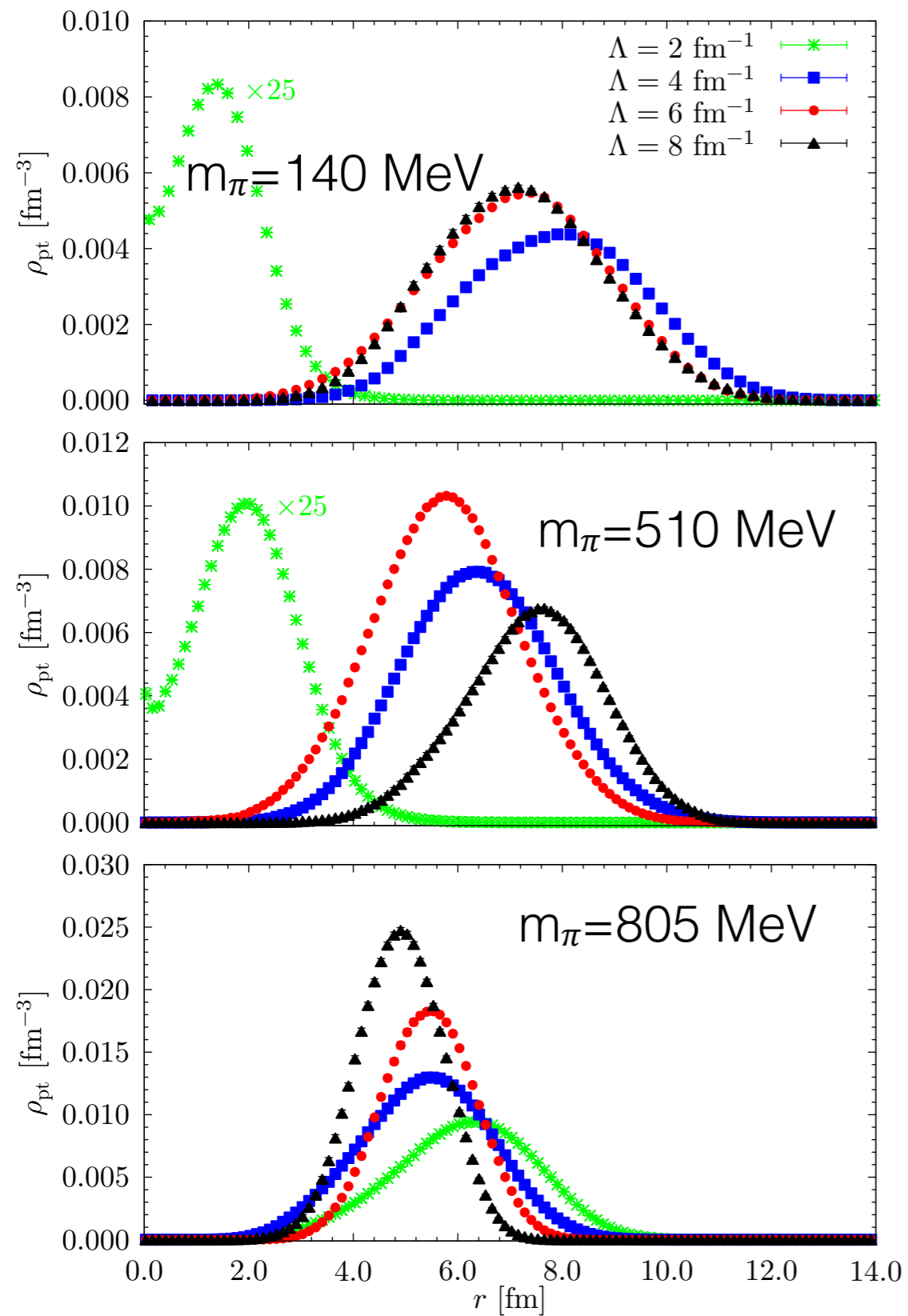
Table 1: ${}^4\text{He}$ energy for different values of the pion mass m_π and the cutoff Λ , compared to experiment and LQCD calculations [1, 2]. See main text and appendix for details on errors and extrapolations.

Λ	$m_\pi = 140 \text{ MeV}$	$m_\pi = 510 \text{ MeV}$	$m_\pi = 805 \text{ MeV}$
2 fm^{-1}	1.374 ± 0.004	1.482 ± 0.003	0.898 ± 0.001
4 fm^{-1}	1.203 ± 0.004	1.133 ± 0.003	0.699 ± 0.001
6 fm^{-1}	1.109 ± 0.003	1.035 ± 0.002	0.609 ± 0.001
8 fm^{-1}	1.054 ± 0.003	0.976 ± 0.001	0.542 ± 0.001
$\rightarrow \infty$	$0.9^{+0.008(\text{sys})}_{+0.2(\text{stat})}$	$0.8^{+0.04(\text{sys})}_{+0.1(\text{stat})}$	$0.25^{+0.05(\text{sys})}_{+0.06(\text{stat})}$
“Exp.”	1.45		

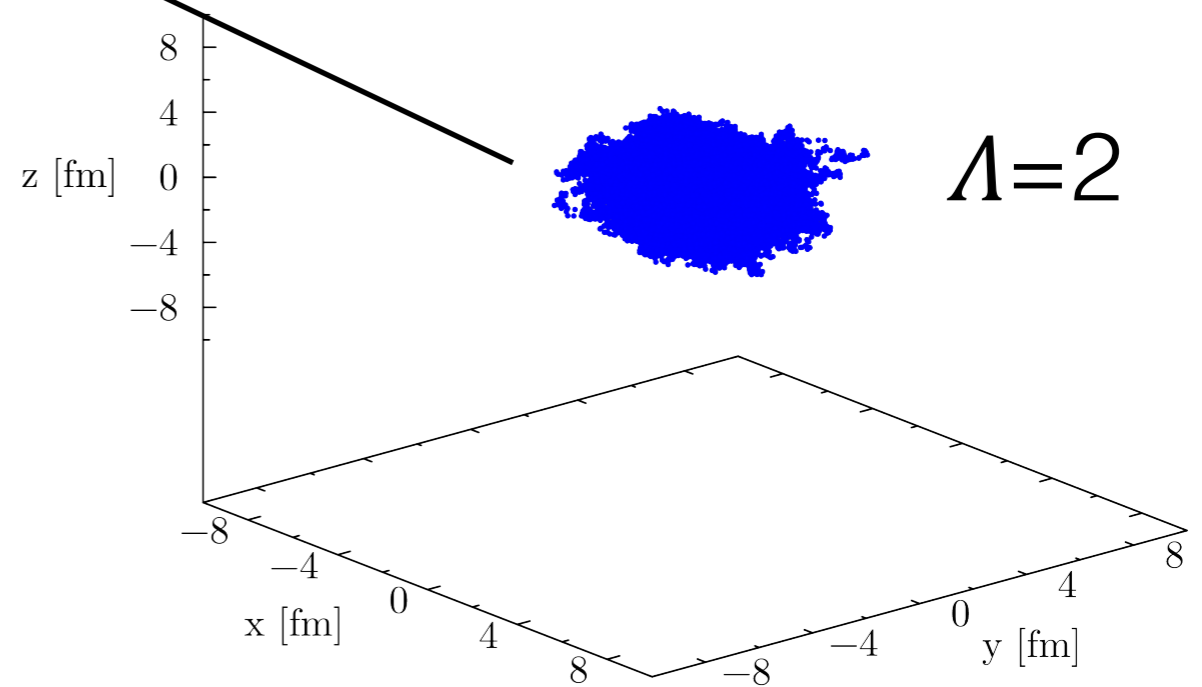
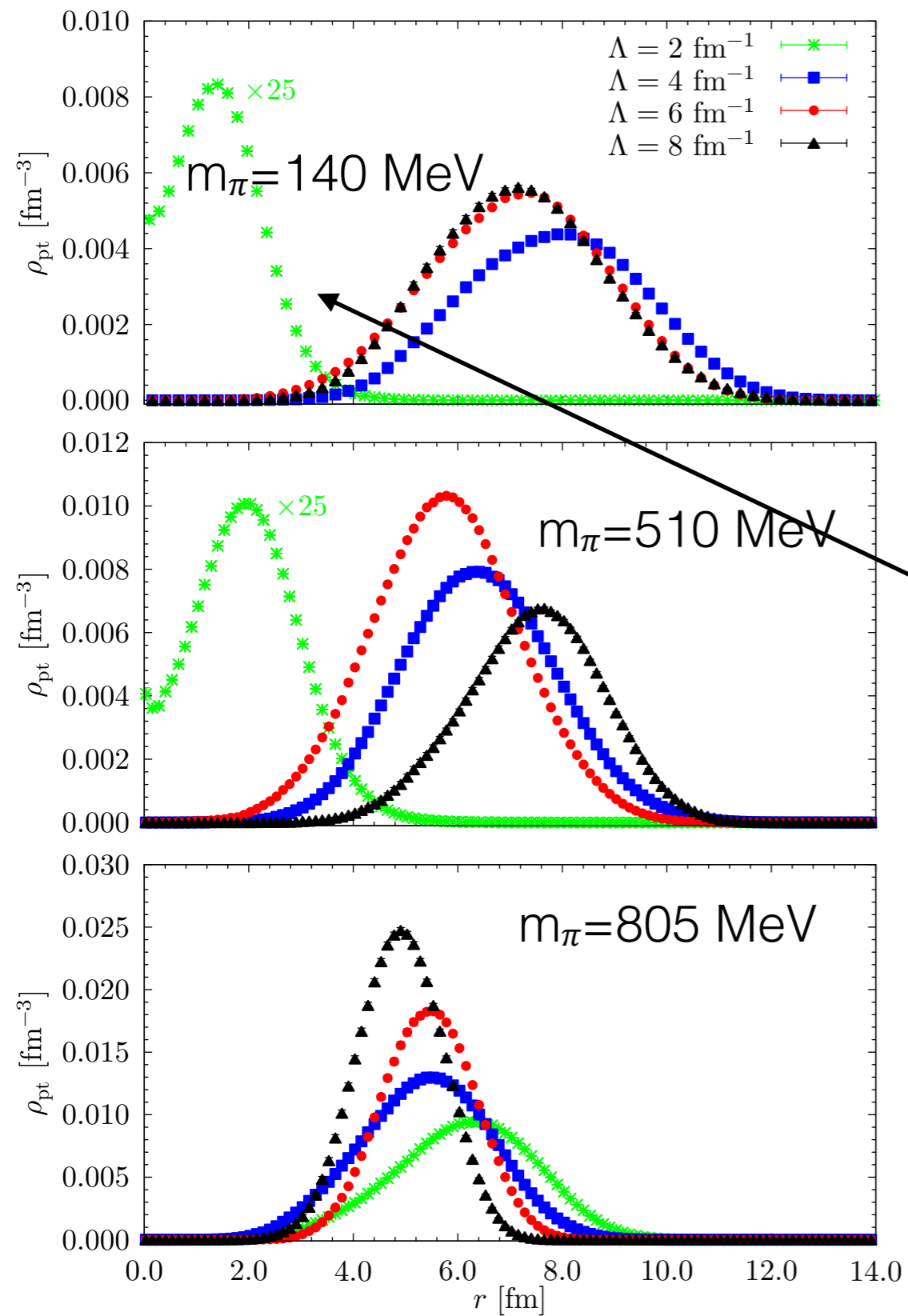
Table 2: ${}^4\text{He}$ point-proton radius for different values of the pion mass m_π and cutoff Λ , compared to experiment and LQCD calculations [1, 2]. See main text and appendix for details on errors and extrapolations.

~30% error at LO expected from theory

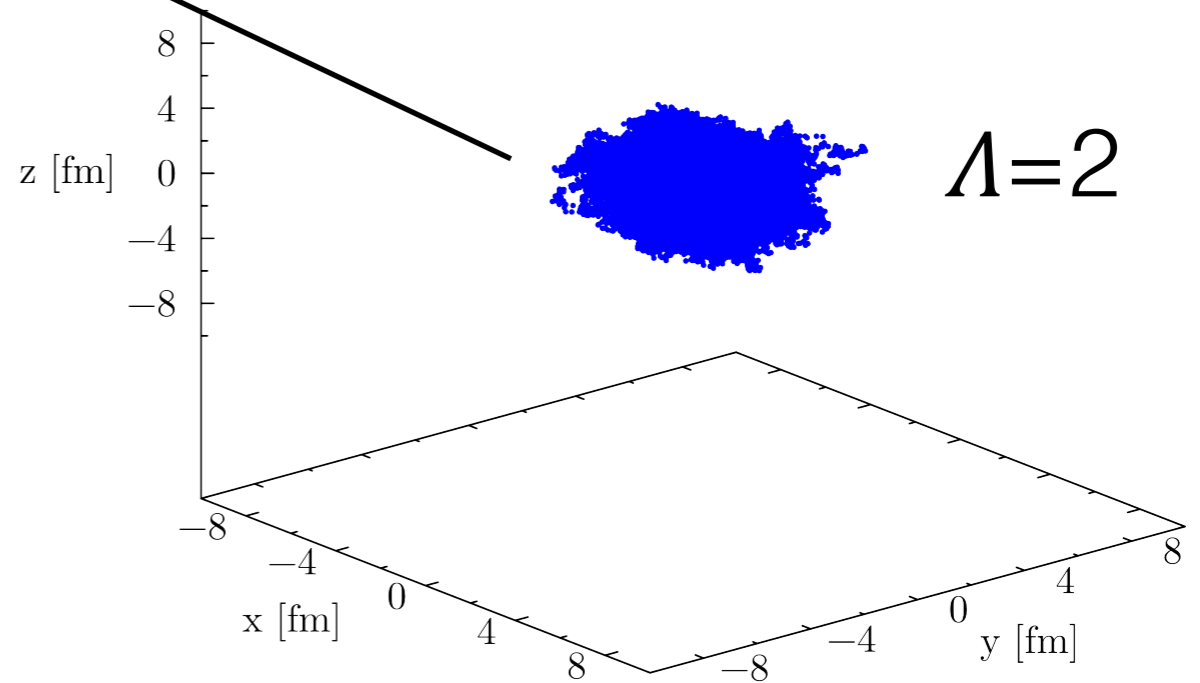
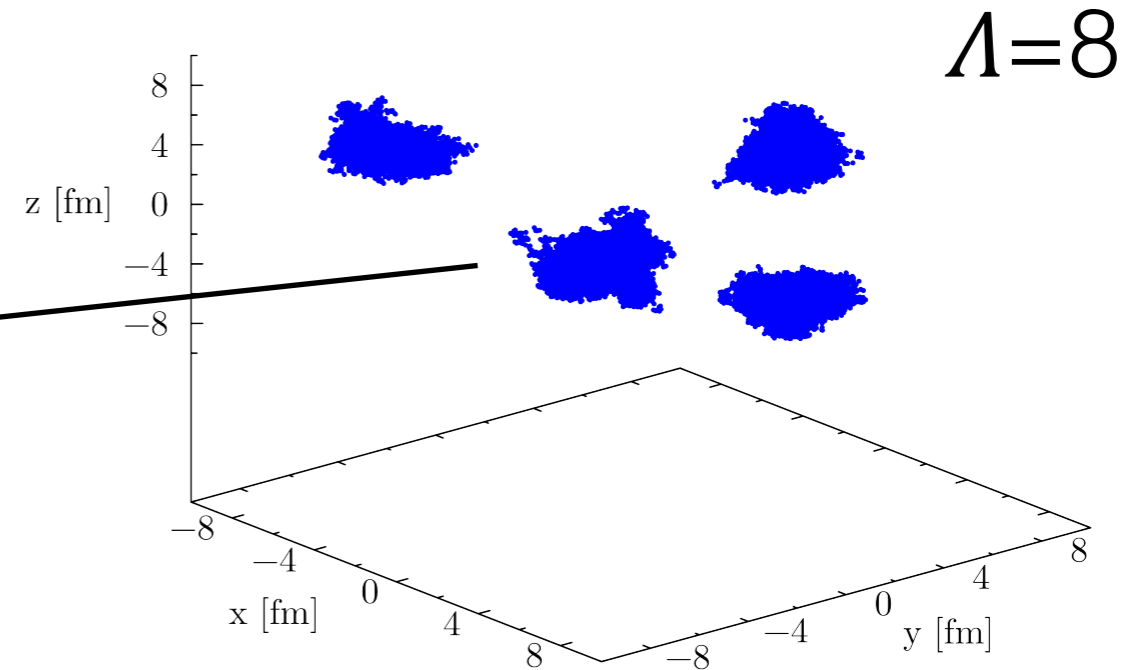
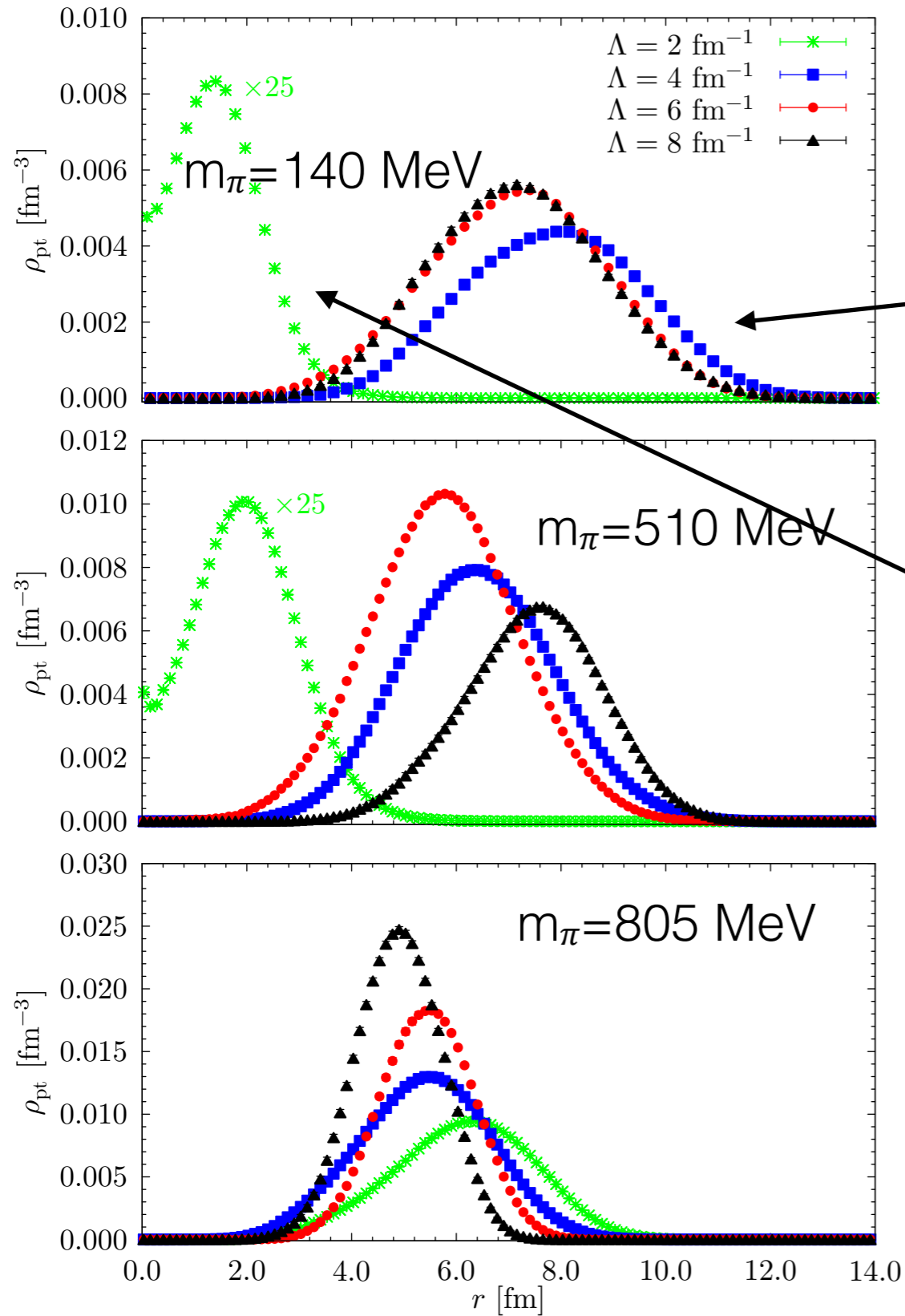
RESULTS FOR ^{16}O



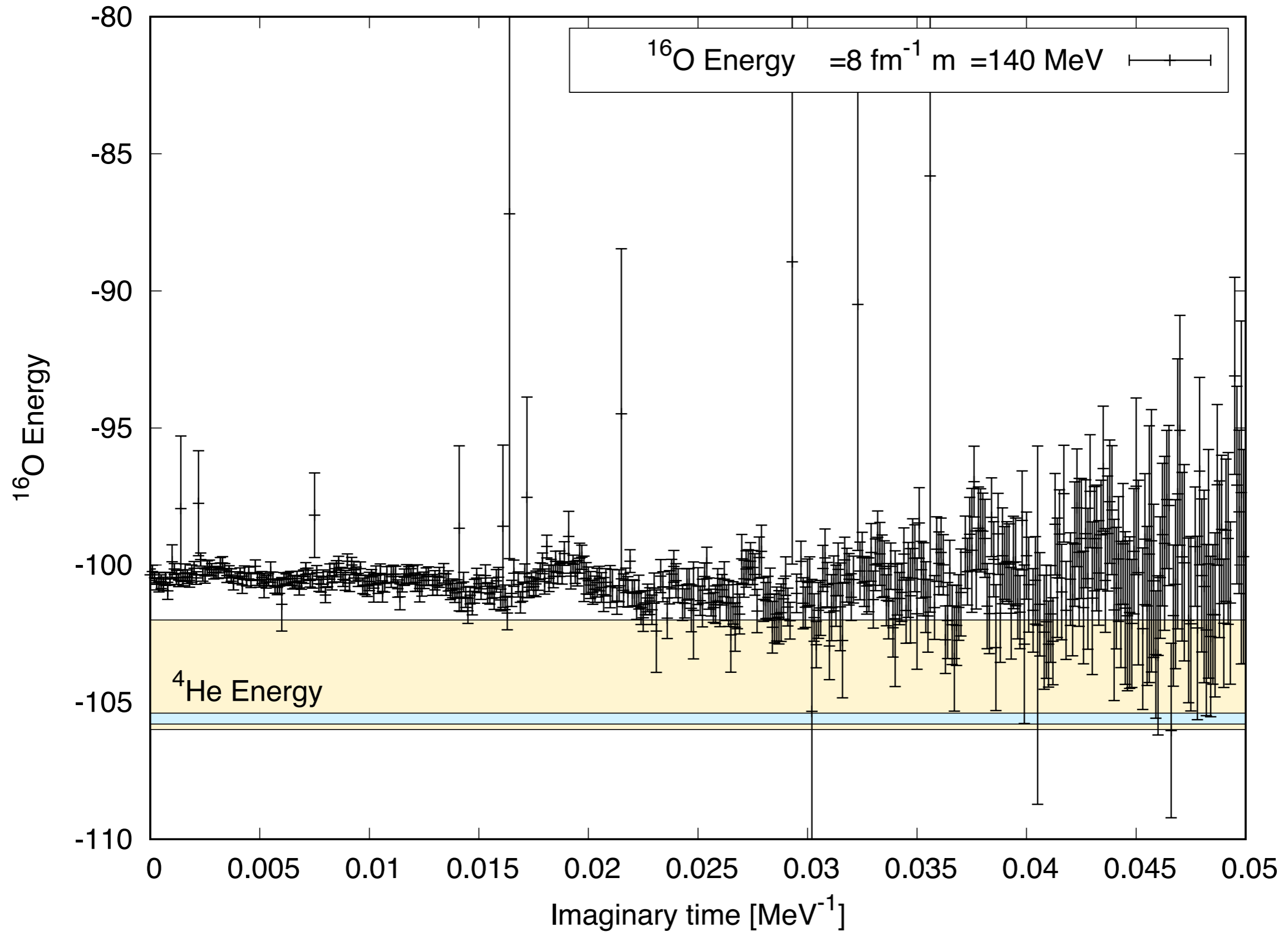
RESULTS FOR ^{16}O



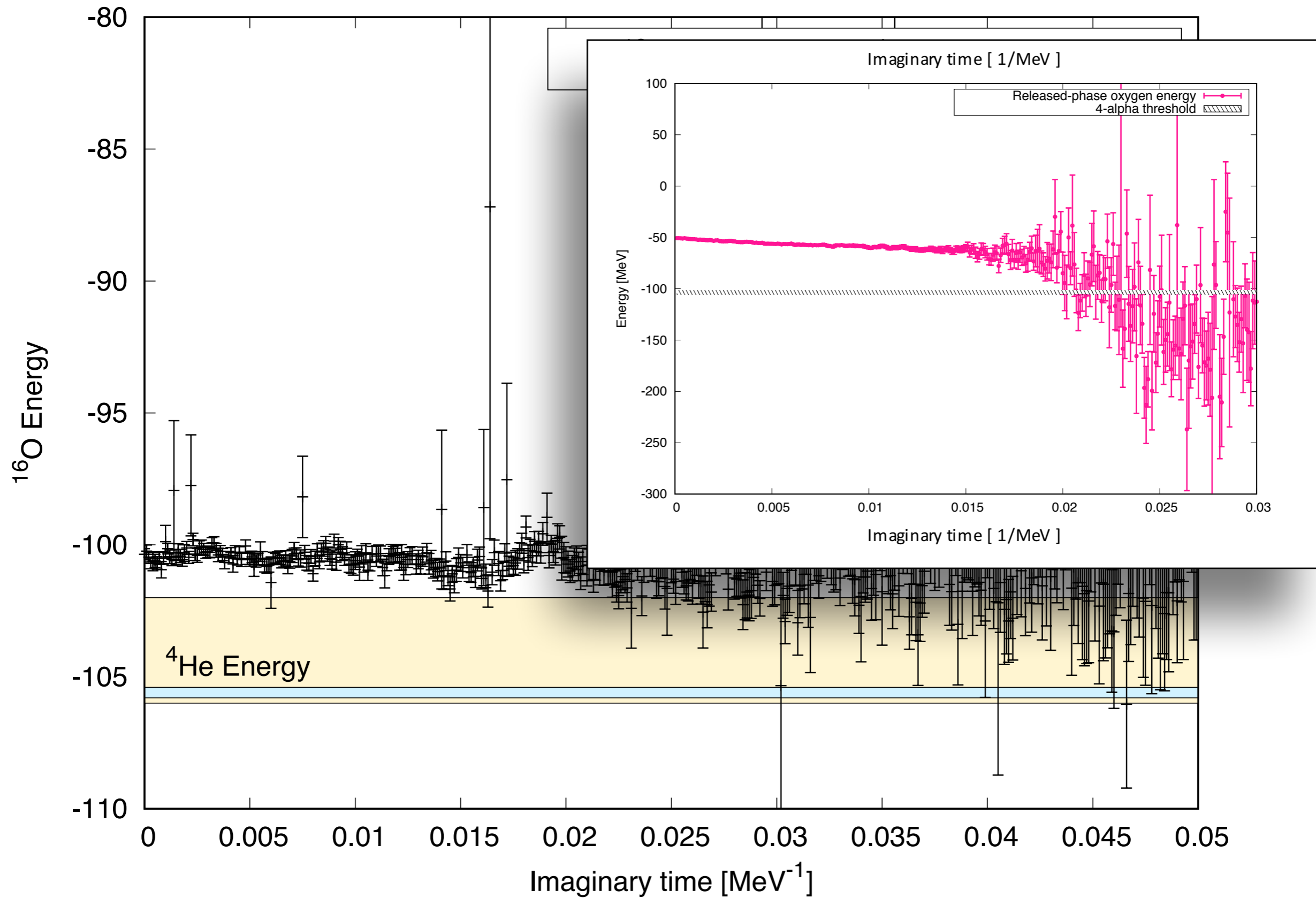
RESULTS FOR ^{16}O



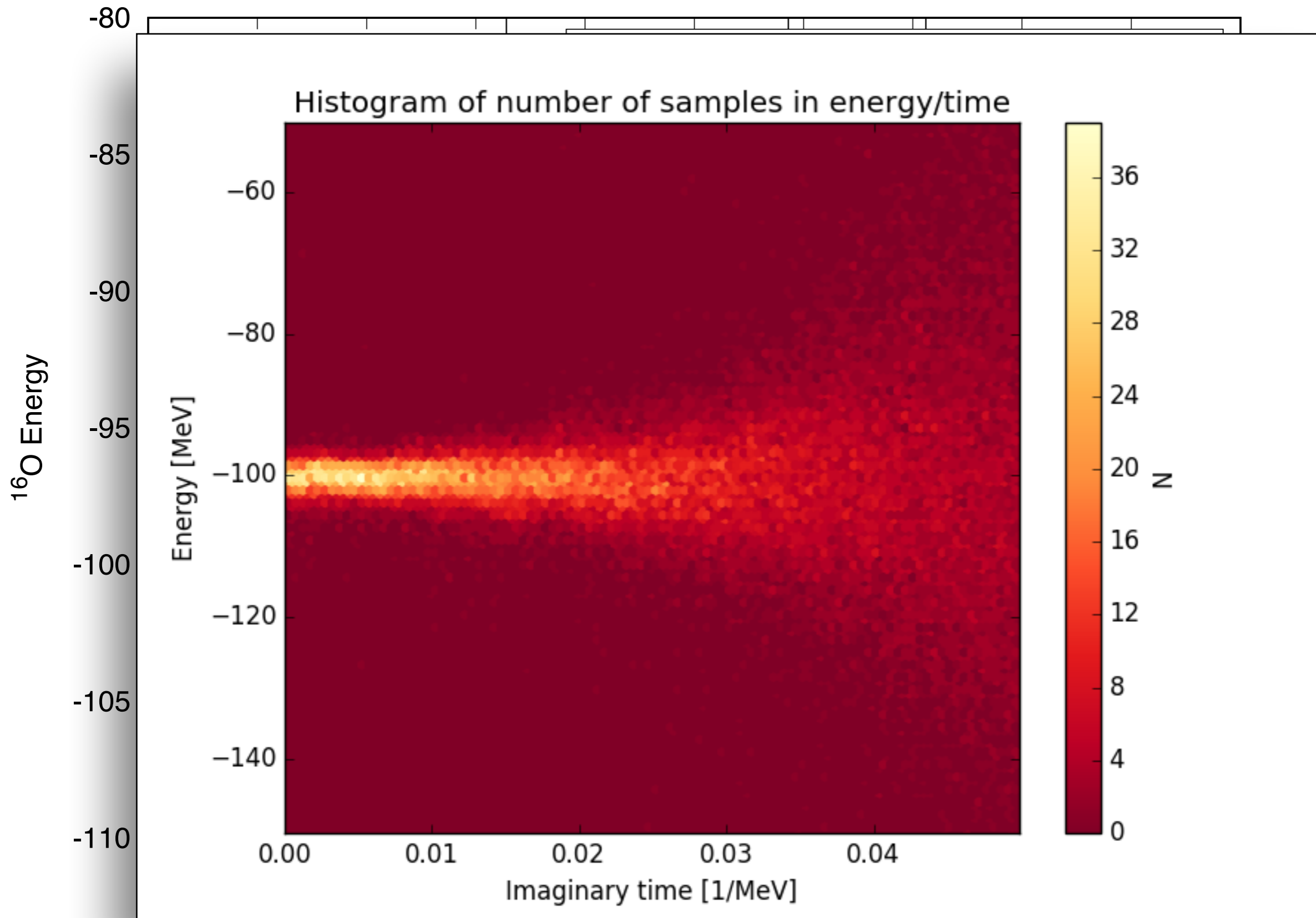
RESULTS FOR ^{16}O



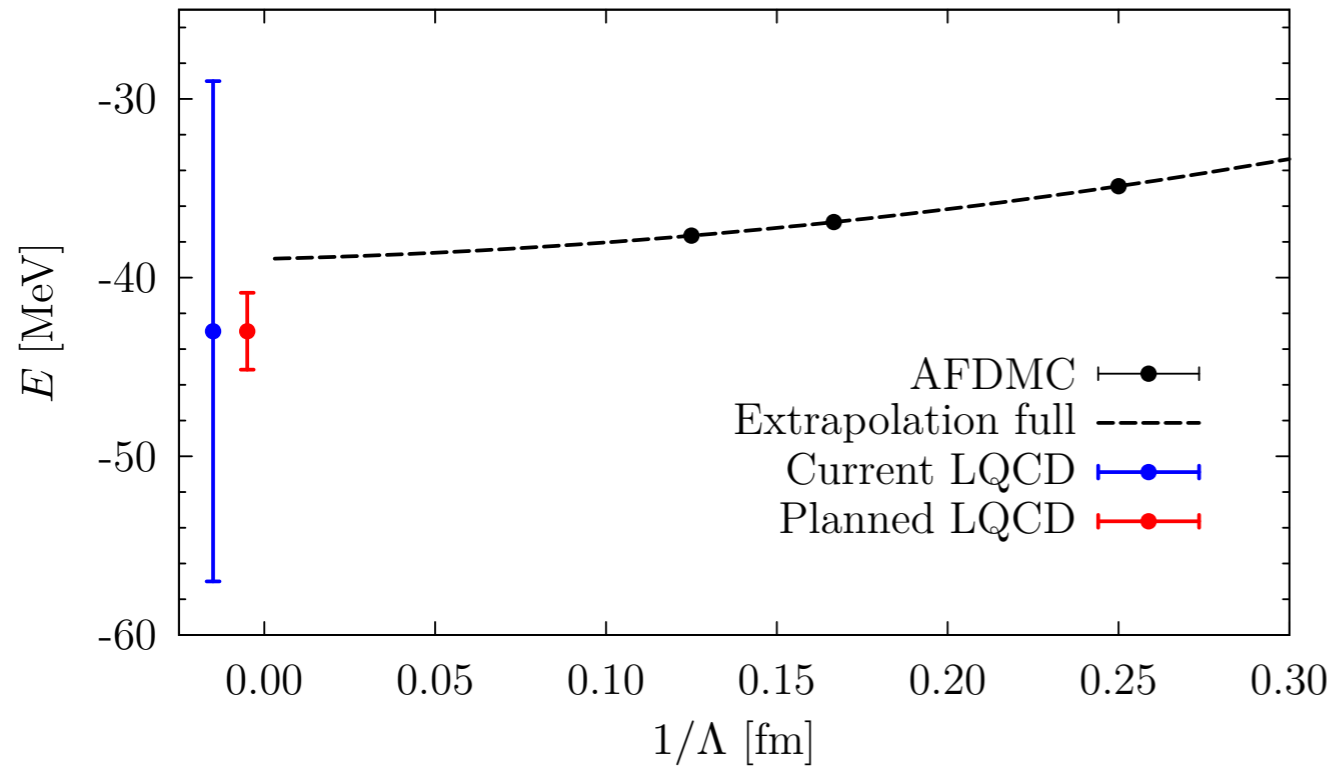
RESULTS FOR ^{16}O



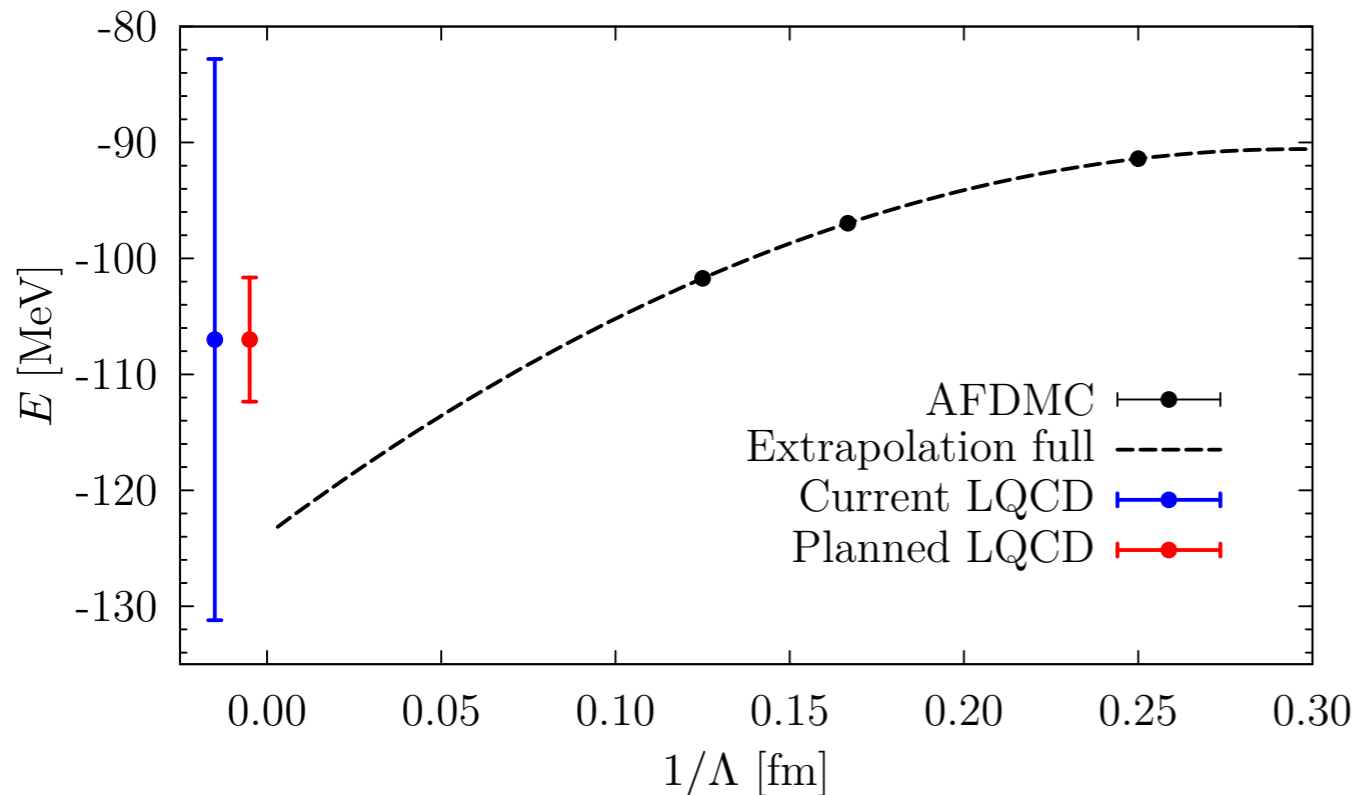
RESULTS FOR ^{16}O



CONSISTENCY OF PREDICTIONS



At present the LQCD data on 2,3 and 4 baryon systems are affected by very large statistical errors.

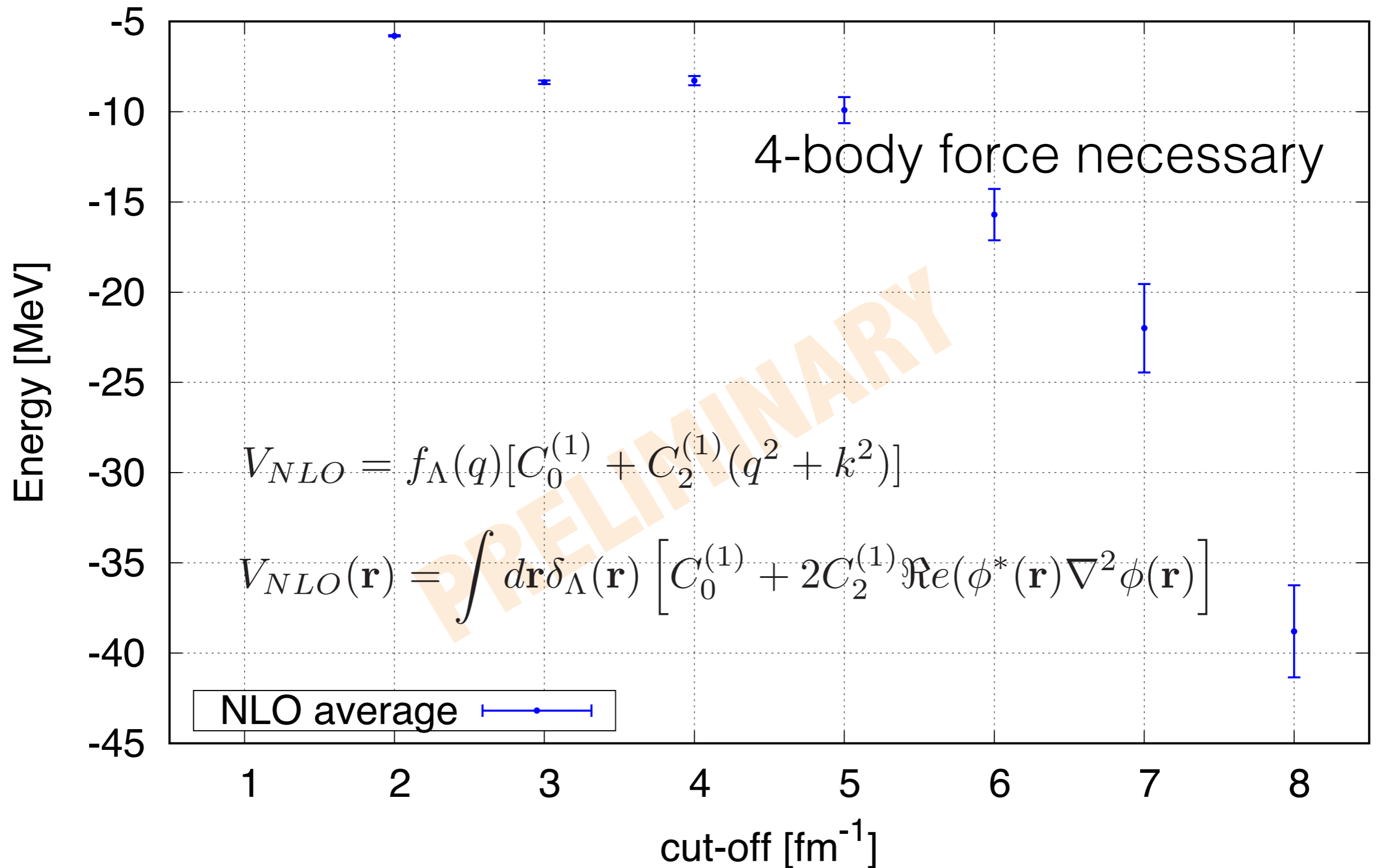


The consistency of theory cannot be fully tested yet.

NEED BETTER LQCD STATISTICS!

BEYOND LO...

^4He NLO energy, $m_\pi = 140$ MeV



CONCLUSIONS

- Pionless EFT is the correct theory to describe LQCD data for $m_\pi > 500\text{MeV}$, and it should work also at the physical value (at least for light nuclei, definitely for $A \leq 4$)
- Three-body forces are necessary already at LO to avoid Thomas collapse. No evidence of the need of a 4-body force (some serious hint that we will need it at NLO...)
- At LO ^{16}O is not bound with respect to breakup in 4α .
- **However:** we can expect LO to have an error of $\sim 30\%$. NLO could definitely give back the missing binding.