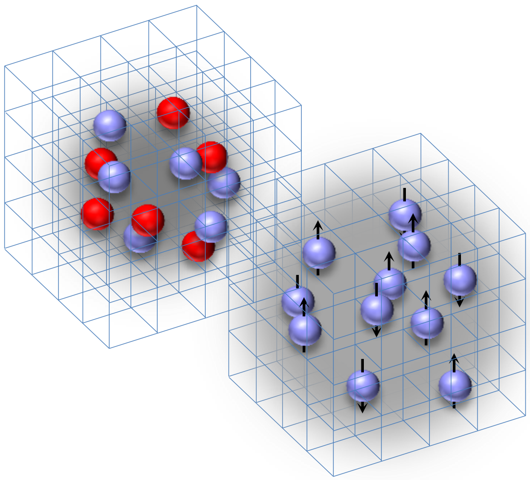
# Nuclear structure and excitations from lattice effective field theory




**Nuclear Lattice EFT Collaboration**

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***Computational and Theoretical Advances for Exotic Isotopes in the Medium Mass Region***
Institute for Nuclear Theory,
University of Washington, Seattle
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# Outline

Introduction and motivation

What is lattice effective field theory?

Lattice interactions and scattering

Euclidean time projection and auxiliary fields

Spectral convexity, pairing, clustering

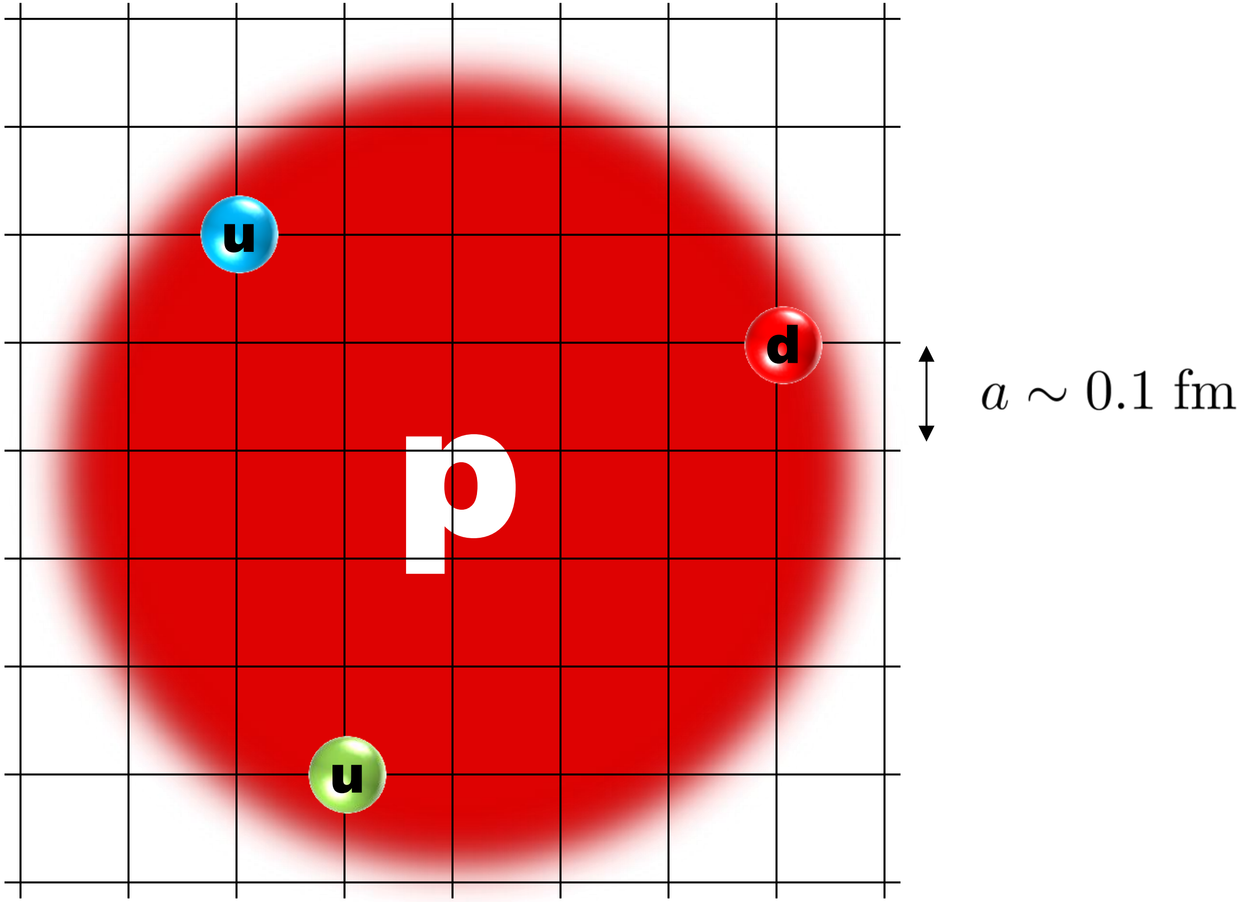
Carbon-12 and the Hoyle state

Light quark mass dependence of helium burning

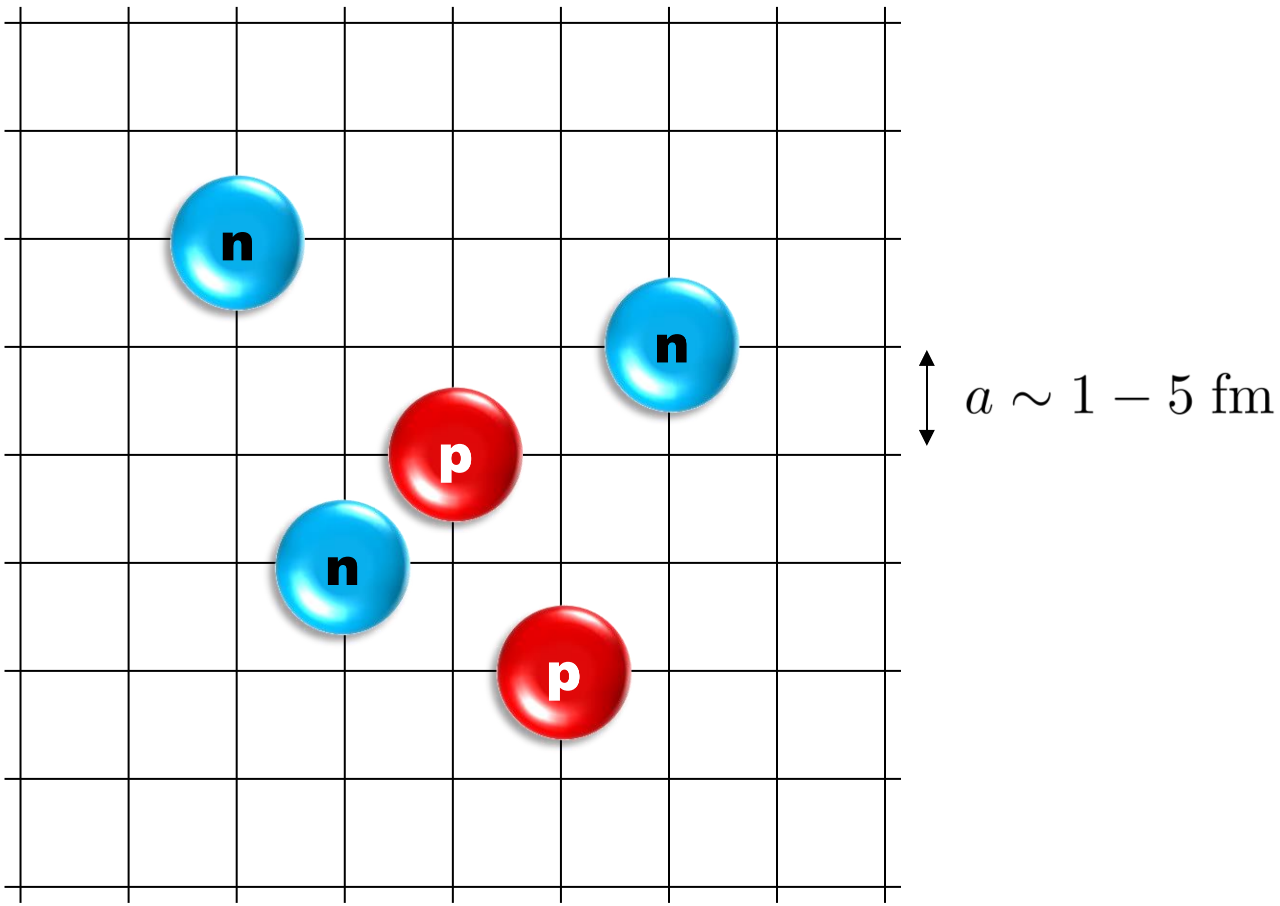
Work in progress:  Oxygen-16

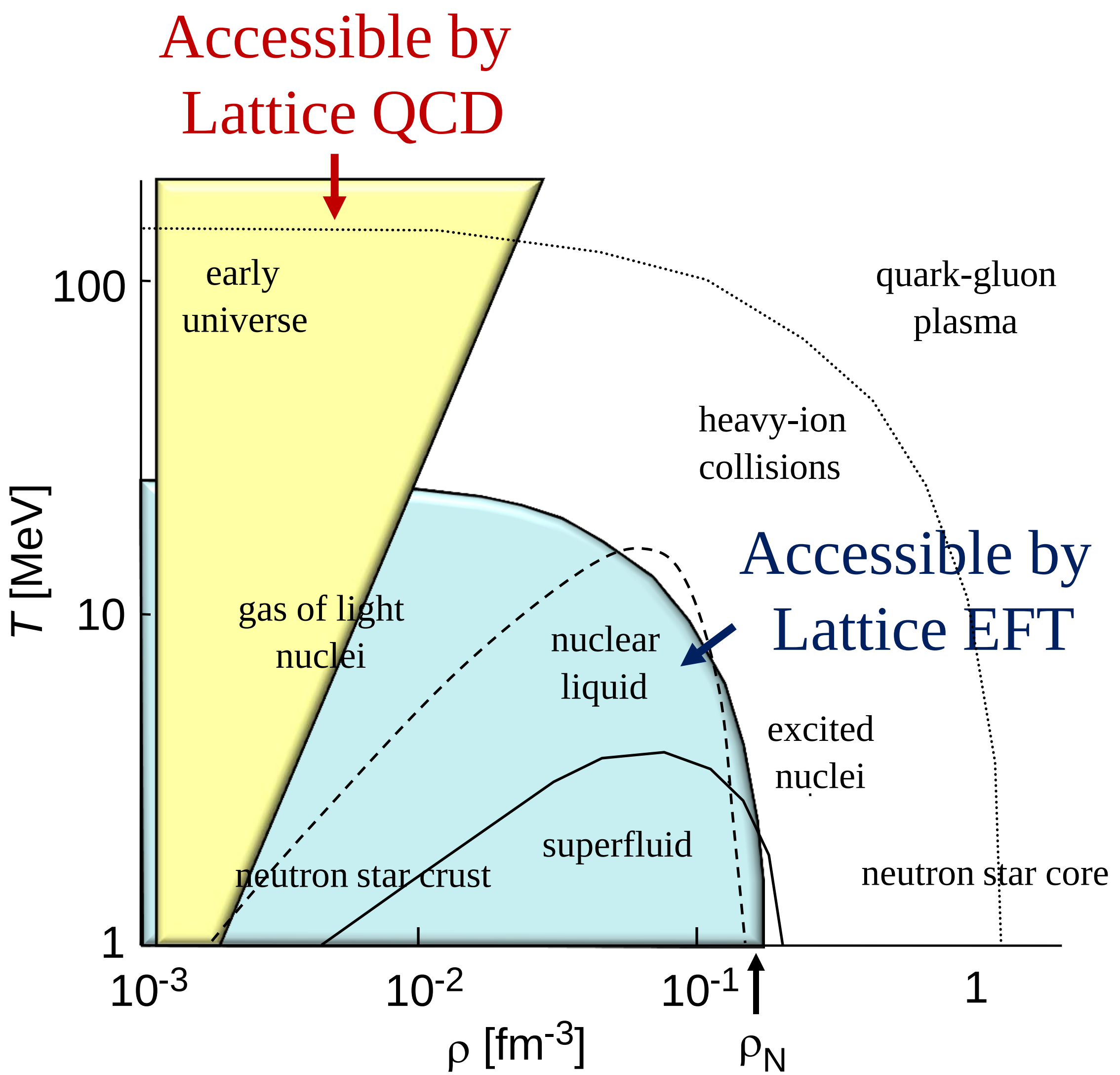
Summary and future directions

# Lattice quantum chromodynamics



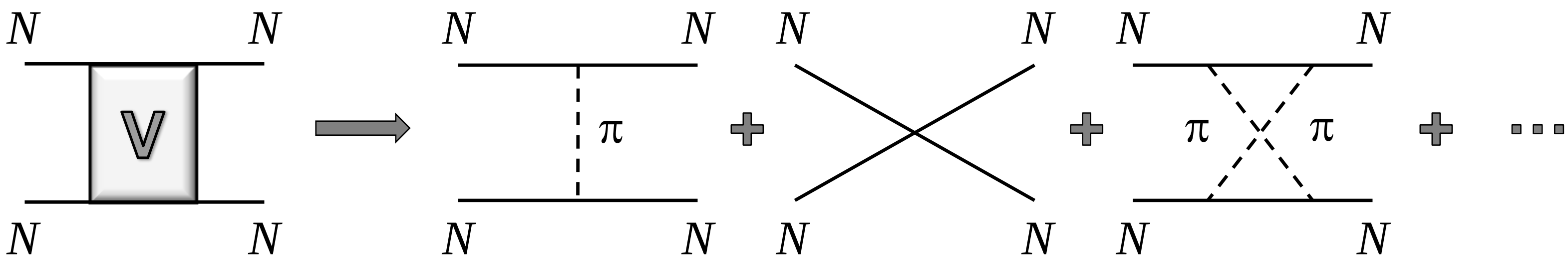
# Lattice effective field theory




Accessible by
Lattice QCD
100
10
1
T [MeV]
early
universe
quark-gluon
plasma
heavy-ion
collisions
Accessible by
Lattice EFT
gas of light
nuclei
nuclear
liquid
excited
nuclei
superfluid
neutron star crust
neutron star core
$10^{-3}$
$10^{-2}$
$10^{-1}$
1
ρ [fm$^{-3}$]
$\rho_N$

# Low energy nucleons: Chiral effective field theory

Construct the effective potential order by order




$V^{\mathrm{OPEP}}$ Contact interactions $V^{\mathrm{TPEP}}$

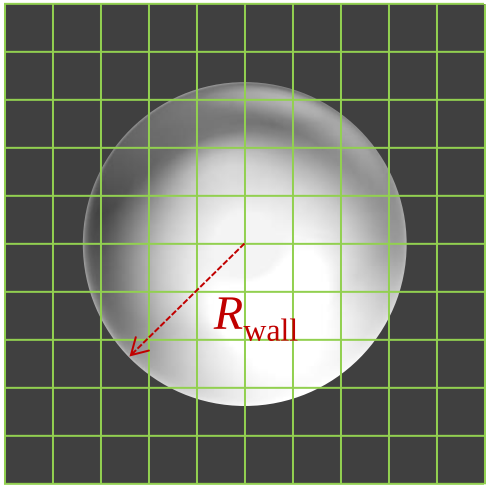
Leading order (LO) Next-to-leading order (NLO)

Physical scattering data → Unknown operator coefficients

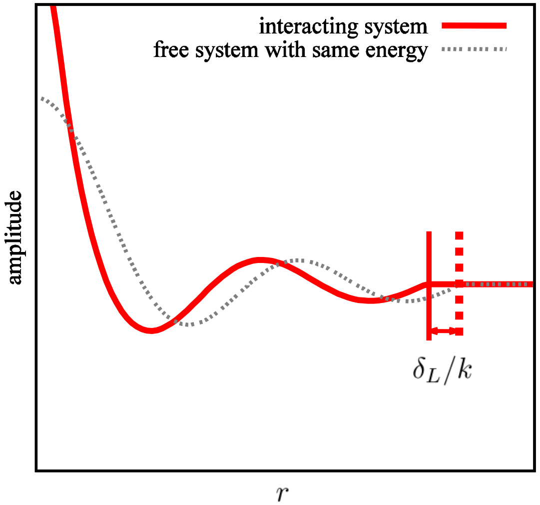
## Spherical wall method

*Borasoy, Epelbaum, Krebs, D.L., Meißner, EPJA 34 (2007) 185*

Spherical wall imposed in the center of mass frame

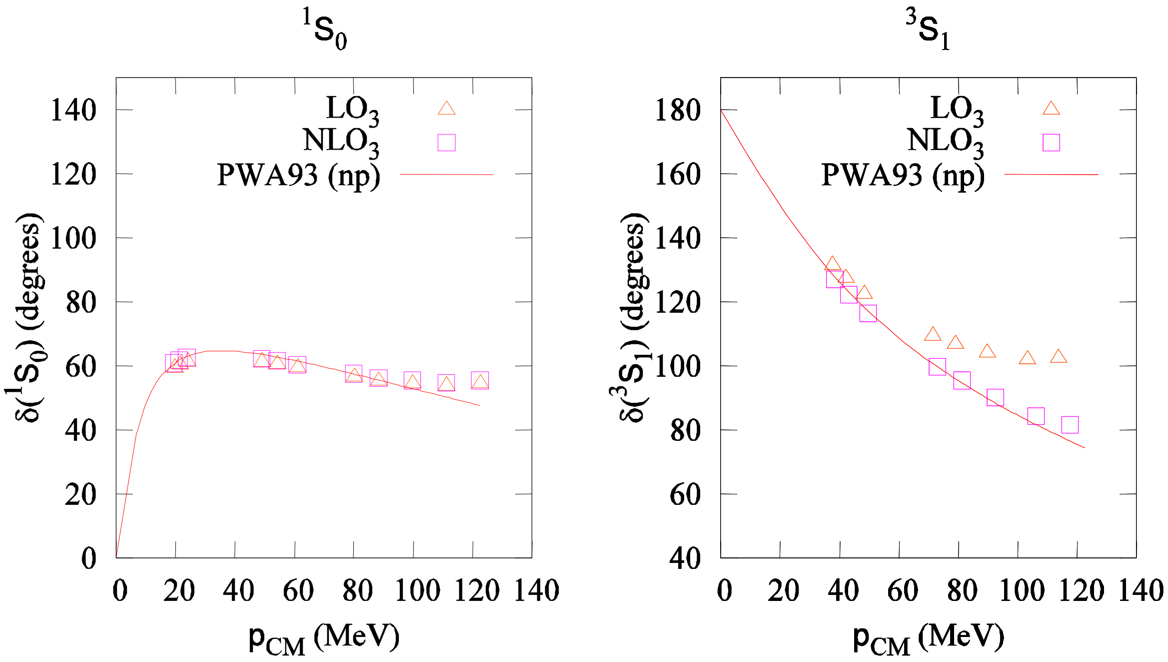



| Representation | $J_z$ | Example |
|---|---|---|
| $A_1$ | $0 \bmod 4$ | $Y_{0,0}$ |
| $T_1$ | $0, 1, 3 \bmod 4$ | $\{Y_{1,0}, Y_{1,1}, Y_{1,-1}\}$ |
| $E$ | $0, 2 \bmod 4$ | $\left\{Y_{2,0}, \frac{Y_{2,-2}+Y_{2,2}}{\sqrt{2}}\right\}$ |
| $T_2$ | $1, 2, 3 \bmod 4$ | $\left\{Y_{2,1}, \frac{Y_{2,-2}-Y_{2,2}}{\sqrt{2}}, Y_{2,-1}\right\}$ |
| $A_2$ | $2 \bmod 4$ | $\frac{Y_{3,2}-Y_{3,-2}}{\sqrt{2}}$ |



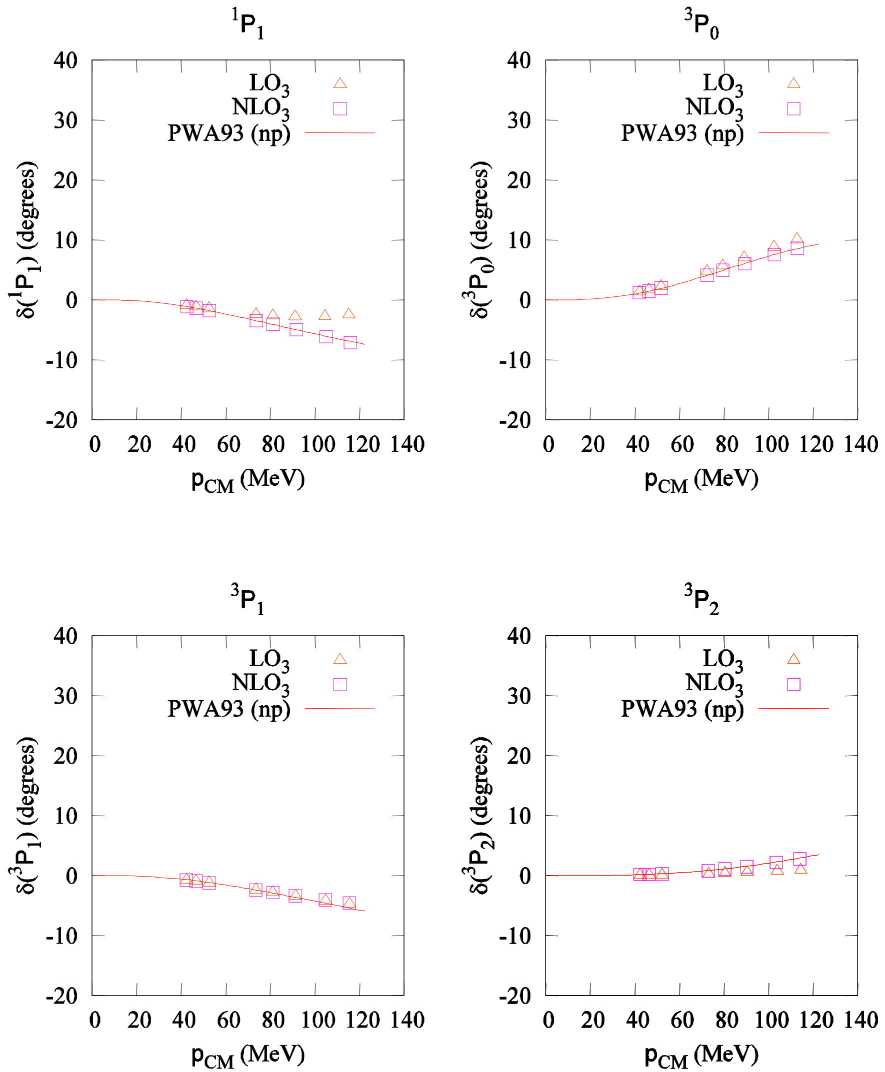
## LO$_3$: S waves

$a = 1.97$ fm



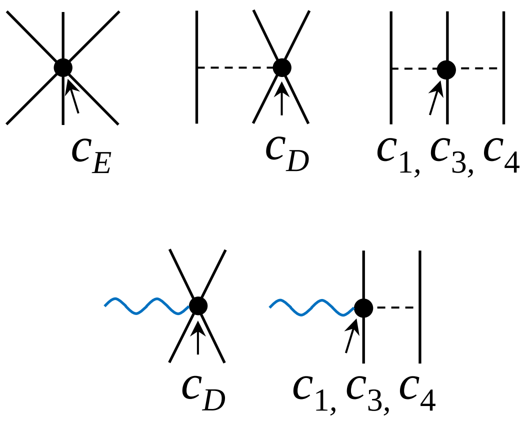
## $\underline{LO_3\text{: P waves}}$

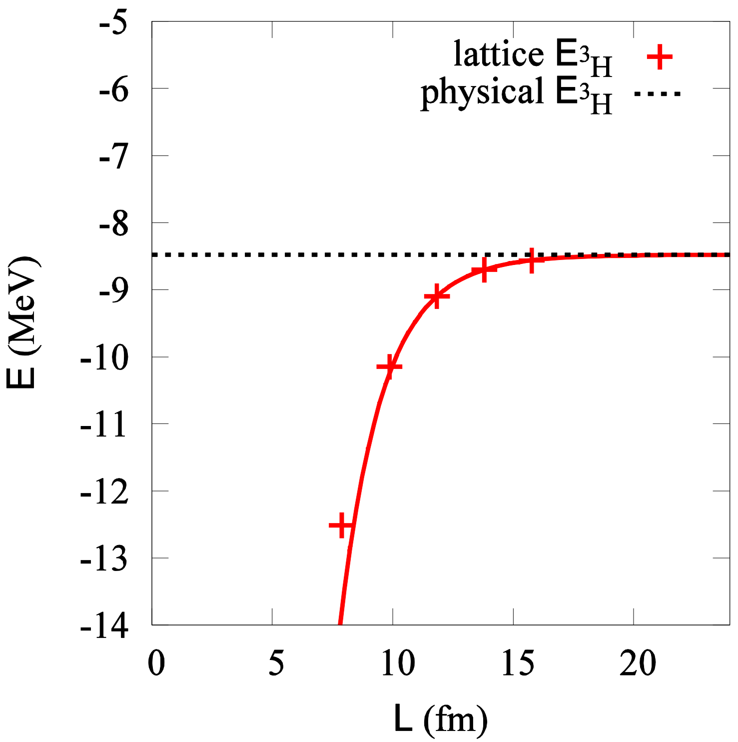
$a = 1.97$ fm



# Three nucleon forces

Two unknown coefficients at NNLO from three-nucleon forces.
Determine $c_D$ and $c_E$ using $^3$H binding energy and the weak axial current at low cutoff momentum.



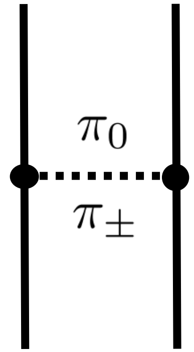




*Park, et al., PRC 67 (2003) 055206,*
*Gårdestig, Phillips, PRL 96 (2006) 232301,*
*Gazit, Quaglioni, Navratil, PRL 103 (2009) 102502*

# <u>Neutrons and protons:  Isospin breaking and Coulomb</u>

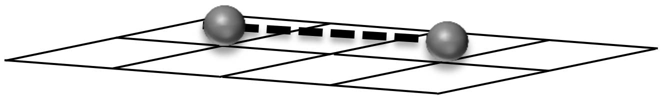
Isospin-breaking and power counting *[Friar , van Kolck, PRC 60 (1999) 034006; Walzl, Meißner, Epelbaum NPA 693 (2001) 663; Friar, van Kolck, Payne, Coon, PRC 68 (2003) 024003; Epelbaum, Meißner, PRC72 (2005) 044001…]*

<u>Pion mass difference</u>

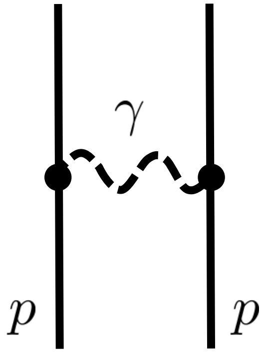


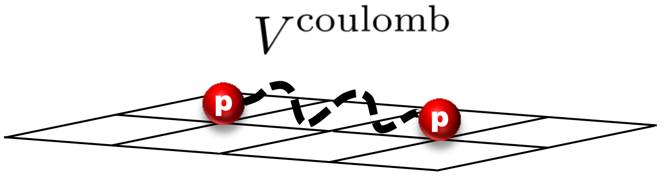

$m_{\pi_0} \neq m_{\pi_\pm}$

$V_{\pi_0}^{\rm OPEP}, V_{\pi_\pm}^{\rm OPEP}$

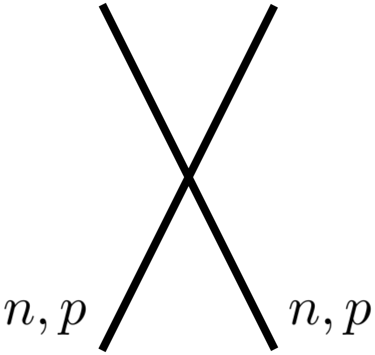


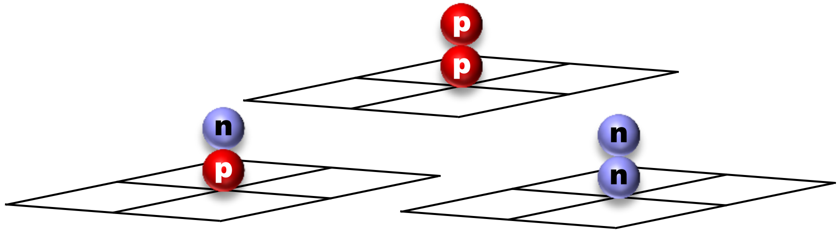
## Coulomb potential



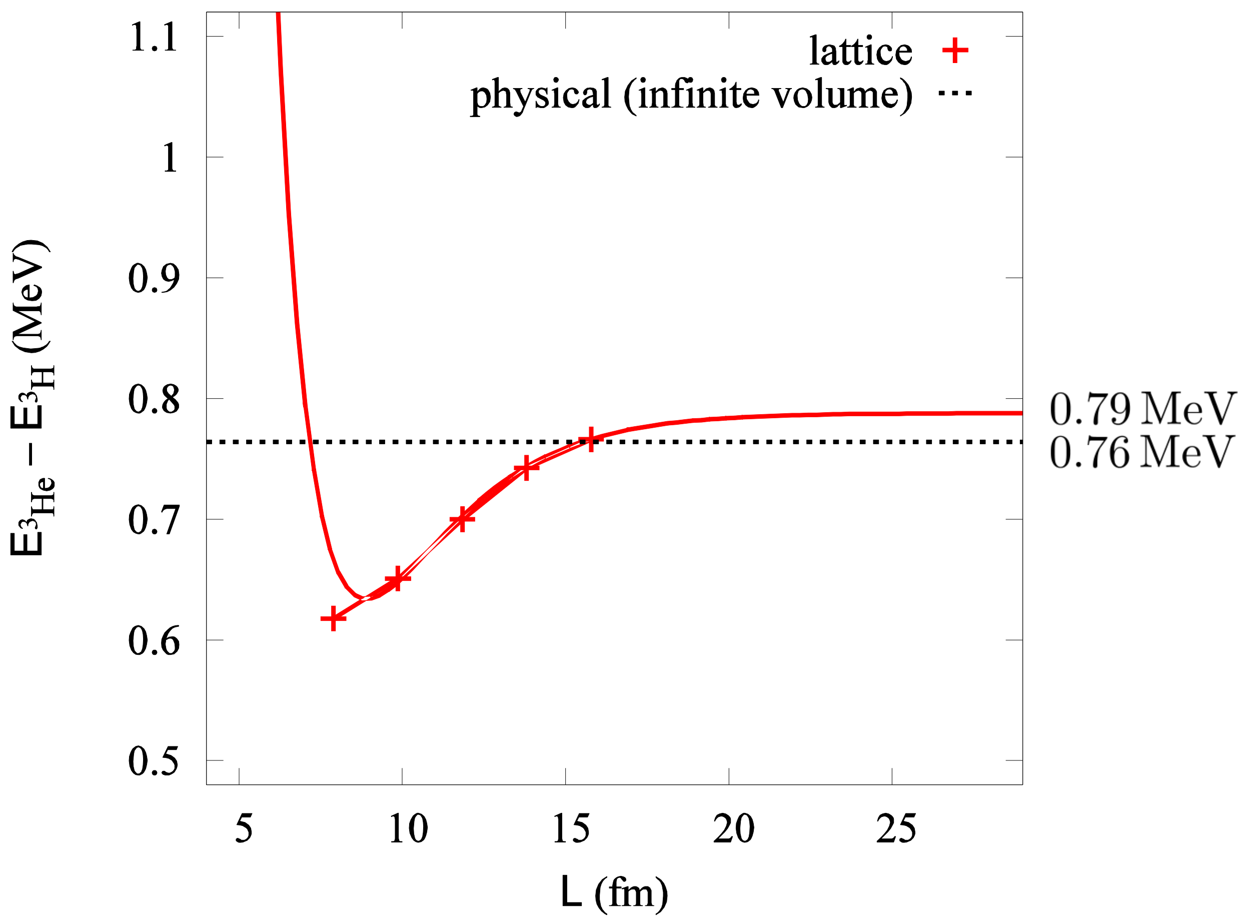

## Charge symmetry breaking
## Charge independence breaking



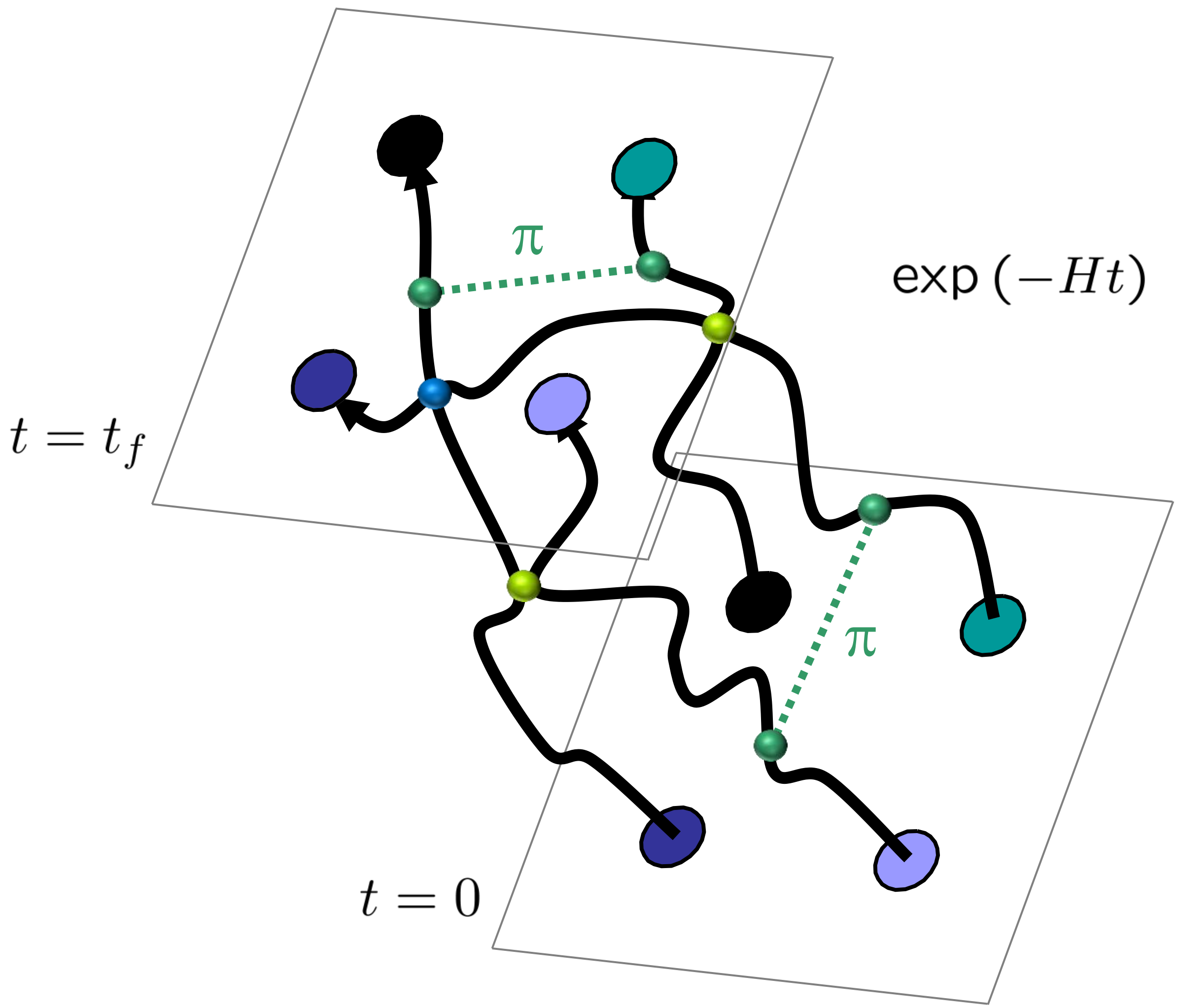



# Triton and Helium-3

$$E_{^3\mathrm{He}} - E_{\mathrm{triton}} = 0.79(5)\ \mathrm{MeV}$$



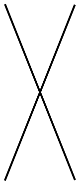
# Euclidean time projection



# Auxiliary field method

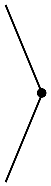
We can write exponentials of the interaction using a Gaussian integral identity

$$\exp\left[-\frac{C}{2}(N^\dagger N)^2\right]$$



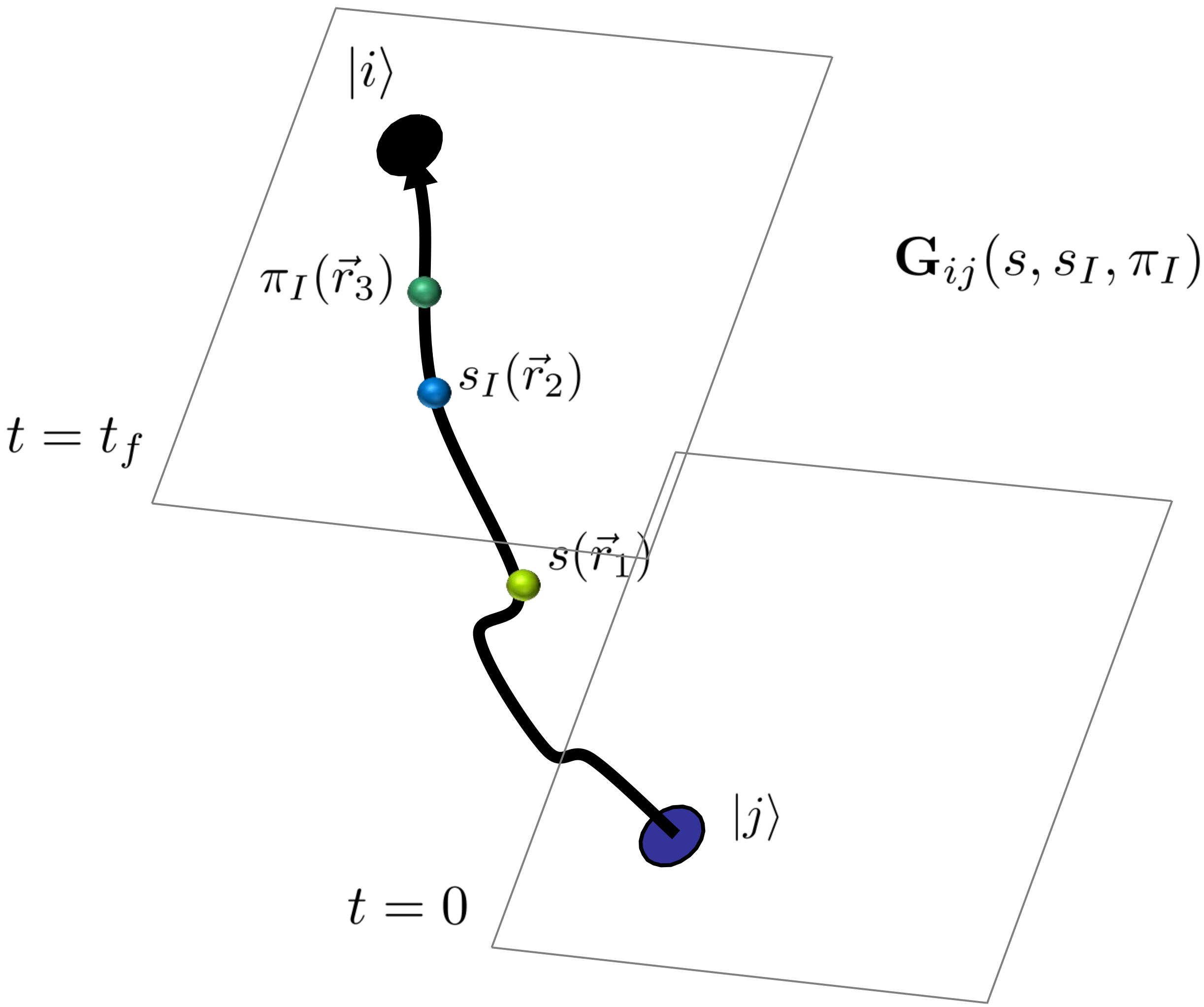
$$(N^\dagger N)^2$$

$$= \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-C}\, s(N^\dagger N)\right]$$

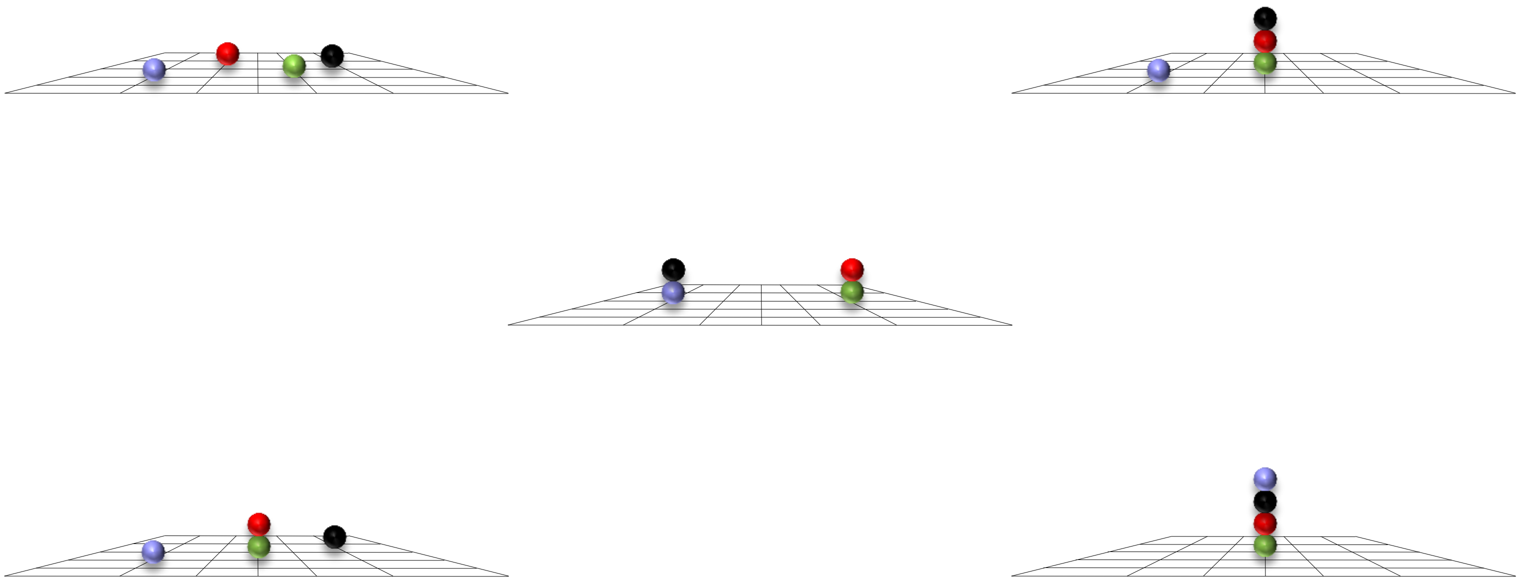


$$sN^\dagger N$$

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.

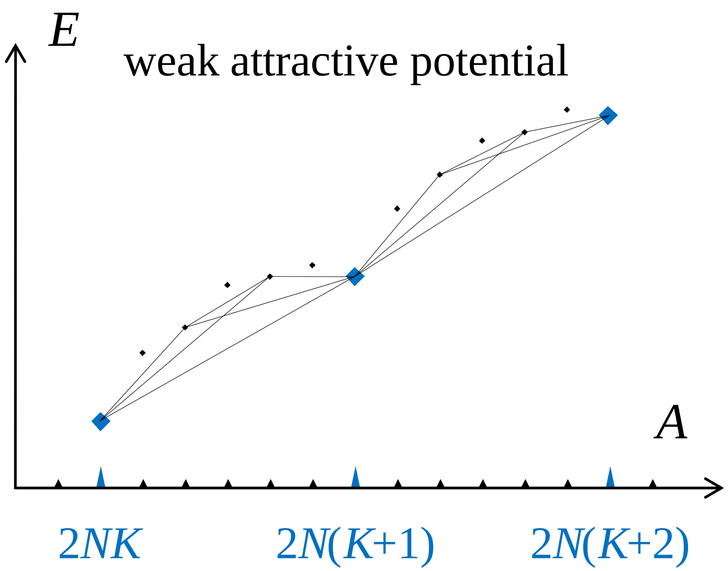

$|i\rangle$
$\mathbf{G}_{ij}(s, s_I, \pi_I)$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$t = t_f$
$s(\vec{r}_1)$
$|j\rangle$
$t = 0$

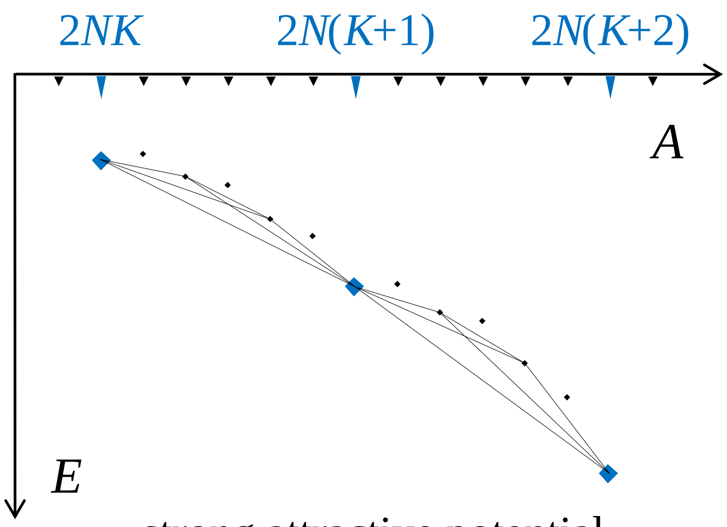
# Particle clustering included automatically



# Spectral convexity, pairing, and clustering

***Theorem:***
Any fermionic theory with SU(2$N$) symmetry and two-body potential with negative semi-definite Fourier transform obeys SU(2$N$) convexity bounds.




***Corollary:***
System can be simulated without sign oscillations

*Chen, D.L. Schäfer, PRL 93 (2004) 242302; D.L., PRL 98 (2007) 182501*

There are $2N$ species of fermions. We calculate the path integral using projection Monte Carlo with one auxiliary field coupled to the total particle density.

The path integral is

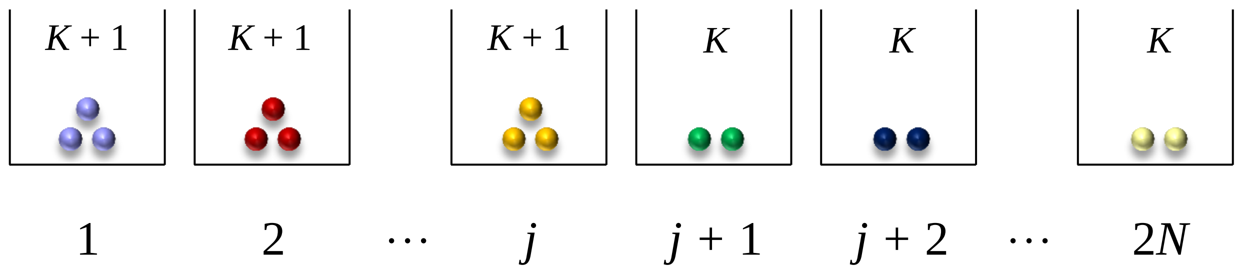
$$\int D\phi \, e^{-S(\phi)} \, \mathrm{det} \, \mathbf{G}(\phi)$$

where the auxiliary field has a quadratic action of the form

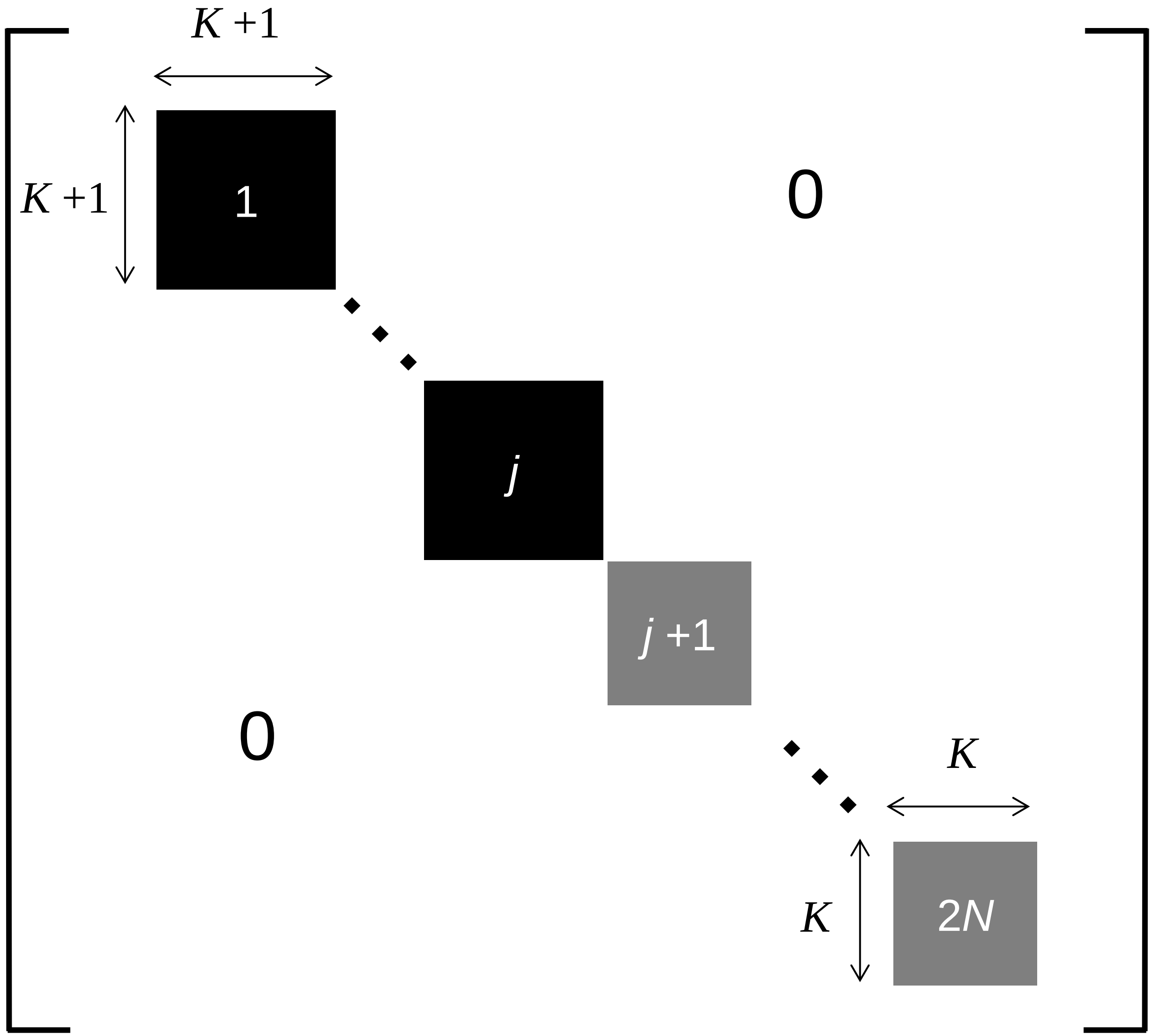
$$S(\phi) = -\frac{\alpha_t}{2} \sum_{n_t} \sum_{\vec{n},\vec{n}'} \phi(\vec{n}, n_t) V^{-1}(\vec{n} - \vec{n}') \phi(\vec{n}', n_t)$$

inverse of potential

We choose the sector with $K + 1$ particles for species 1 to $j$, and $K$ particles for species $j + 1$ to $2N$.




The auxiliary field is coupled to the total particle density. The total particle density is an operator which diagonal in particle species. Therefore the matrix has the following block diagonal structure…



$K+1$
$K+1$
1
0
$j$
$j+1$
0
$K$
$K$
$2N$

The path integral is then

$$Z_{j,K+1;2N-j,K} = \int D\phi \; e^{-S(\phi)} \; \left[\det \mathbf{M}_{(K+1)\times(K+1)}(\phi)\right]^{j} \left[\det \mathbf{M}_{K\times K}(\phi)\right]^{2N-j}$$

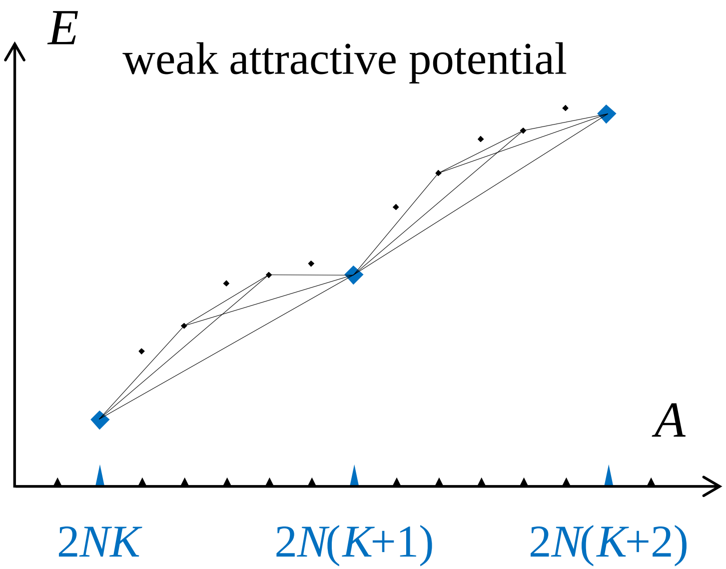
The Hölder inequality states that for any positive *p*, *q* satisfying

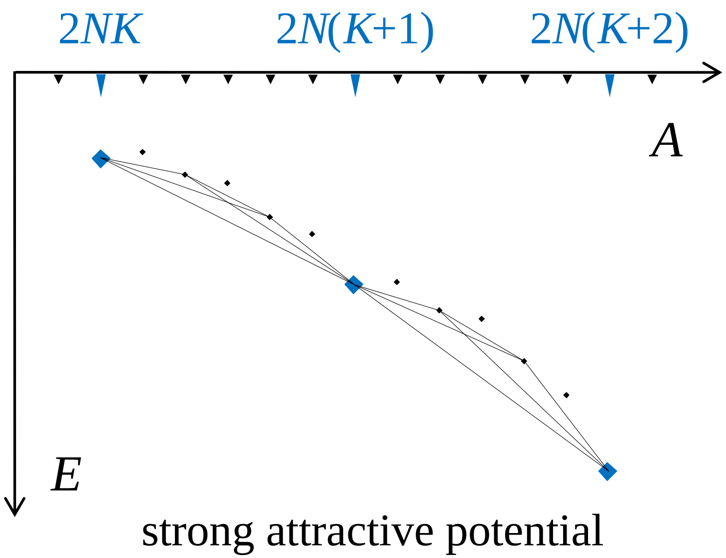
$$1/p + 1/q = 1$$

we have

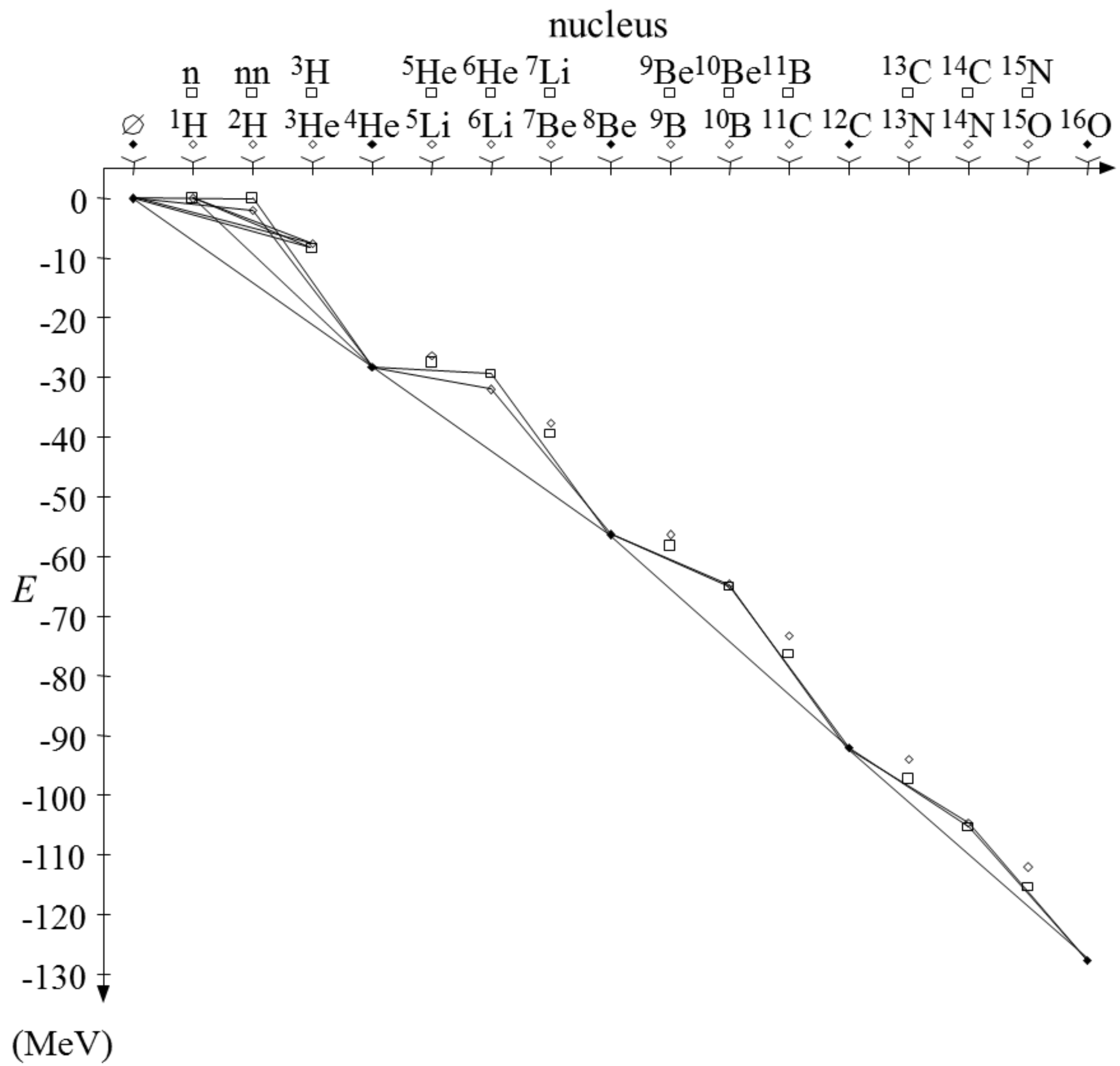
$$\int dx \; |f(x)g(x)| \leq \left[\int dx \; |f(x)|^{p}\right]^{1/p} \times \left[\int dx \; |g(x)|^{q}\right]^{1/q}$$

Application of the Hölder inequality leads to the spectral convexity theorem

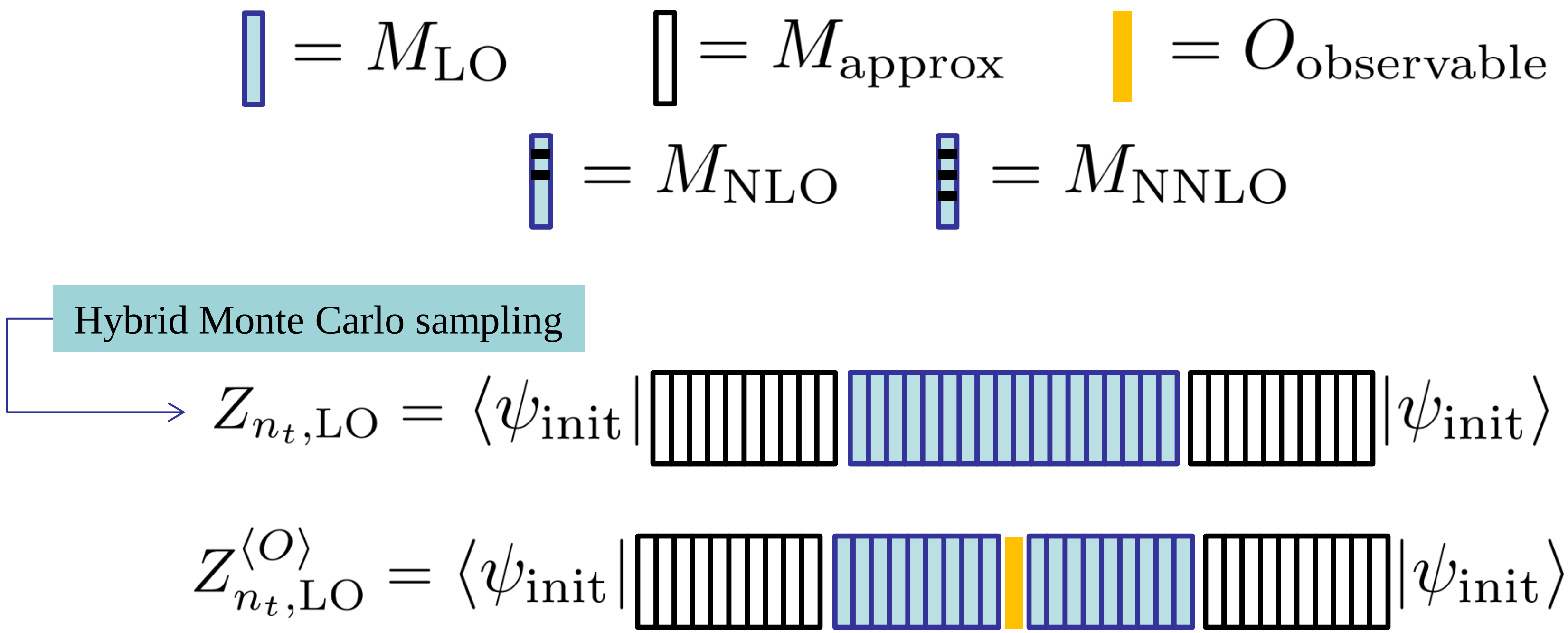

E
weak attractive potential
A
2NK
2N(K+1)
2N(K+2)


2NK
2N(K+1)
2N(K+2)
A
E
strong attractive potential

# SU(4) convexity bounds

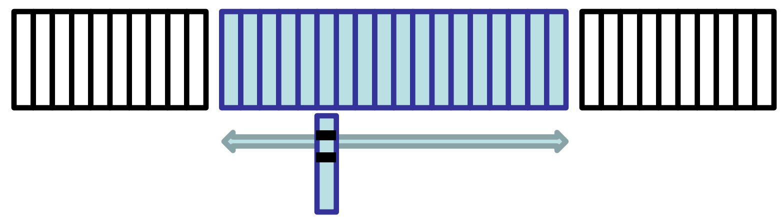


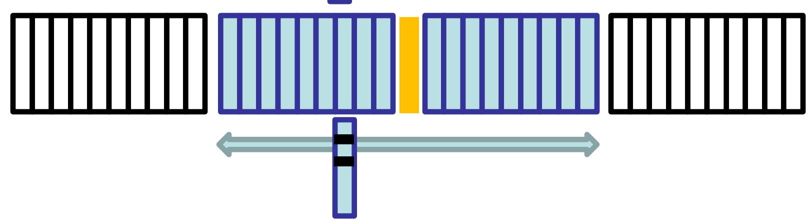
# Schematic of lattice Monte Carlo calculation




$$e^{-E_{0,\mathrm{LO}} a_t} = \lim_{n_t \to \infty} Z_{n_t+1,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

$$\langle O \rangle_{0,\mathrm{LO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

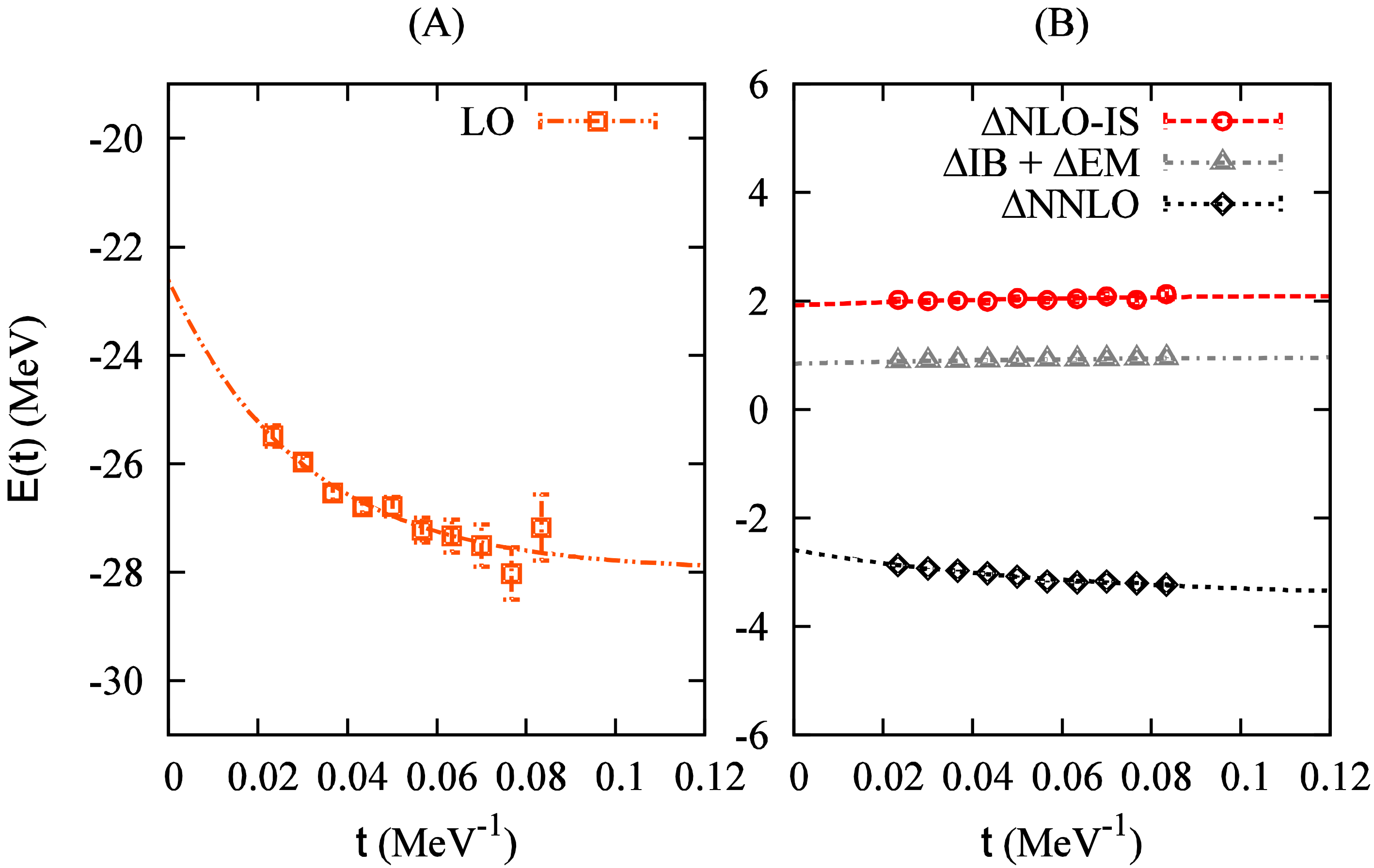
$Z_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$  $| \psi_{\mathrm{init}} \rangle$

$Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$  $| \psi_{\mathrm{init}} \rangle$

$$\langle O \rangle_{0,\mathrm{NLO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} / Z_{n_t,\mathrm{NLO}}$$

# Ground state of Helium-4

$L = 11.8\,\mathrm{fm}$




*Epelbaum, Krebs, D.L, Meißner, PRL 106 (2011) 192501*
*Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 109 (2012) 252501*

## Ground state of Helium-4

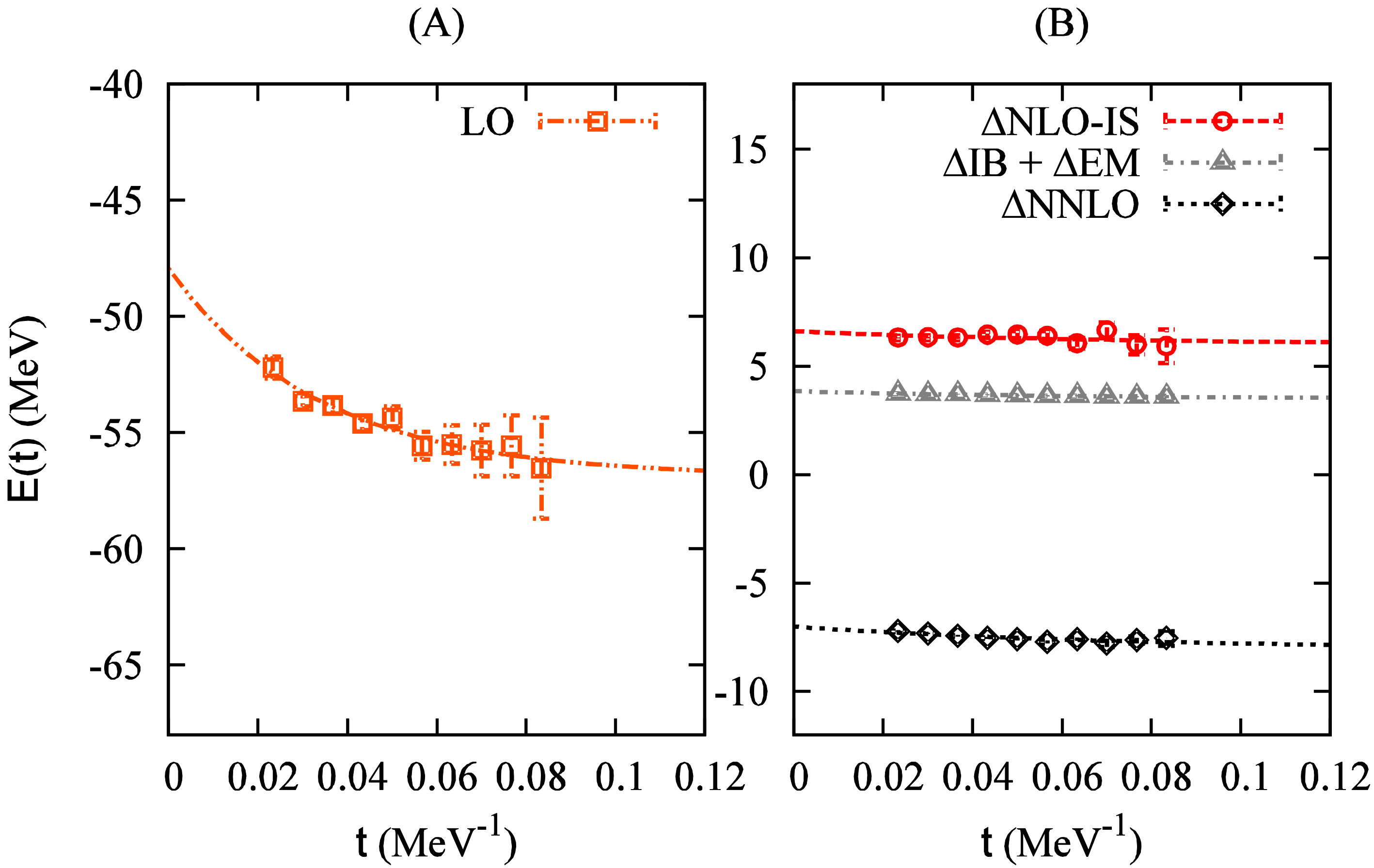
$$L = 11.8\,\mathrm{fm}$$

| | |
|---|---|
| LO* ($O(Q^0)$) | –28.0(3) MeV |
| NLO ($O(Q^2)$) | –24.9(5) MeV |
| NNLO ($O(Q^3)$) | –28.3(6) MeV |
| Experiment | –28.3 MeV |

*contains some interactions promoted from NLO

# Ground state of Beryllium-8

$L = 11.8\,\mathrm{fm}$




*Epelbaum, Krebs, D.L, Meißner, PRL 106 (2011) 192501*
*Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 109 (2012) 252501*

## Ground state of Beryllium-8

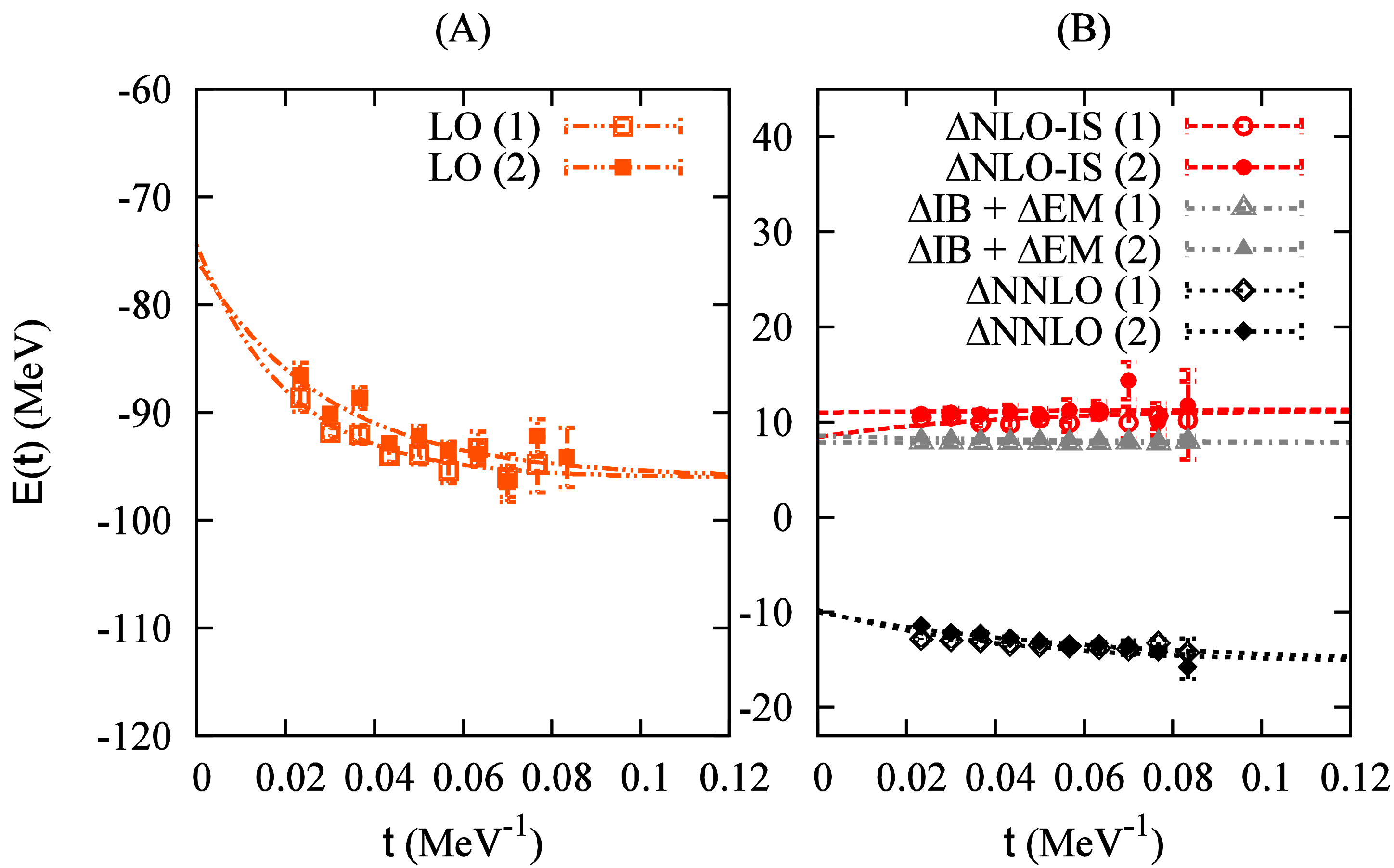
$$L = 11.8\,\mathrm{fm}$$

| | |
|---|---|
| LO* ($O(Q^0)$) | –57(2) MeV |
| NLO ($O(Q^2)$) | –47(2) MeV |
| NNLO ($O(Q^3)$) | –55(2) MeV |
| Experiment | –56.5 MeV |

*contains some interactions promoted from NLO

# Ground state of Carbon-12

$$L = 11.8\,\mathrm{fm}$$




*Epelbaum, Krebs, D.L, Meißner, PRL 106 (2011) 192501*
*Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 109 (2012) 252501*

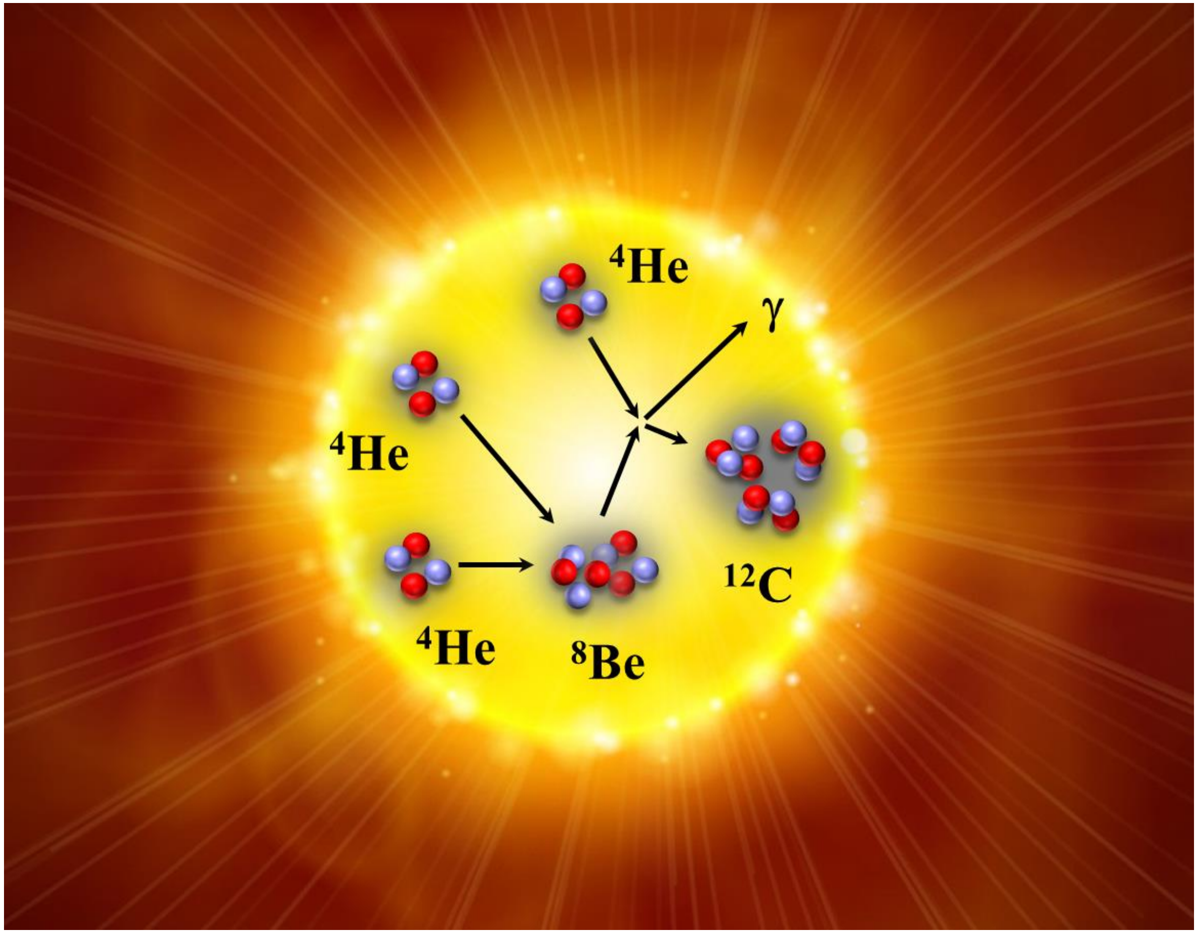
## Ground state of Carbon-12

$$L = 11.8\,\mathrm{fm}$$

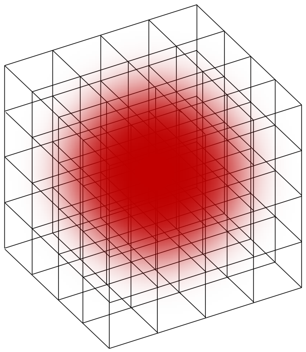
| | |
|---|---|
| LO* ($O(Q^0)$) | –96(2) MeV |
| NLO ($O(Q^2)$) | –77(3) MeV |
| NNLO ($O(Q^3)$) | –92(3) MeV |
| Experiment | –92.2 MeV |

*contains some interactions promoted from NLO

# Carbon-12 spectrum and the Hoyle state



## Simulations using general initial/final state wavefunctions



$$\bigwedge_{j=1,\cdots,A} |\psi_j(\vec{n})\rangle$$

Construct states with well-defined momentum using all possible translations.

$$L^{-3/2}\sum_{\vec{m}} e^{i\vec{P}\cdot\vec{m}} \bigwedge_{j=1,\cdots,A} |\psi_j(\vec{n}-\vec{m})\rangle$$

Shell model wavefunctions

$$\psi_j(\vec{n}) = \exp(-c\vec{n}^2)$$
$$\psi'_j(\vec{n}) = n_x \exp(-c\vec{n}^2)$$
$$\psi''_j(\vec{n}) = n_y \exp(-c\vec{n}^2)$$
$$\psi'''_j(\vec{n}) = n_z \exp(-c\vec{n}^2)$$
$$\vdots$$

Alpha cluster wavefunctions

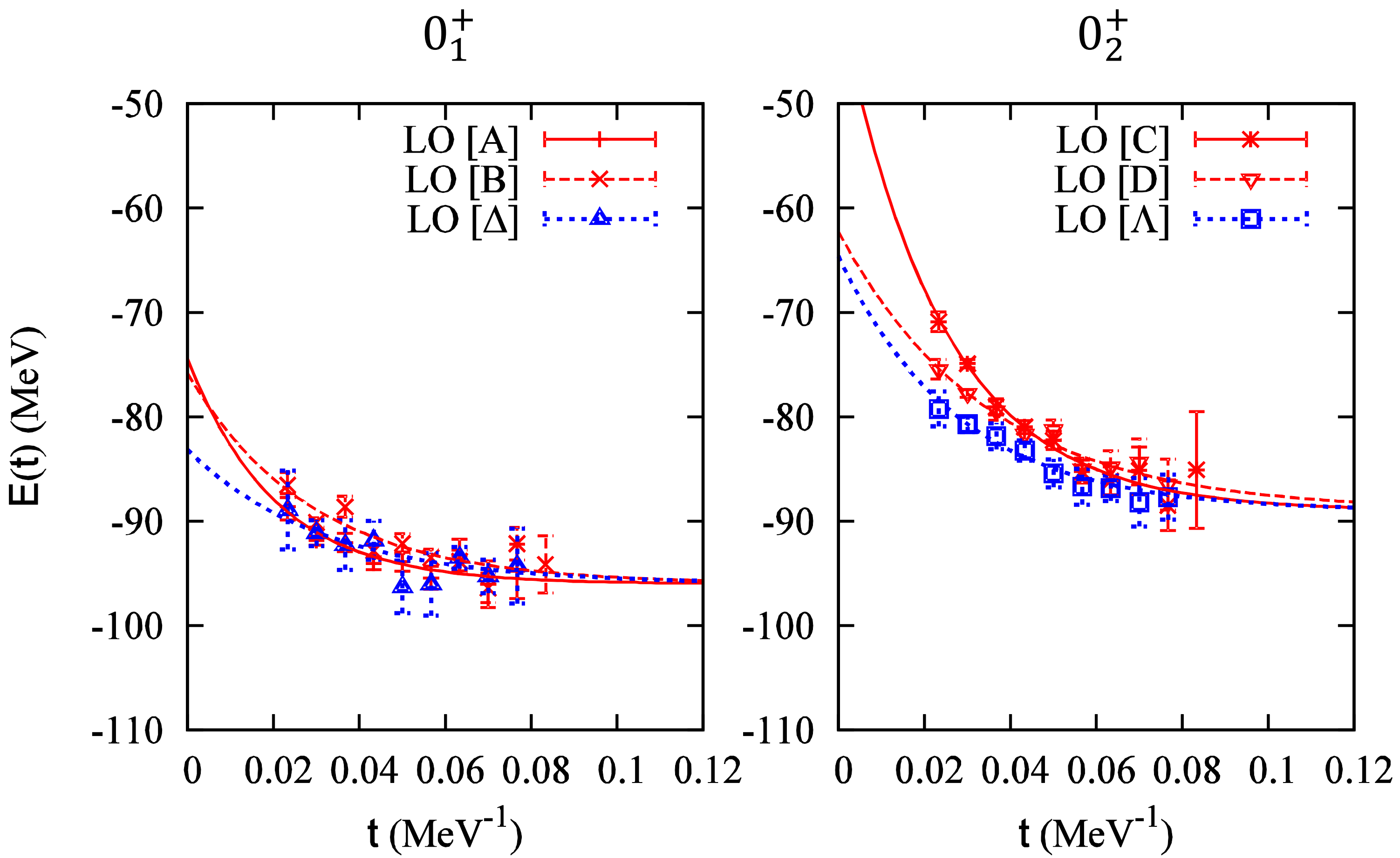
$$\psi_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m})^2]$$
$$\psi'_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m}')^2]$$
$$\psi''_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m}'')^2]$$
$$\vdots$$

Shell model wavefunctions by themselves do not have enough local four nucleon correlations,

$$< (N^\dagger N)^4 >$$

Needs to develop the four nucleon correlations via Euclidean time projection.

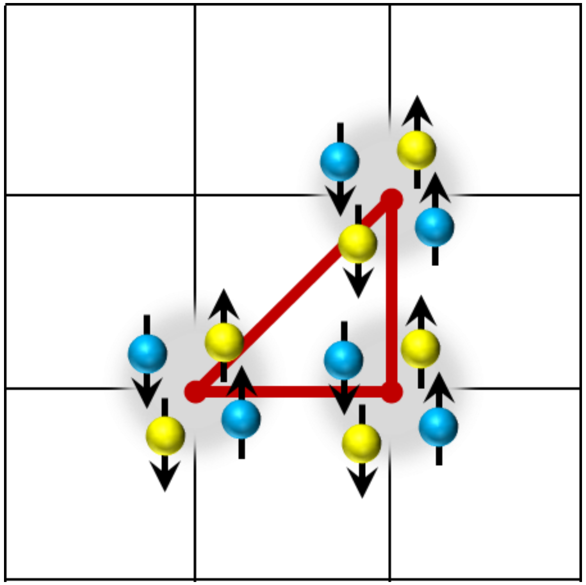
But can reproduce same results starting directly from alpha cluster wavefunctions [$\Delta$ and $\Lambda$ in plots on next slide].




*Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 109 252501 (2012)*

# Structure of ground state and first 2+

Strong overlap with compact triangle configuration

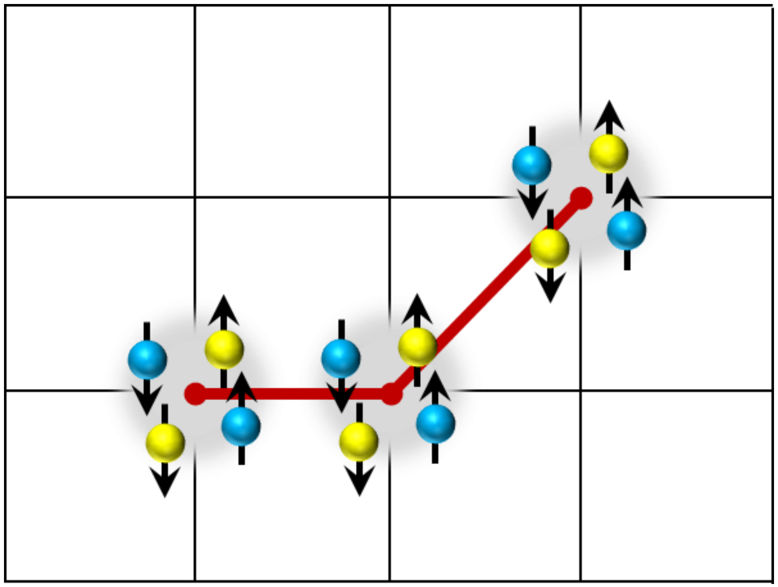


**12 rotational orientations**

$$a = 1.97 \text{ fm}$$

Structure of Hoyle state and second 2+

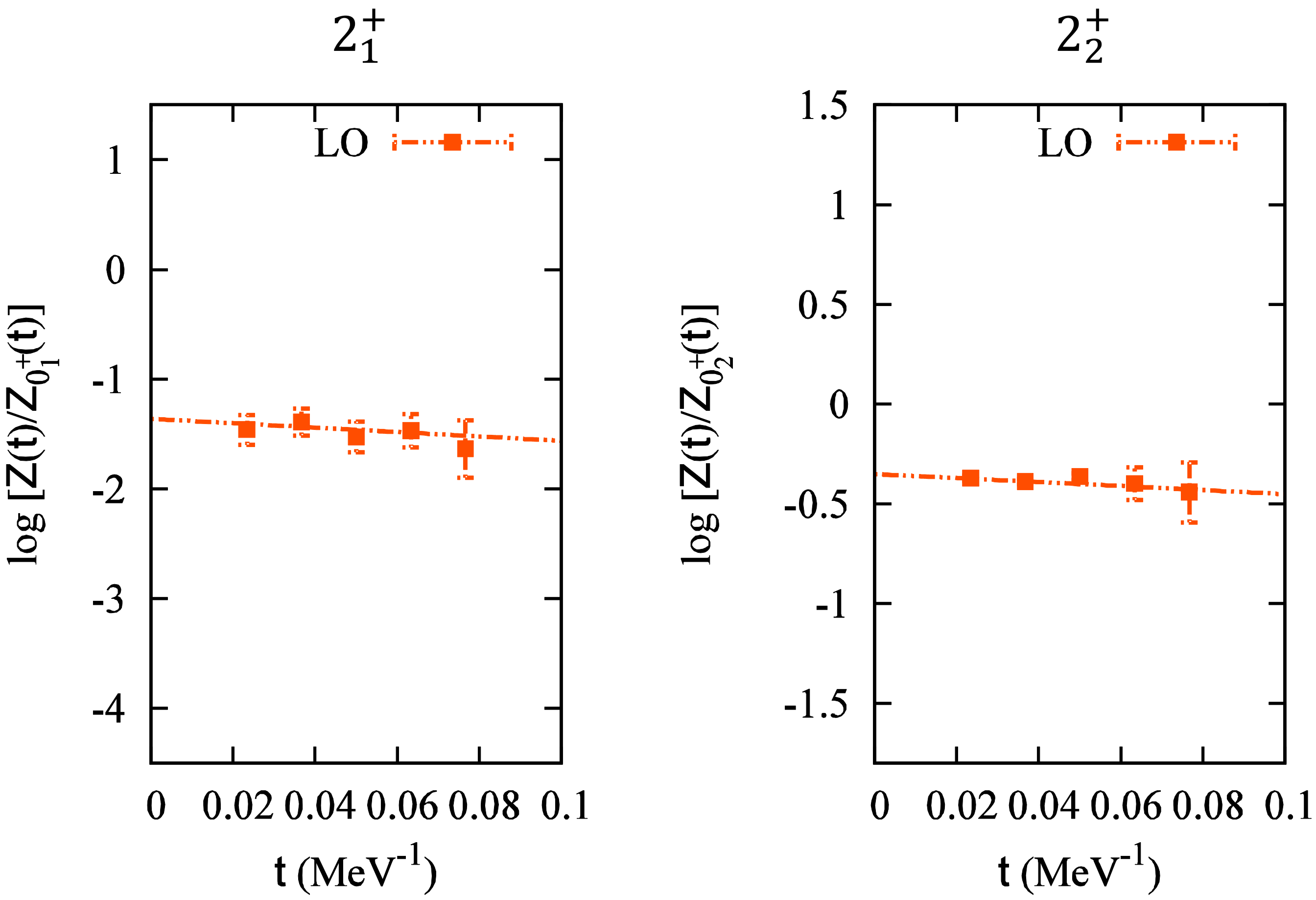
Strong overlap with bent arm configuration



**24 rotational orientations**

$$a = 1.97 \text{ fm}$$

# Rotational excitations – $2_1^+$, $2_2^+$



# Excited state spectrum of carbon-12 (even parity)

| | $2_1^+$ | $0_2^+$ | $2_2^+$ |
|---|---|---|---|
| LO* ($O(Q^0)$) | –94(2) MeV | –89(2) MeV | –88(2) MeV |
| NLO ($O(Q^2)$) | –74(3) MeV | –72(3) MeV | –70(3) MeV |
| NNLO ($O(Q^3)$) | –89(3) MeV | –85(3) MeV | –83(3) MeV |
| Experiment | –87.72 MeV | –84.51 MeV | –82.6(1) MeV (*A*,*B*)<br>–81.1(3) MeV (*C*)<br>–82.13(11) MeV (*D*) |

*contains some interactions promoted from NLO

*A – Freer et al., PRC 80 (2009) 041303*

*B – Zimmerman et al., PRC 84 (2011) 027304*

*C – Hyldegaard et al., PRC 81 (2010) 024303*

*D – Itoh et al., PRC 84 (2011) 054308*

*Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 109 252501 (2012)*

## RMS charge radius

| | LO | Experiment |
|---|---|---|
| $r_{0_1^+}$ [fm] | 2.2(2) | 2.47(2) |
| $r_{2_1^+}$ [fm] | 2.2(2) | – |
| $r_{0_2^+}$ [fm] | 2.4(2) | – |
| $r_{2_2^+}$ [fm] | 2.4(2) | – |

*Schaller, et al.*
*NPA 379 (1982) 523*

bound states at leading order

## Quadrupole moment

| | LO | Experiment |
|---|---|---|
| $Q_{2_1^+}$ [$e$ fm$^2$] | 6(2) | 6(3) |
| $Q_{2_2^+}$ [$e$ fm$^2$] | –7(2) | – |

*Vermeer, et al.*
*PLB 122 (1983) 23*

# Electromagnetic transition strengths

| | LO | Experiment |
|---|---|---|
| $B(E2, 2_1^+ \to 0_1^+)$ $[e^2 \text{ fm}^4]$ | 5(2) | 7.6(4) |
| $B(E2, 2_1^+ \to 0_2^+)$ $[e^2 \text{ fm}^4]$ | 1.5(7) | 2.6(4) |
| $B(E2, 2_2^+ \to 0_1^+)$ $[e^2 \text{ fm}^4]$ | 2(1) | 0.73(13) |
| $B(E2, 2_2^+ \to 0_2^+)$ $[e^2 \text{ fm}^4]$ | 6(2) | – |
| $m(E0, 0_2^+ \to 0_1^+)$ $[e \text{ fm}^2]$ | 3(1) | 5.5(1) |

*Ajzenberg-Selove, NPA 506 (1990) 1*

*Zimmerman, et al., arXiv:1303.4326*

*Chernykh, et al., PRL 105 (2010) 022501*

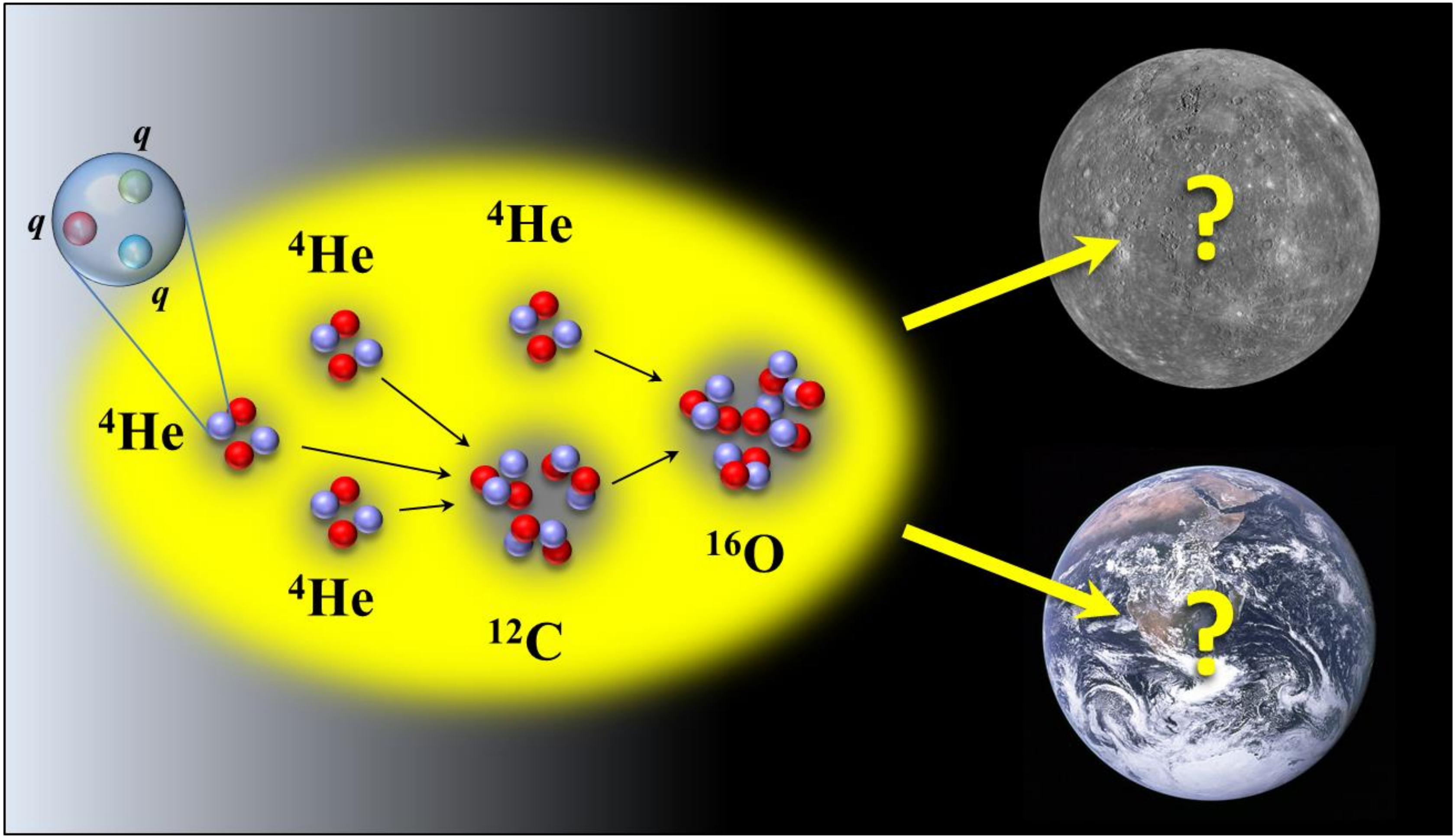
See also other recent calculations using fermionic molecular dynamics

*Chernykh, et al., PRL 98 (2007) 032501*

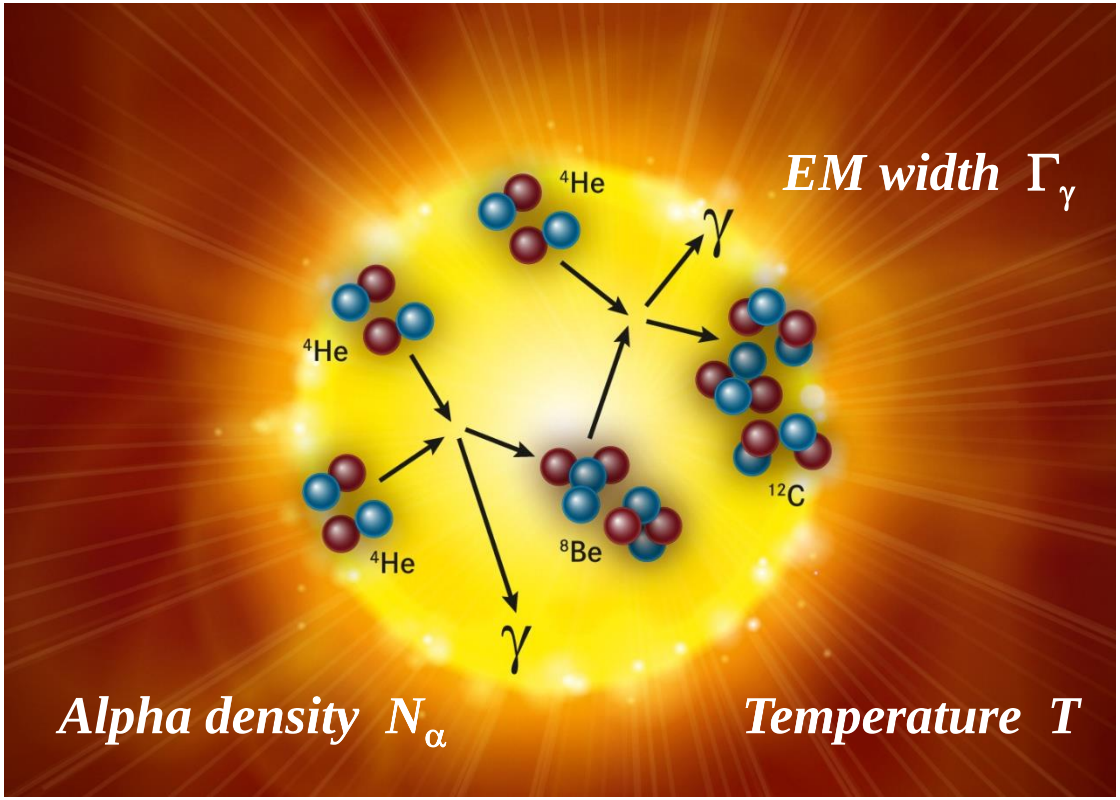
and no-core shell model

*Forssen, Roth, Navratil, arXiv:1110.0634v2*

# Light quark mass dependence of helium burning



# Triple alpha reaction rate




$$r_{3\alpha} \propto \Gamma_\gamma \, (N_\alpha / k_B T)^3 \times \exp(-\varepsilon / k_B T)$$

$\varepsilon = E_h - 3E_\alpha$ Hoyle relative to triple-alpha

# Is nature fine-tuned?

$$\varepsilon = E_h - 3E_\alpha = 379\,\mathrm{keV}$$

$\varepsilon > 479\,\mathrm{keV}$

Less resonance enhancement.
Rate of carbon production smaller by several orders of magnitude.
Low carbon abundance is unfavorable for carbon-based life.

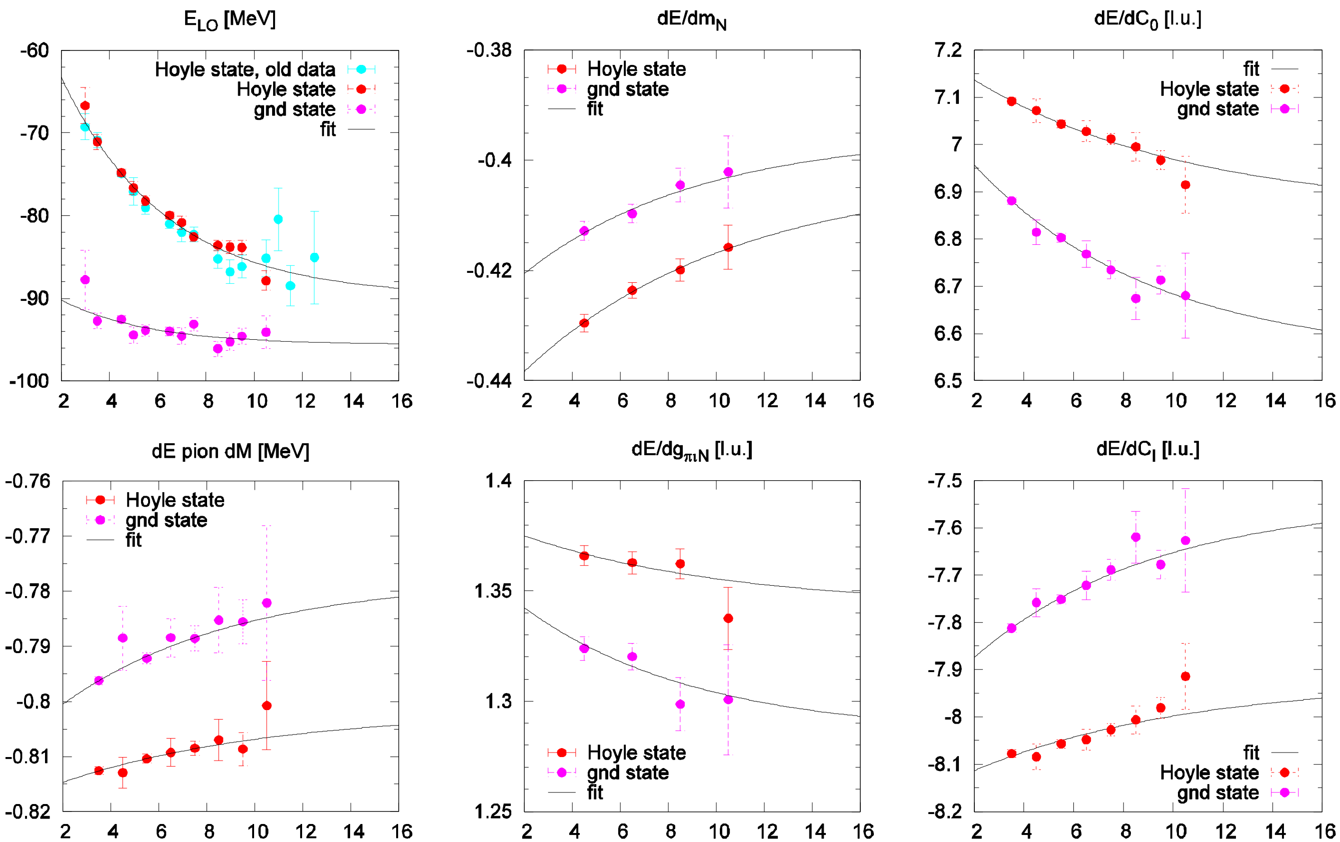
$\varepsilon < 279\,\mathrm{keV}$

Carbon production occurs at lower stellar temperatures and oxygen production greatly reduced.
Low oxygen abundance is unfavorable for carbon-based life.

*Schlattl et al., Astrophys. Space Sci., 291, 27–56 (2004)*

We investigate the dependence on the fundamental parameters of the standard model such as the light quark masses. Can be parameterized by the pion mass.

# Lattice results for pion mass dependence



| | |
|---|---|
| $\Delta E_h = E_h - E_b - E_\alpha$ | Hoyle relative to Be-8-alpha |
| $\Delta E_b = E_b - 2E_\alpha$ | Be-8 relative to alpha-alpha |
| $\varepsilon = E_h - 3E_\alpha$ | Hoyle relative to triple-alpha |

$$\left.\frac{\partial \Delta E_h}{\partial M_\pi}\right|_{M_\pi^{\rm ph}} = -0.455(35)\bar{A}_s - 0.744(24)\bar{A}_t + 0.051(19)$$

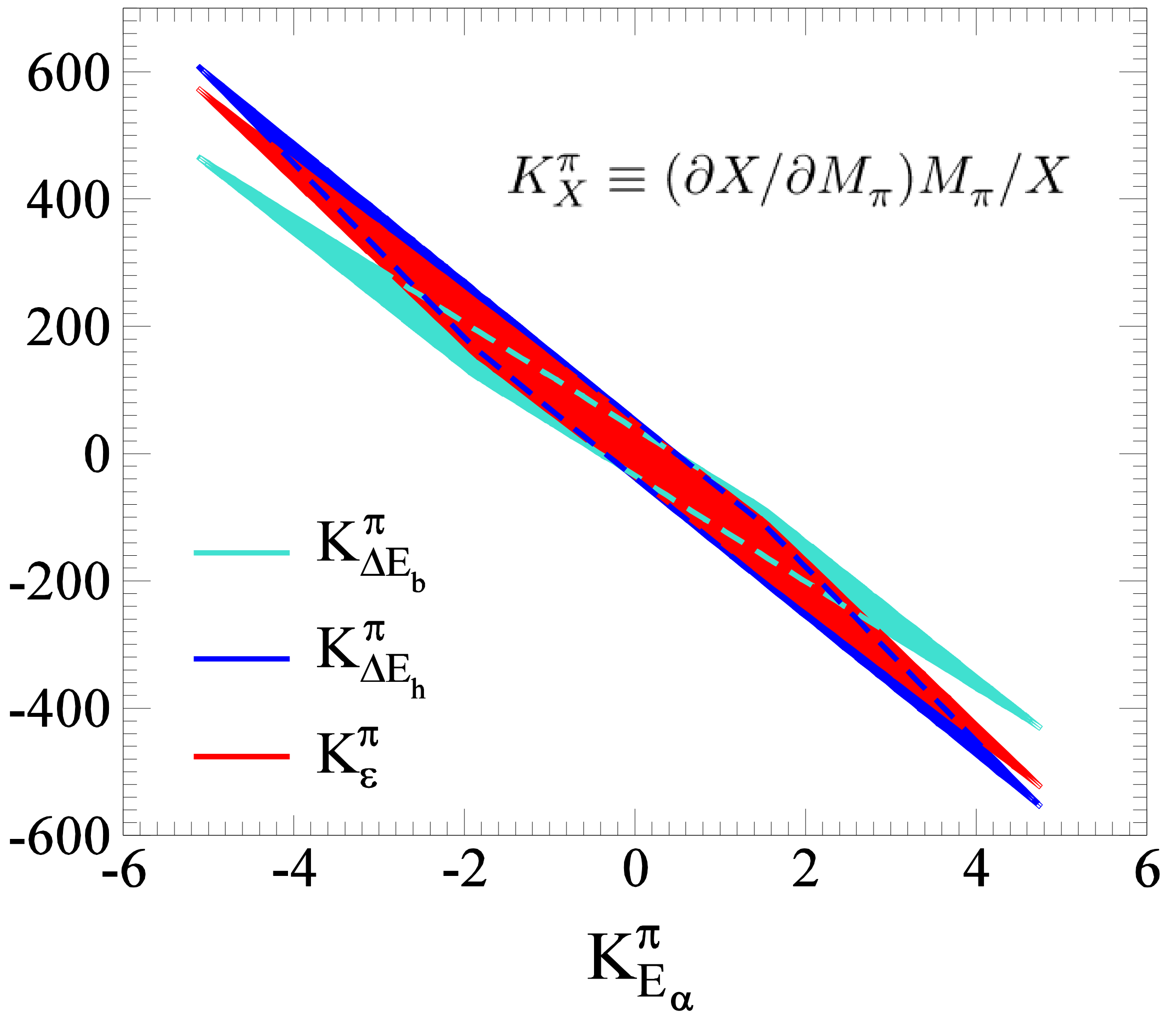
$$\left.\frac{\partial \Delta E_b}{\partial M_\pi}\right|_{M_\pi^{\rm ph}} = -0.117(34)\bar{A}_s - 0.189(24)\bar{A}_t + 0.013(12)$$

$$\left.\frac{\partial \varepsilon}{\partial M_\pi}\right|_{M_\pi^{\rm ph}} = -0.572(19)\bar{A}_s - 0.933(15)\bar{A}_t + 0.064(16)$$

$$\bar{A}_s \equiv \partial a_s^{-1}/\partial M_\pi\big|_{M_\pi^{\rm ph}} \qquad \bar{A}_t \equiv \partial a_t^{-1}/\partial M_\pi\big|_{M_\pi^{\rm ph}}$$

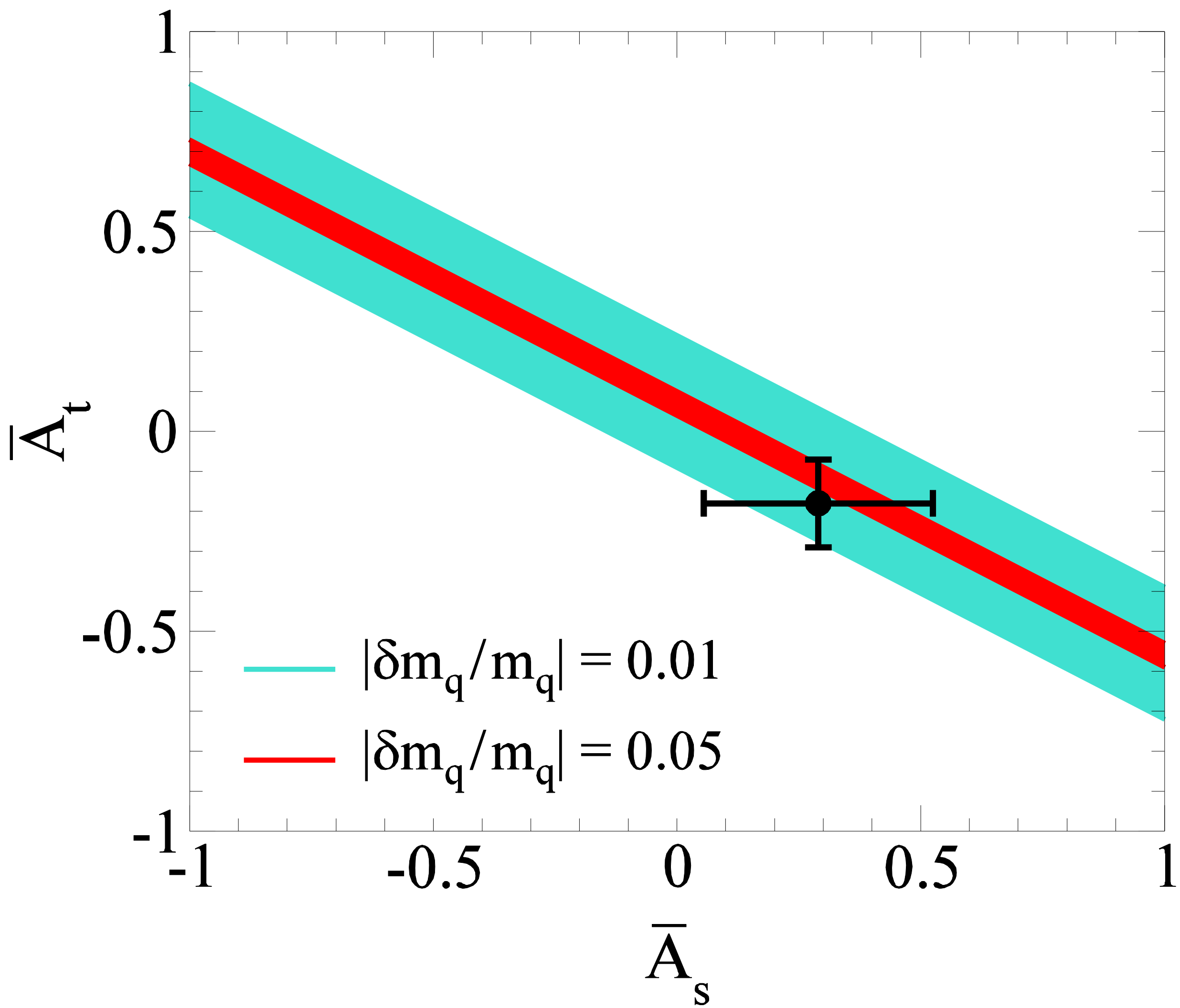
*Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 110 (2013) 112502; ibid., arXiv:1303.4856*
*Berengut et al., arXiv:1301.1738*

## Evidence for correlation with alpha binding energy



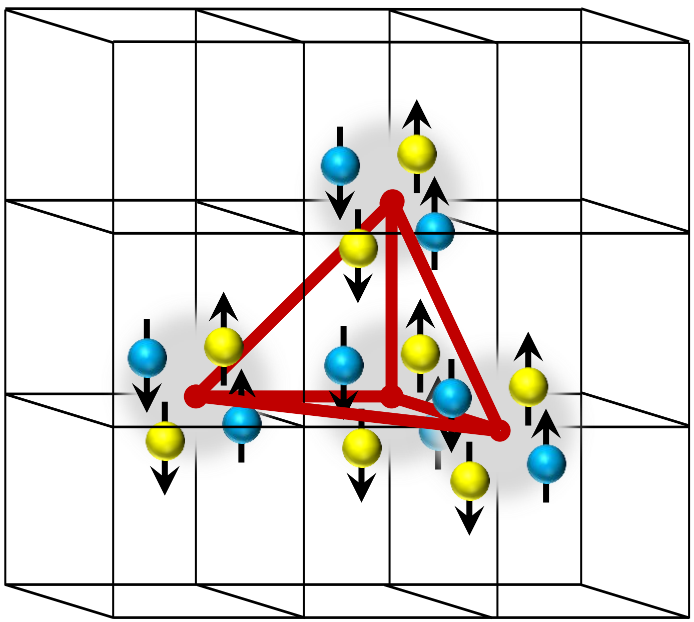

*Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 110 (2013) 112502; ibid., arXiv:1303.4856*

<u>"End of the world" plot</u>



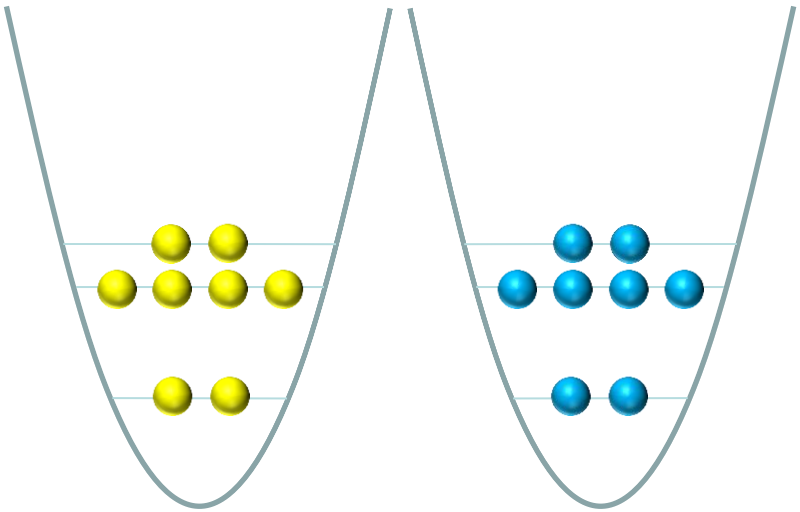
# Work in progress: Oxygen-16

Dual structure of 0+ ground state



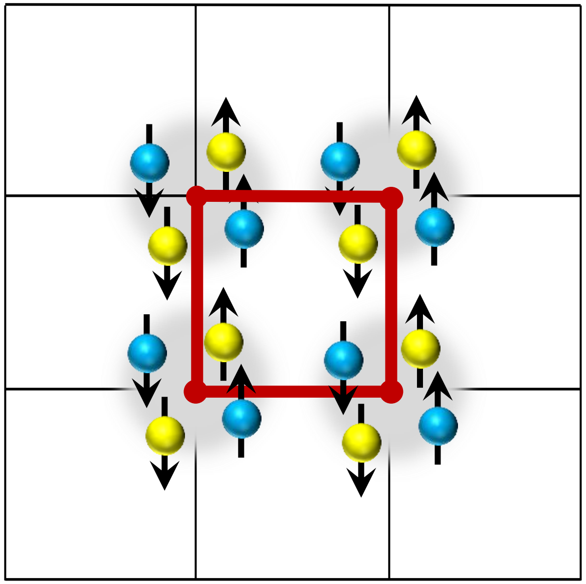
**8 rotational orientations**

$a = 1.97$ fm



Particle-hole excitations: 3–, 1–, etc.

Cluster structure of second 0+ state and first 2+ state



$a = 1.97\ \mathrm{fm}$

**6 rotational orientations**

# Summary and future directions

A golden age for nuclear theory from first principles. Big science discoveries being made and many more around the corner.

Lattice effective field theory is a relatively new and promising tool that combines the framework of effective field theory and computational lattice methods. May play a significant role in the future of *ab initio* nuclear theory.

*Topics to be addressed in the near future…*

Different lattice spacings, spectrum of oxygen-16, adiabatic Hamiltonians for scattering and reactions, alpha clustering in nuclei, transition from S-wave to P-wave pairing in superfluid neutron matter, weak matrix elements, etc.