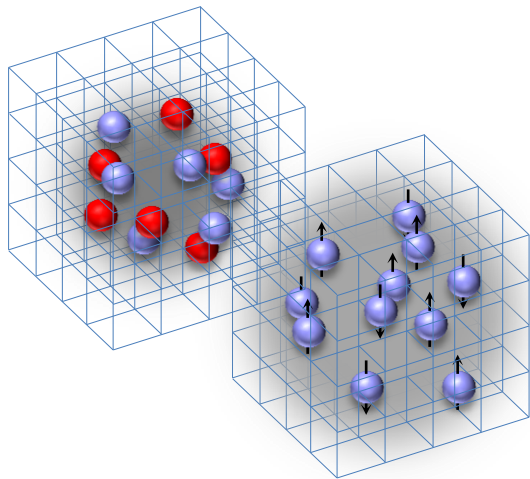


# Nuclear structure and excitations from lattice effective field theory



## Nuclear Lattice EFT Collaboration

Evgeny Epelbaum (Bochum)  
Hermann Krebs (Bochum)  
Timo Lähde (Jülich)  
Dean Lee (NC State)  
Ulf-G. Meißner (Bonn/Jülich)  
Gautam Rupak (MS State)

*From Few-Nucleon Forces  
to Many-Nucleon Structures*

ECT\* and HIC for FAIR Workshop, Trento  
June 11, 2013



## Outline

What is lattice effective field theory?

Carbon-12 spectrum and the Hoyle state

Light quark mass dependence of helium burning

*Ab initio* lattice calculations up to  $A = 28$

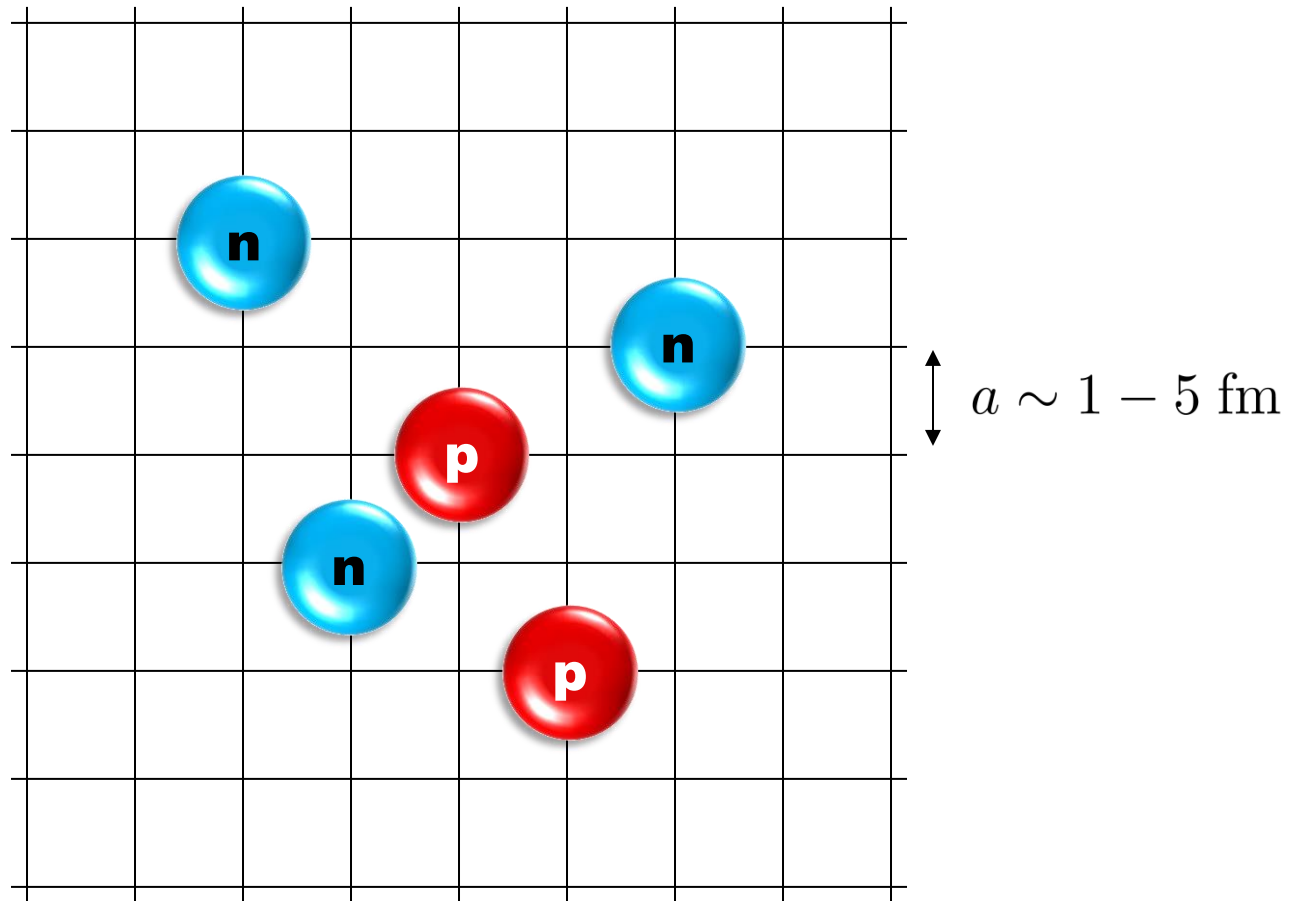
Oxygen-16 structure and spectrum

Properties of neutron matter

Scattering and reactions on the lattice

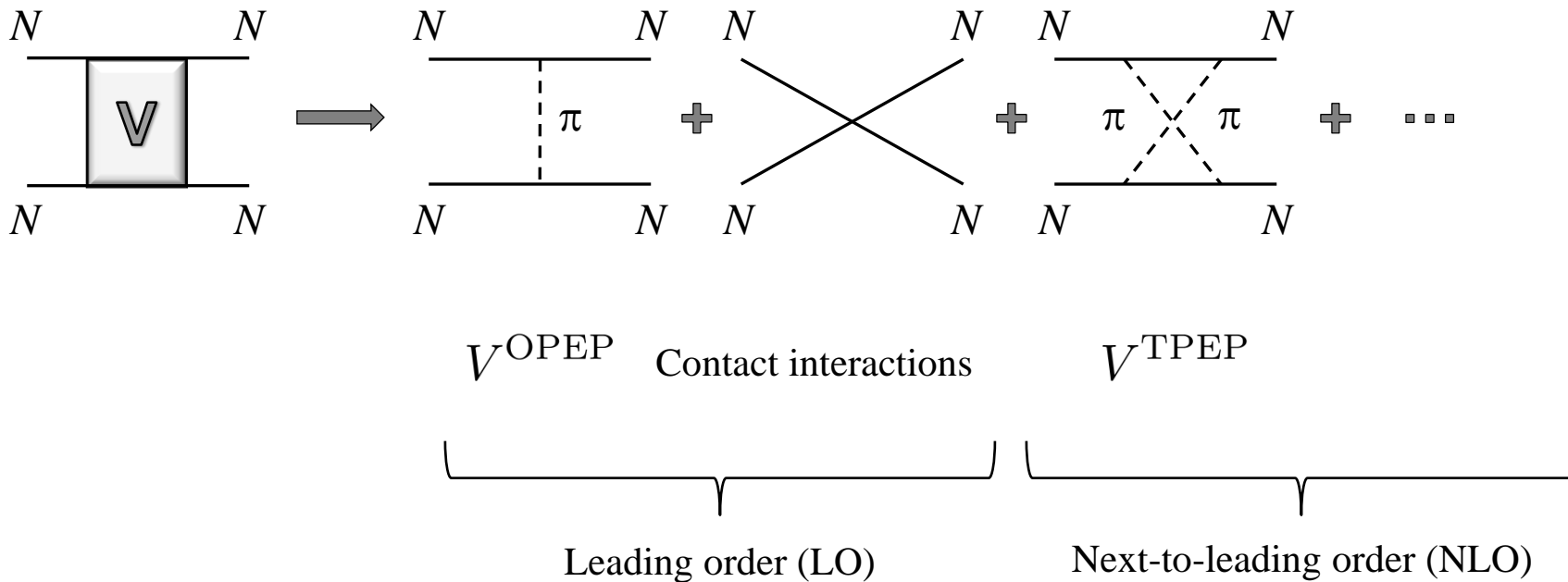
Summary and future directions

# Lattice effective field theory



# Low energy nucleons: Chiral effective field theory

Construct the effective potential order by order



Physical  
scattering data

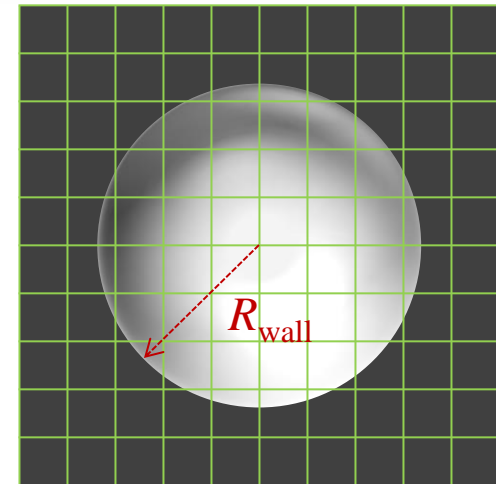


Unknown operator  
coefficients

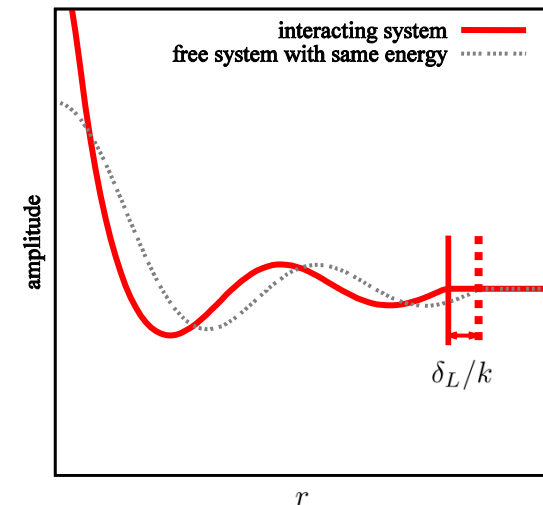
### Spherical wall method

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

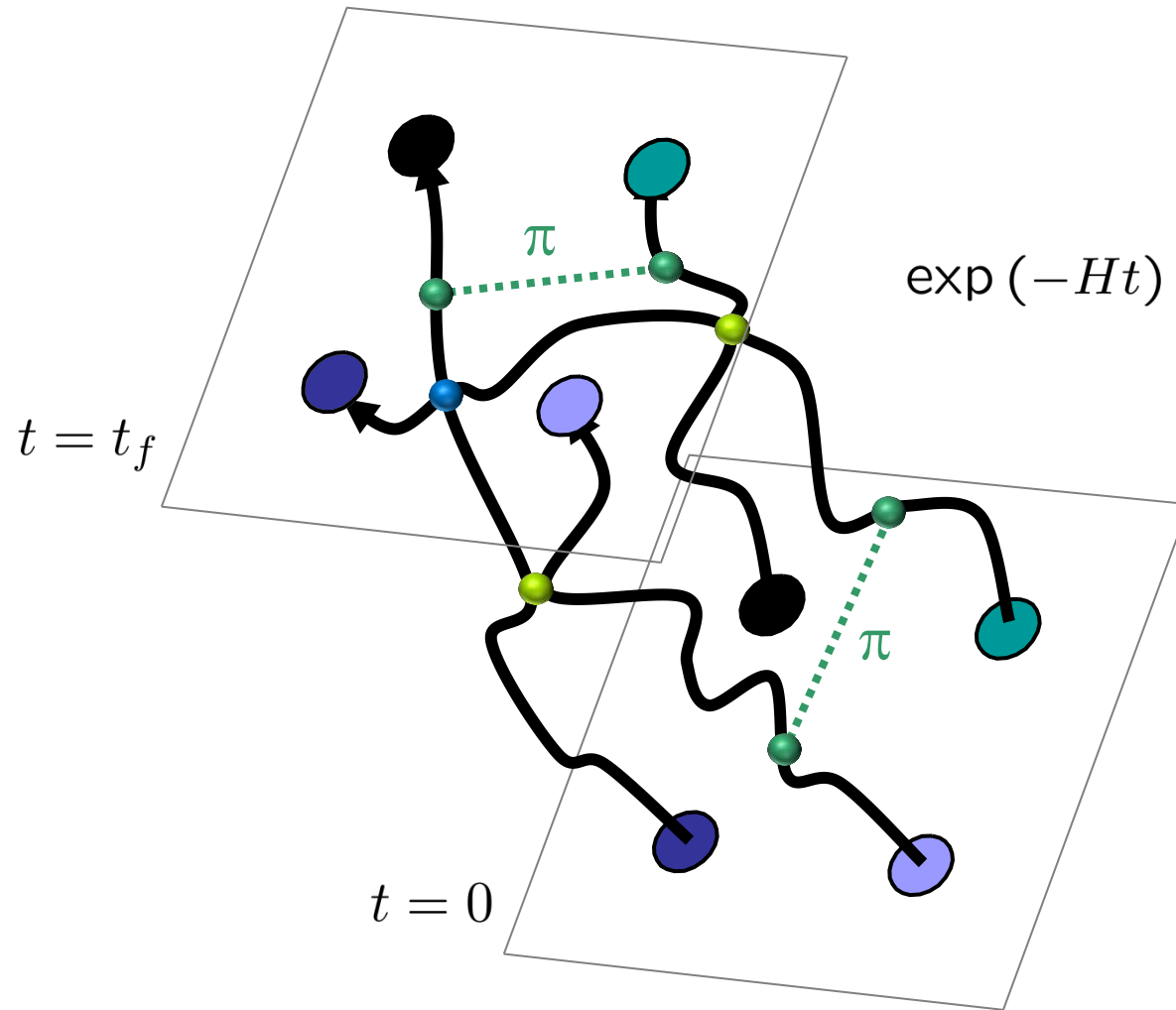
Spherical wall imposed in the center of mass  
frame



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



## Euclidean time projection

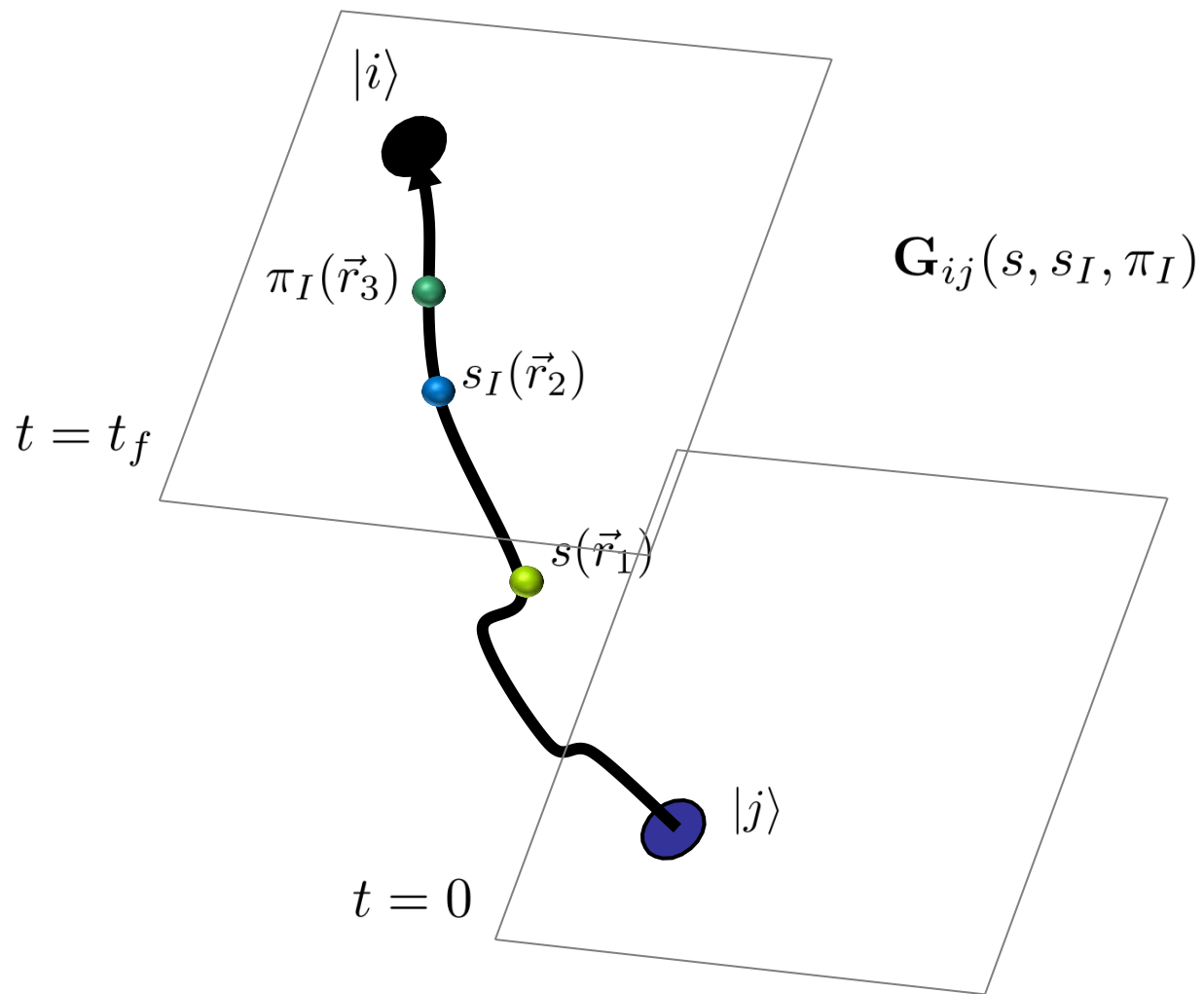


## Auxiliary field method

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

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

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





## Schematic of lattice Monte Carlo calculation

$$\begin{array}{ccc}
 \boxed{\phantom{M}} = M_{\text{LO}} & \boxed{\phantom{M}} = M_{\text{approx}} & \boxed{\phantom{O}} = O_{\text{observable}} \\
 \boxed{\phantom{M}} = M_{\text{NLO}} & \boxed{\phantom{M}} = M_{\text{NNLO}} & 
 \end{array}$$

Hybrid Monte Carlo sampling

$$Z_{n_t, \text{LO}} = \langle \psi_{\text{init}} | \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} | \psi_{\text{init}} \rangle$$

$$Z_{n_t, \text{LO}}^{\langle O \rangle} = \langle \psi_{\text{init}} | \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} \boxed{\phantom{M}} | \psi_{\text{init}} \rangle$$

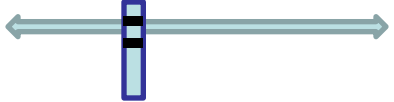
$$e^{-E_{0, \text{LO}} a t} = \lim_{n_t \rightarrow \infty} Z_{n_t+1, \text{LO}} / Z_{n_t, \text{LO}}$$

$$\langle O \rangle_{0, \text{LO}} = \lim_{n_t \rightarrow \infty} Z_{n_t, \text{LO}}^{\langle O \rangle} / Z_{n_t, \text{LO}}$$

$$Z_{n_t, \text{NLO}} = \langle \psi_{\text{init}} | \left[ \text{black bars} \right] \left[ \text{blue bars} \right] \left[ \text{black bars} \right] | \psi_{\text{init}} \rangle$$

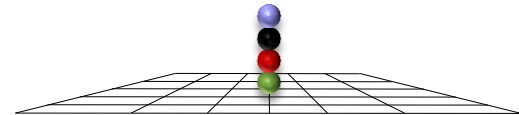
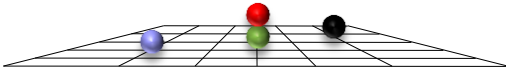
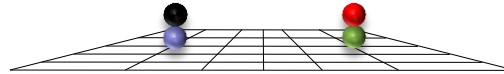
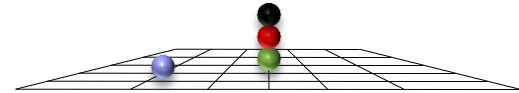


$$Z_{n_t, \text{NLO}}^{\langle O \rangle} = \langle \psi_{\text{init}} | \left[ \text{black bars} \right] \left[ \text{blue bars} \right] \left[ \text{yellow bar} \right] \left[ \text{blue bars} \right] \left[ \text{black bars} \right] | \psi_{\text{init}} \rangle$$

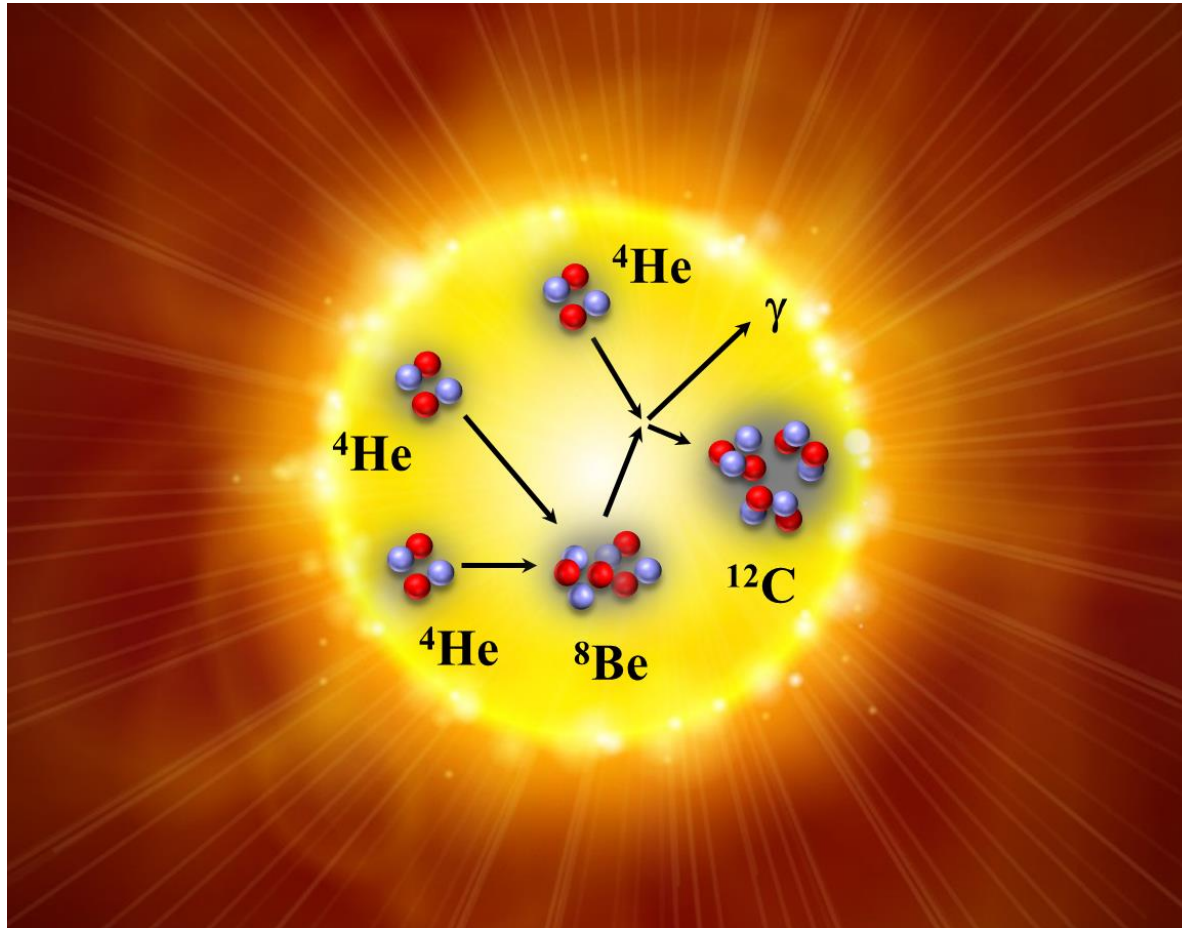


$$\langle O \rangle_{0, \text{NLO}} = \lim_{n_t \rightarrow \infty} Z_{n_t, \text{NLO}}^{\langle O \rangle} / Z_{n_t, \text{NLO}}$$

# Particle clustering included automatically

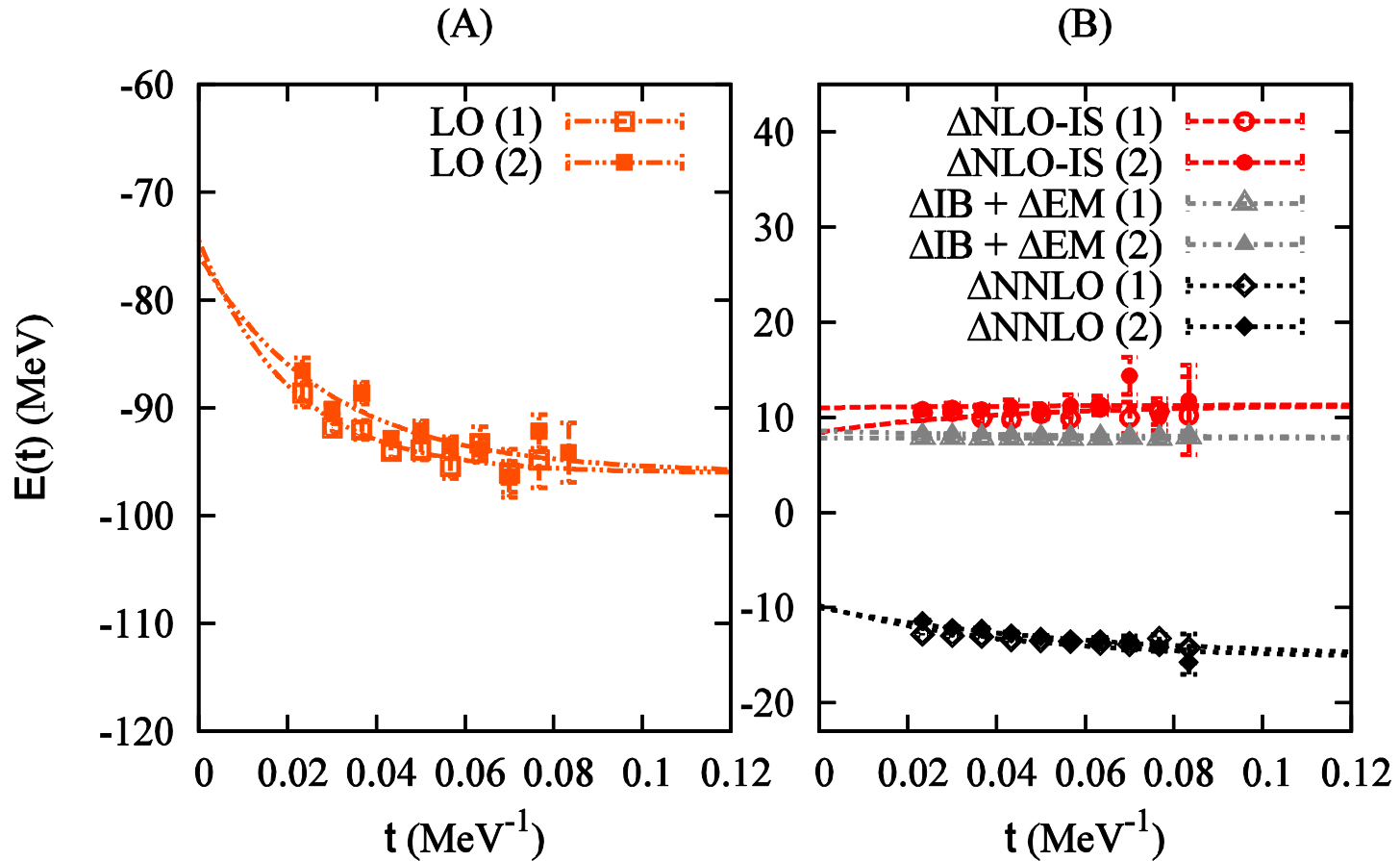


## Carbon-12 spectrum and the Hoyle state



# Ground state of Carbon-12

$L = 11.8$  fm



*Epelbaum, Krebs, D.L, Meißner, PRL 106 (2011) 192501*

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

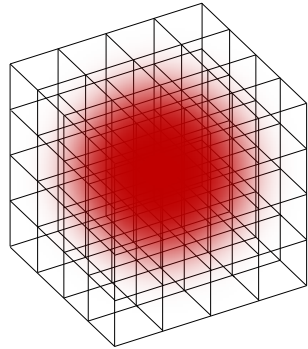
## Ground state of Carbon-12

$$L = 11.8 \text{ fm}$$

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

## Simulations using general initial/final state wavefunctions



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

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

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

## Shell model wavefunctions

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

## Alpha cluster wavefunctions

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

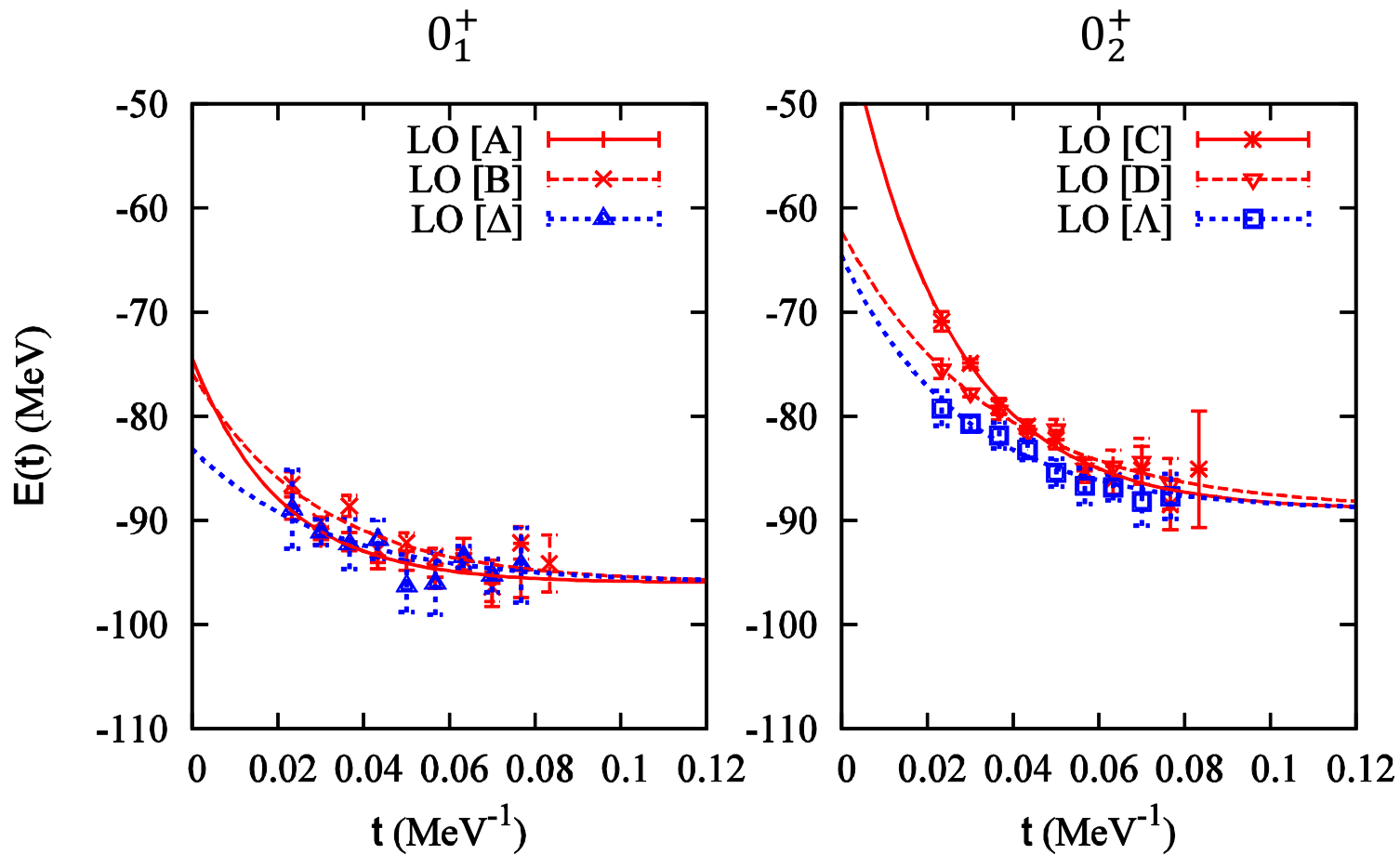


Shell model wavefunctions by themselves do not have enough local four nucleon correlations,

$$\langle (N^\dagger N)^4 \rangle$$

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

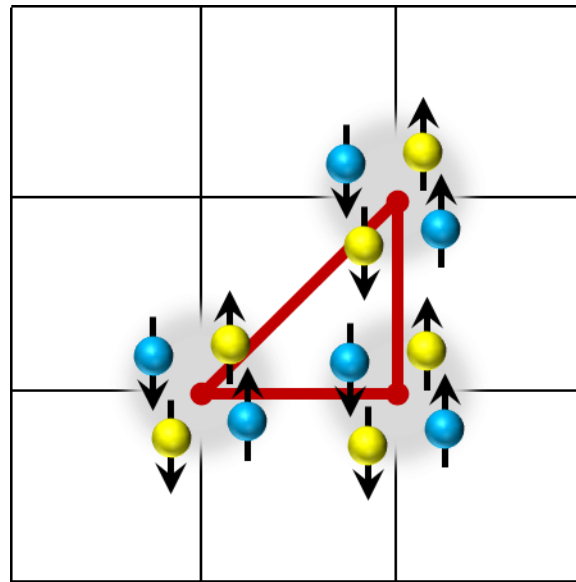
But can reproduce same results starting directly from alpha cluster wavefunctions [ $\Delta$  and  $\Lambda$  in plots on next slide].



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

## Structure of ground state and first 2+

Strong overlap with compact triangle configuration

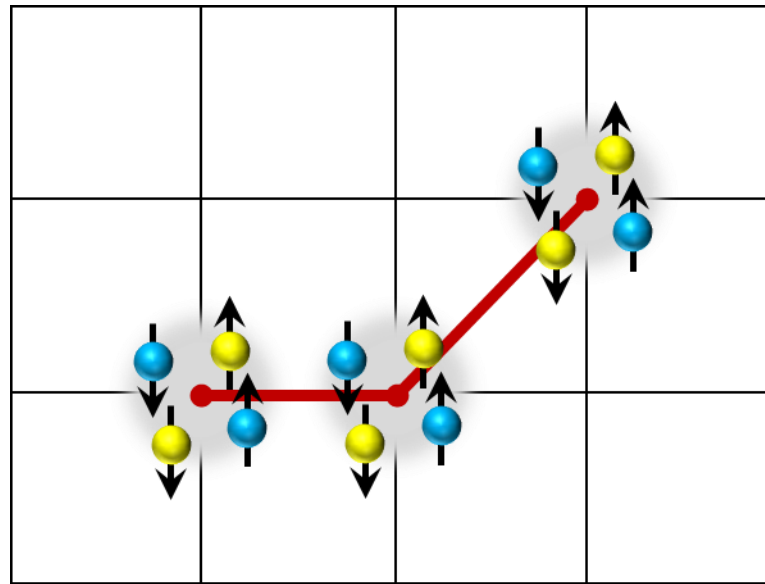


**12 rotational orientations**

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

## Structure of Hoyle state and second 2+

Strong overlap with bent arm configuration



**24 rotational orientations**

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

## 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) -81.1(3) MeV (C) -82.13(11) MeV (D)

\*contains some interactions  
promoted from NLO

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

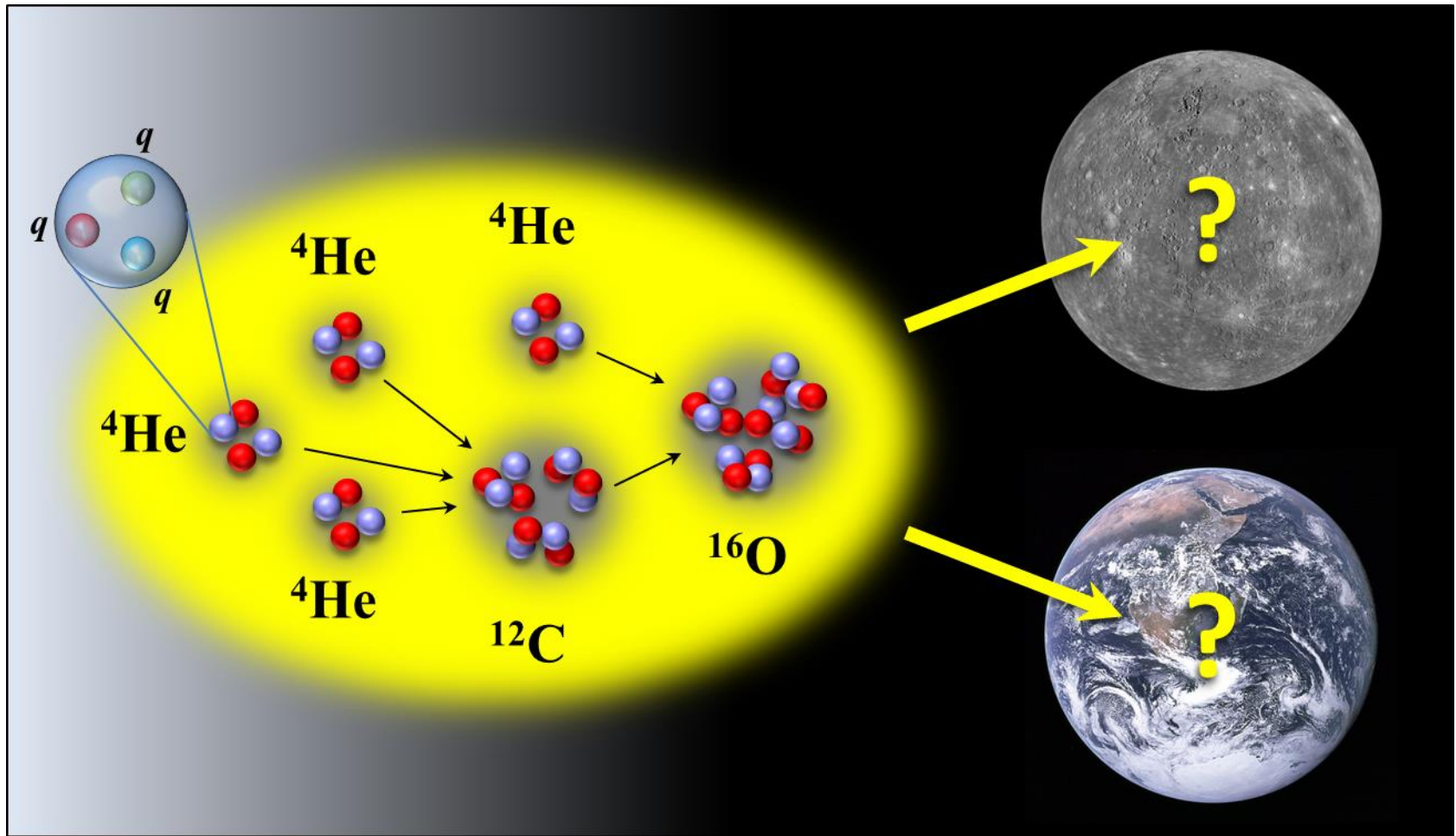
*B – Zimmerman et al., PRC 84 (2011) 027304*

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

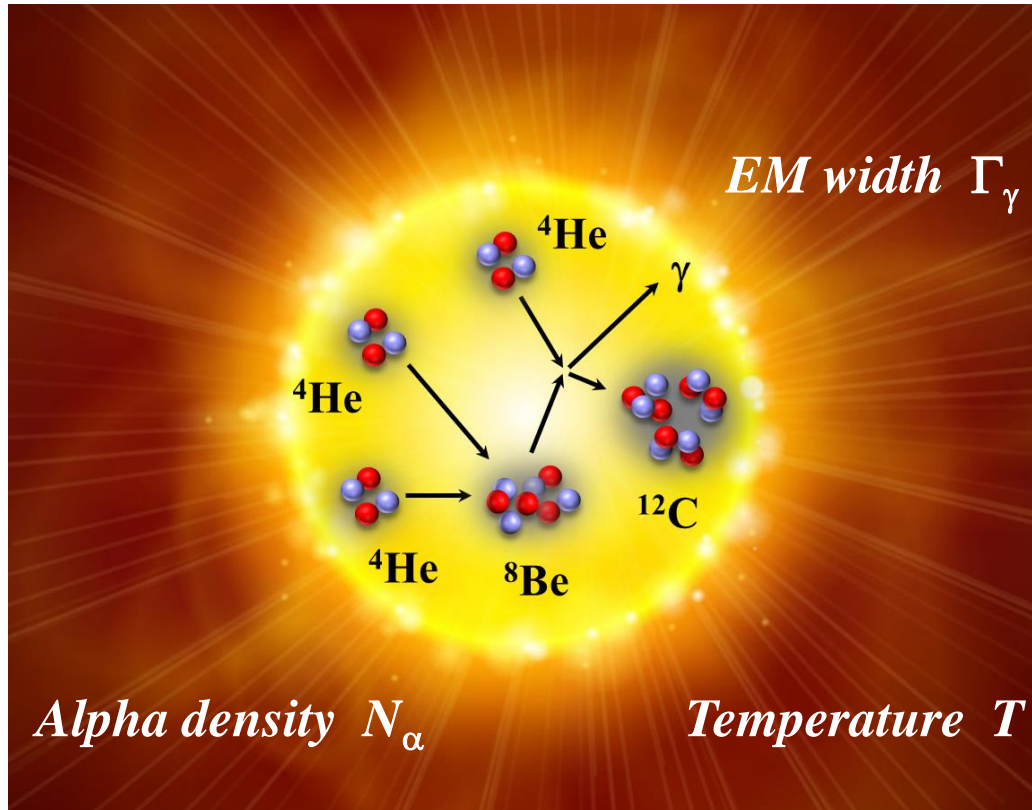
*D – Itoh et al., PRC 84 (2011) 054308*

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

## Light quark mass dependence of helium burning



## Triple alpha reaction rate



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

$$\varepsilon = E_h - 3E_\alpha \quad \text{Hoyle relative to triple-alpha}$$

## Is nature fine-tuned?

$$\varepsilon = E_h - 3E_\alpha \approx 380 \text{ keV}$$

$$\varepsilon > 480 \text{ keV}$$

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

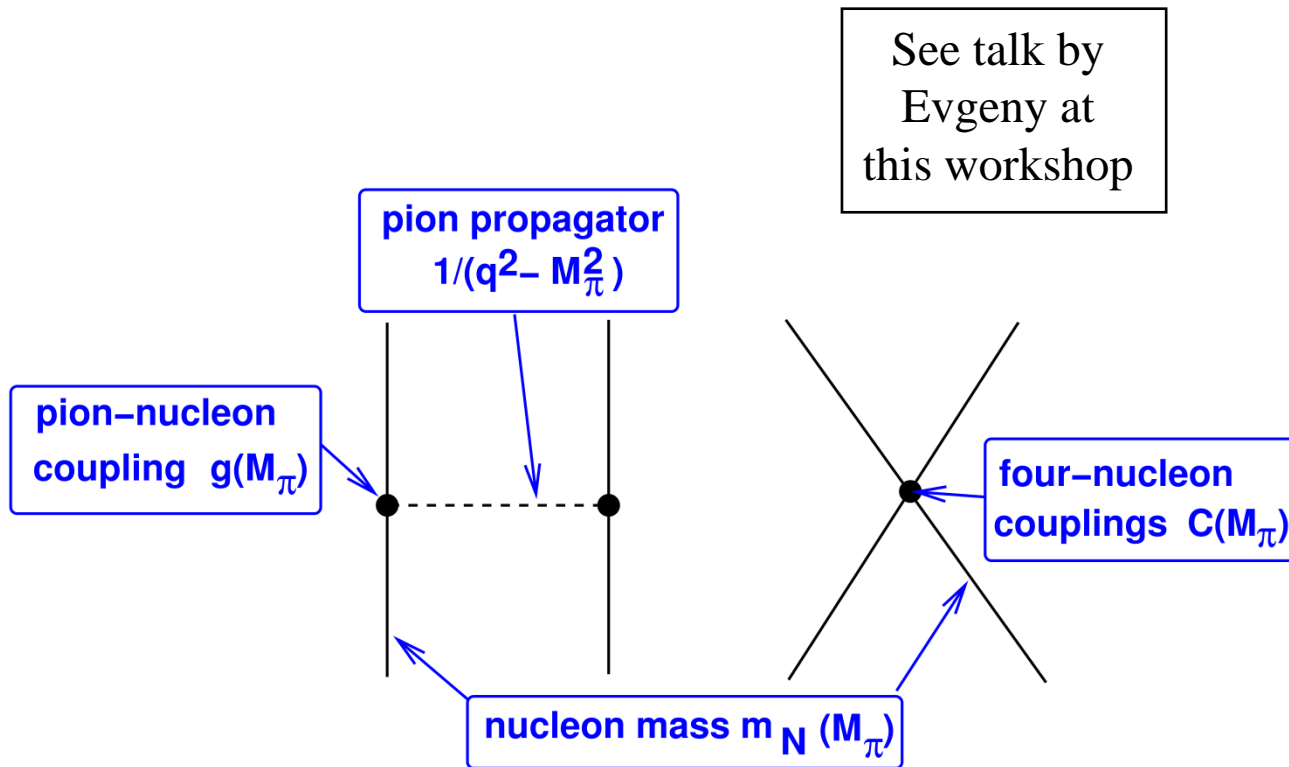
$$\varepsilon < 280 \text{ keV}$$

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.

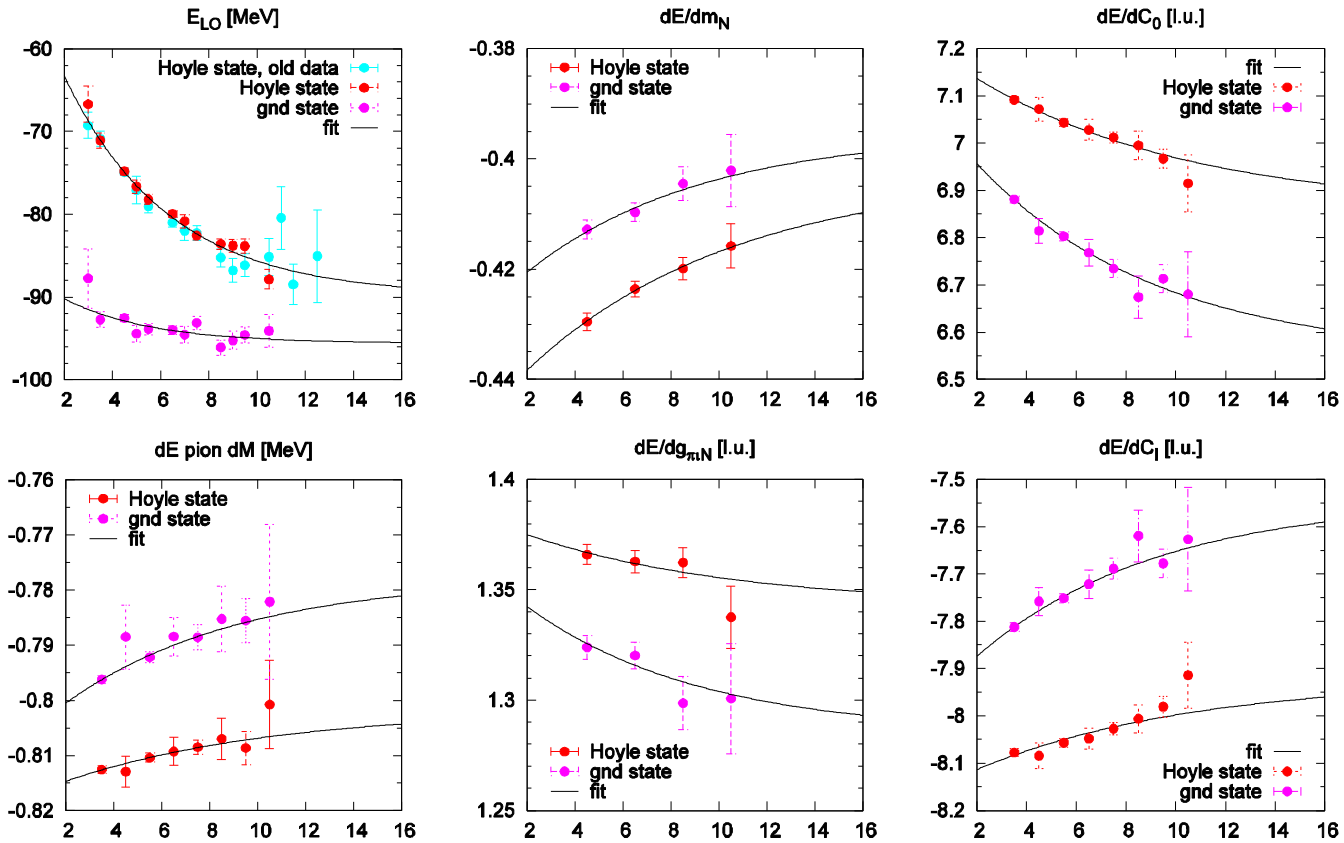




*Figure courtesy of U.-G. Meißner*

*Epelbaum, Krebs, Lähde, D.L. Meißner, PRL 110 (2013) 112502; ibid., arXiv:1303.4856  
 Berengut et al., Phys. Rev. D 87 (2013) 085018*

# Lattice results for pion mass dependence



$$\Delta E_h = E_h - E_b - E_\alpha \quad \text{Hoyle relative to Be-8-alpha}$$

$$\Delta E_b = E_b - 2E_\alpha \quad \text{Be-8 relative to alpha-alpha}$$

$$\varepsilon = E_h - 3E_\alpha \quad \text{Hoyle relative to triple-alpha}$$

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

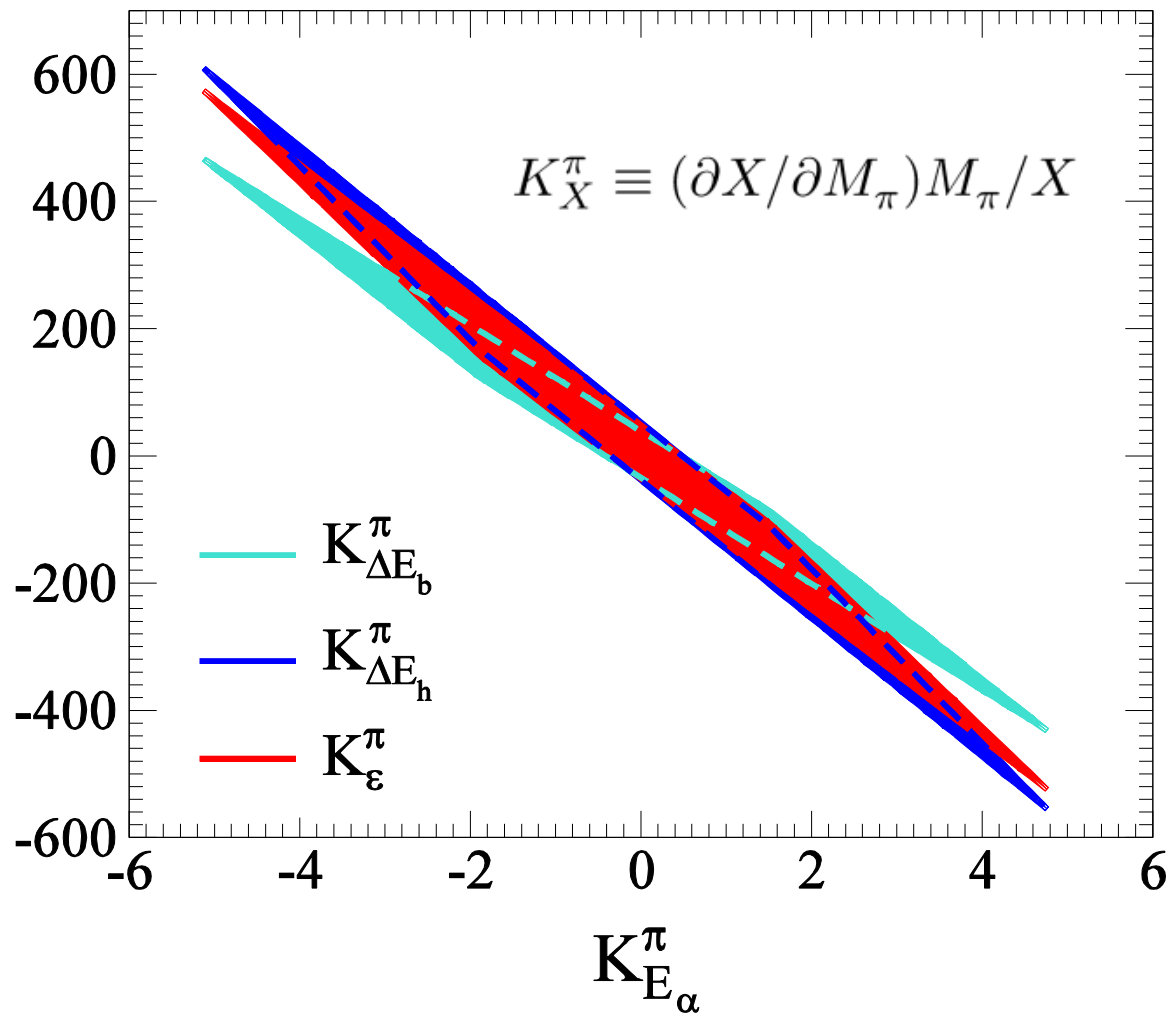
$$\left. \frac{\partial \Delta E_b}{\partial M_\pi} \right|_{M_\pi^{\text{ph}}} = -0.117(34) \bar{A}_s - 0.189(24) \bar{A}_t + 0.013(12)$$

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

$$\bar{A}_s \equiv \partial a_s^{-1} / \partial M_\pi \Big|_{M_\pi^{\text{ph}}} \quad \bar{A}_t \equiv \partial a_t^{-1} / \partial M_\pi \Big|_{M_\pi^{\text{ph}}}$$

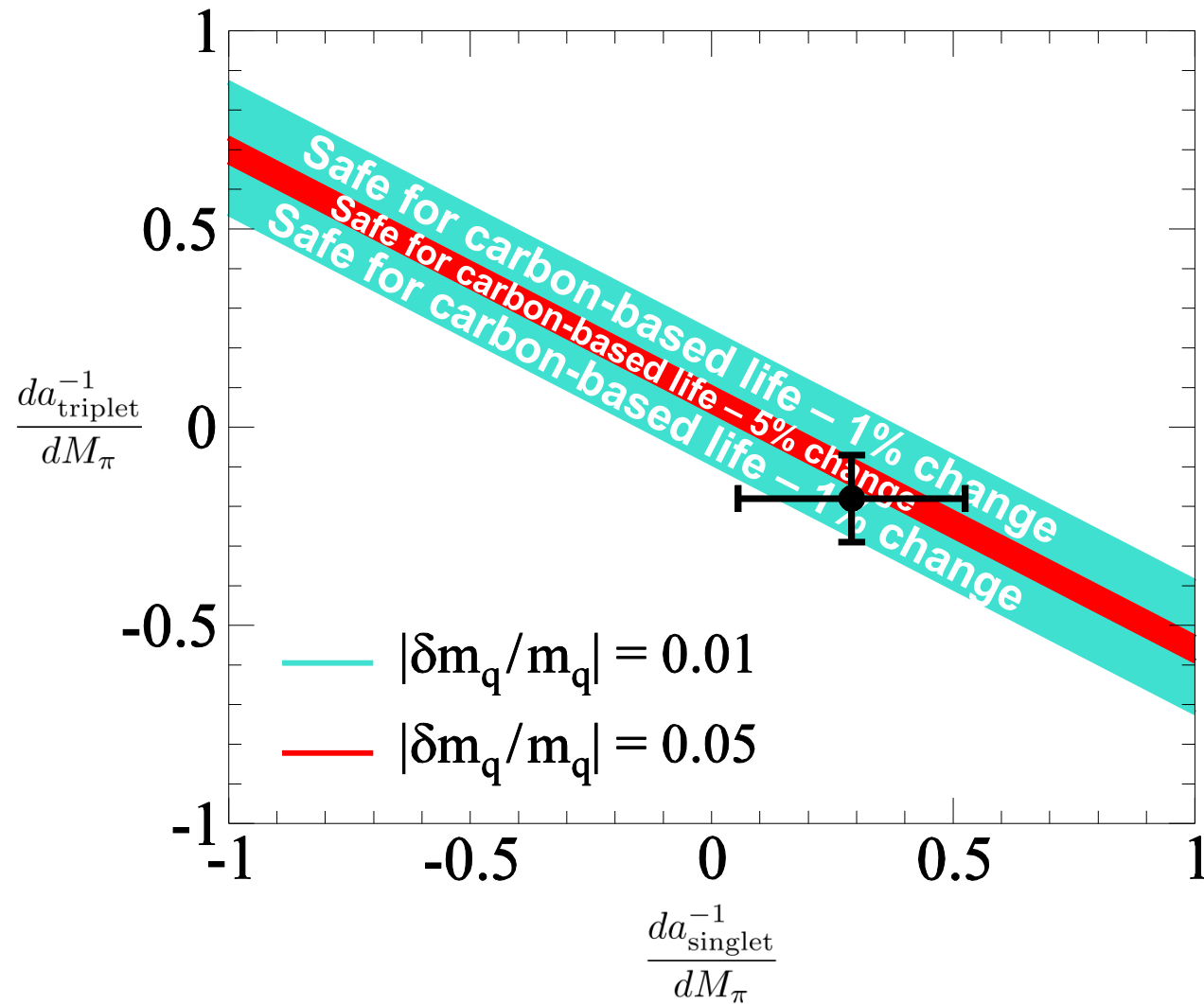
*Epelbaum, Krebs, Lähde, D.L. Meißner, PRL 110 (2013) 112502; ibid., arXiv:1303.4856*  
*Berengut et al., Phys. Rev. D 87 (2013) 085018*

## Evidence for correlation with alpha binding energy



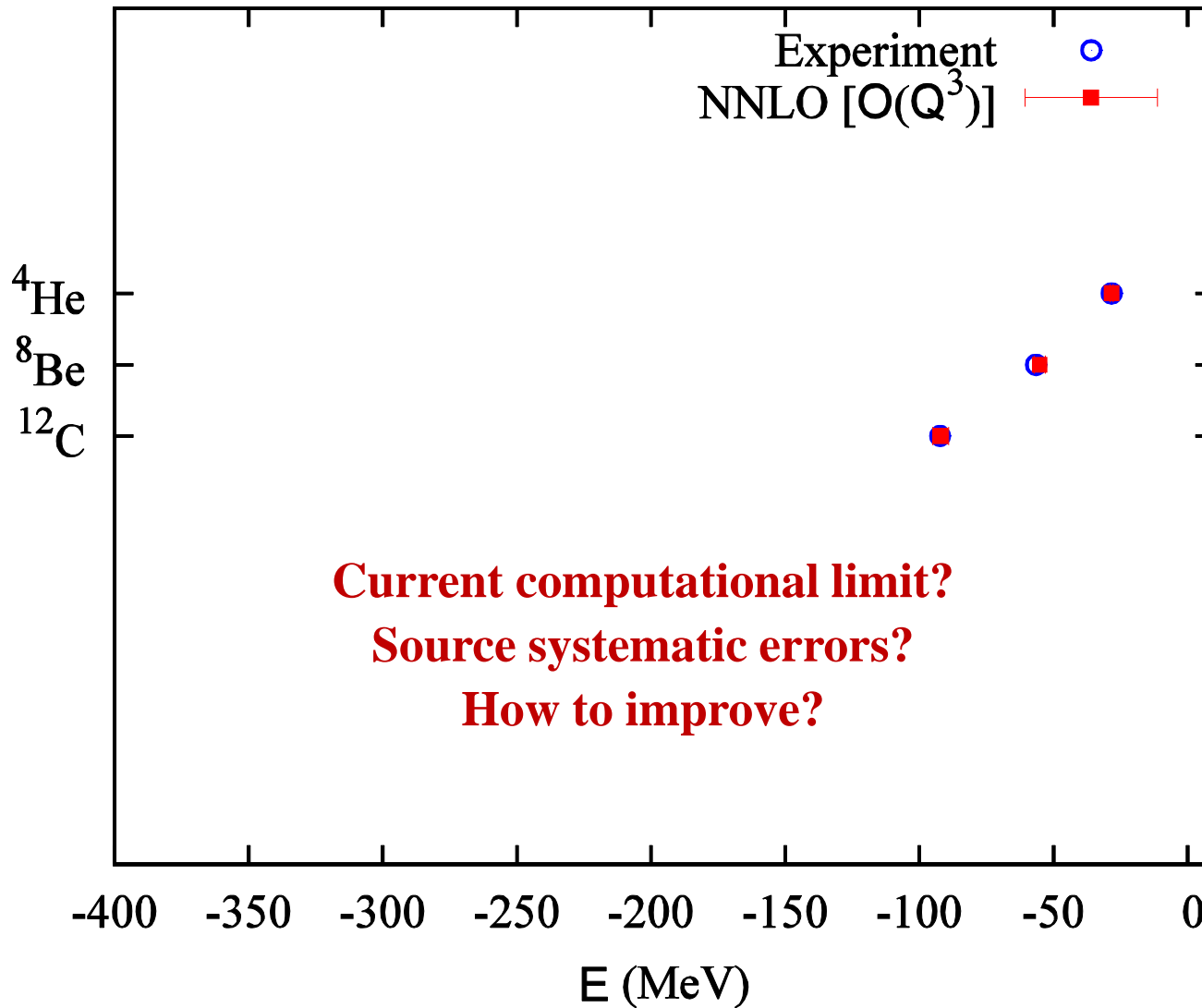
*Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 110 (2013) 112502; ibid., arXiv:1303.4856*

## “End of the world” plot

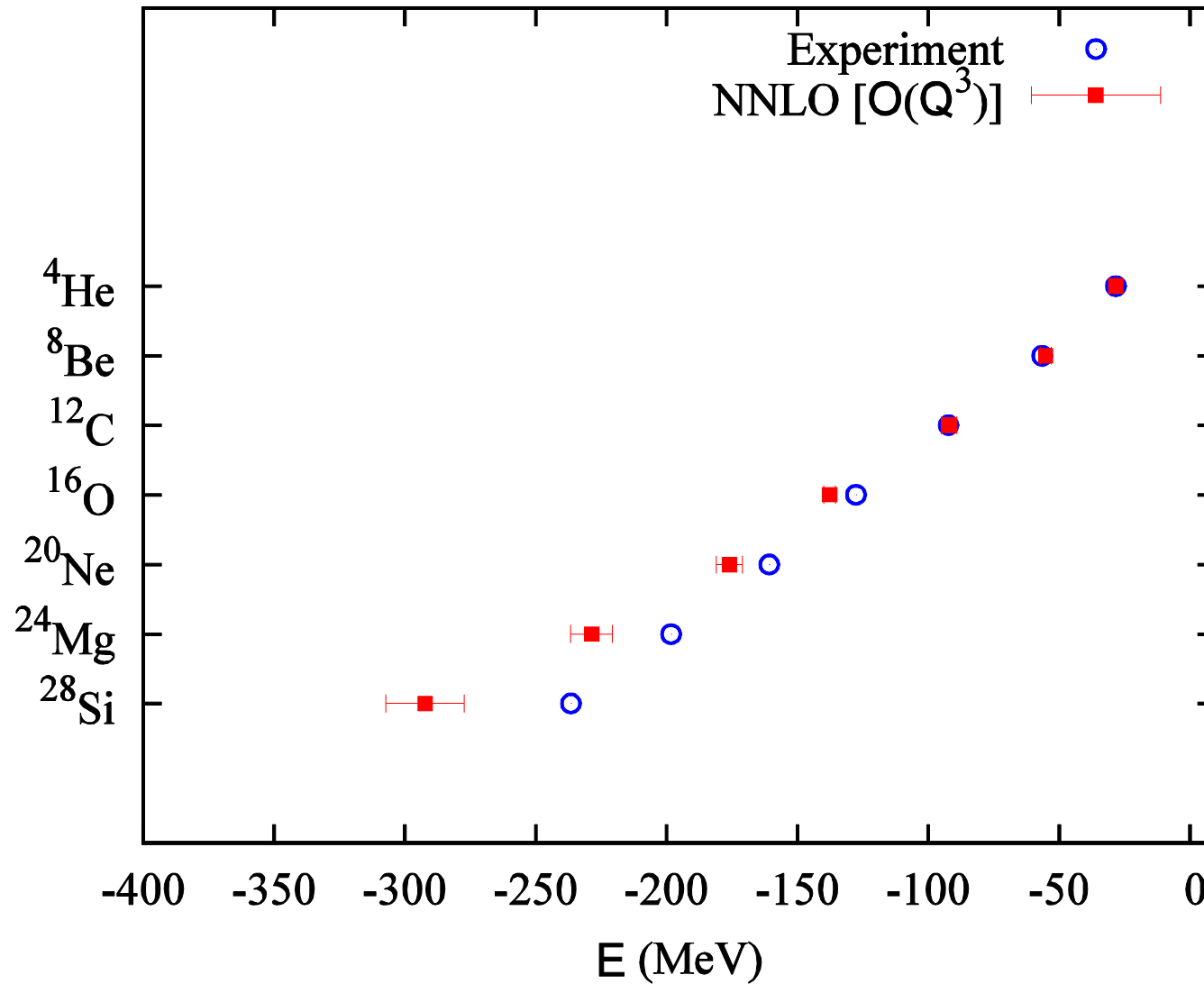


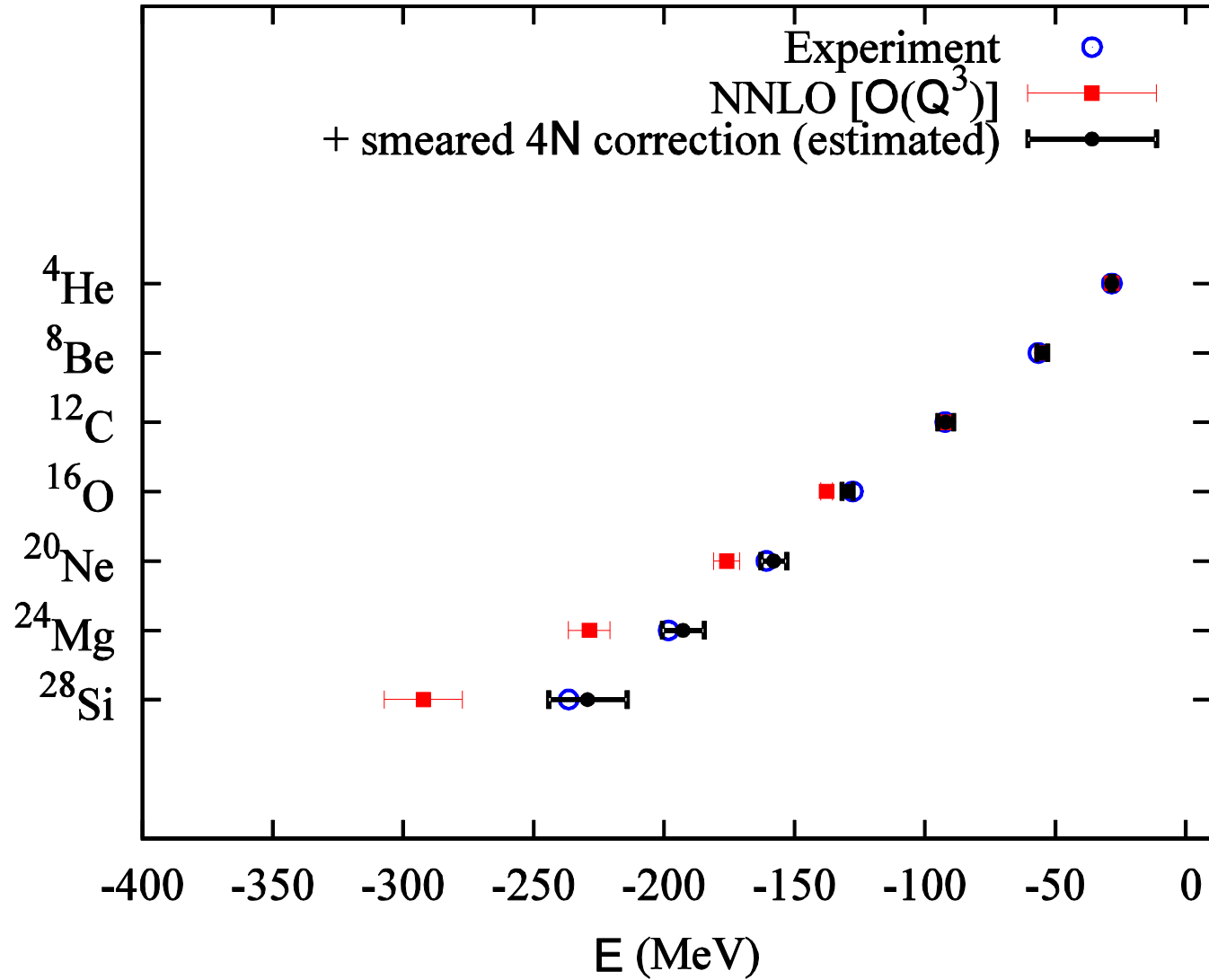
*Epelbaum, Krebs, Lähde, D.L. Meißner, PRL 110 (2013) 112502; ibid., arXiv:1303.4856*

Preliminary: *Ab initio* lattice calculations up to  $A = 28$



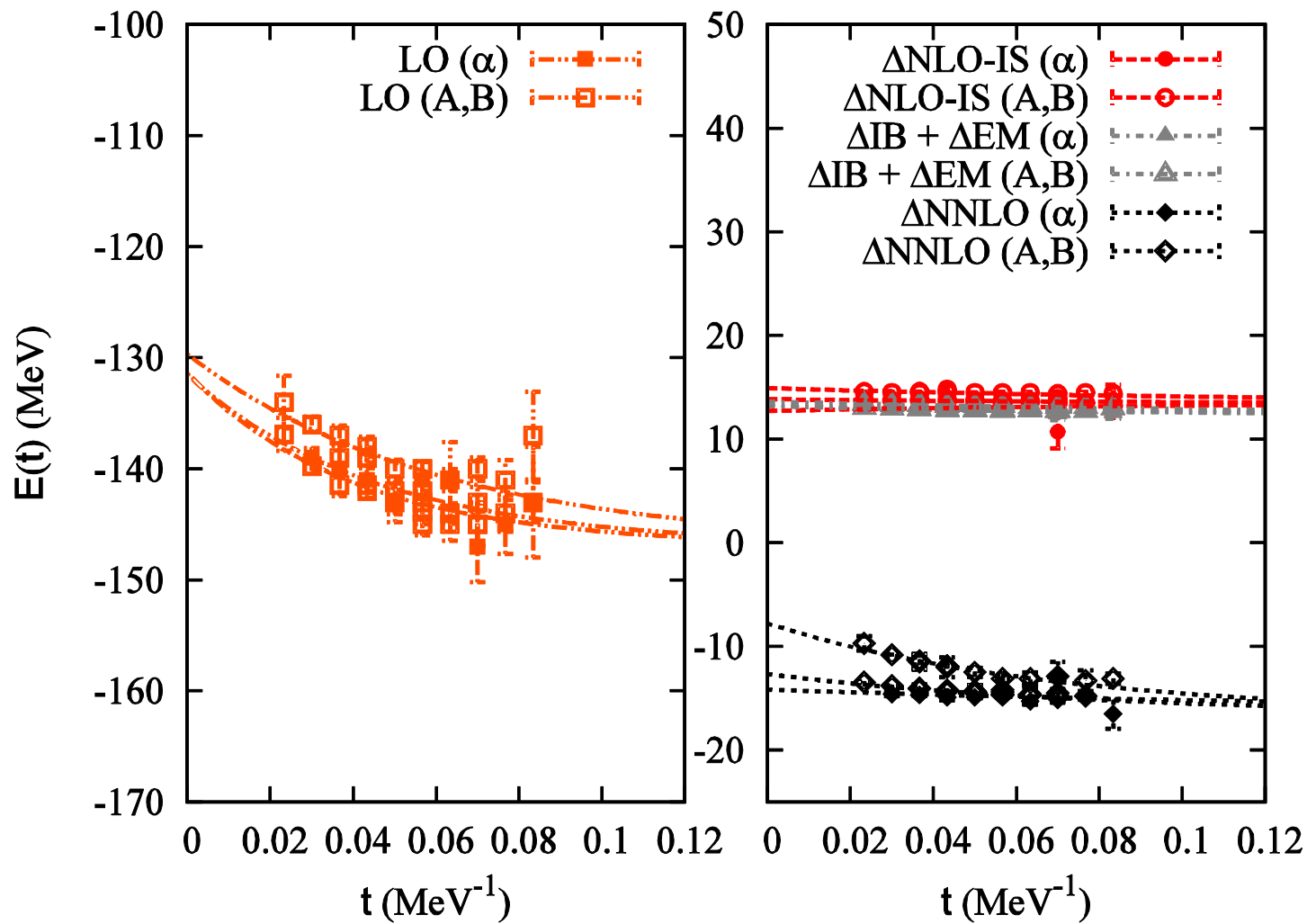
Preliminary: *Ab initio* lattice calculations up to  $A = 28$



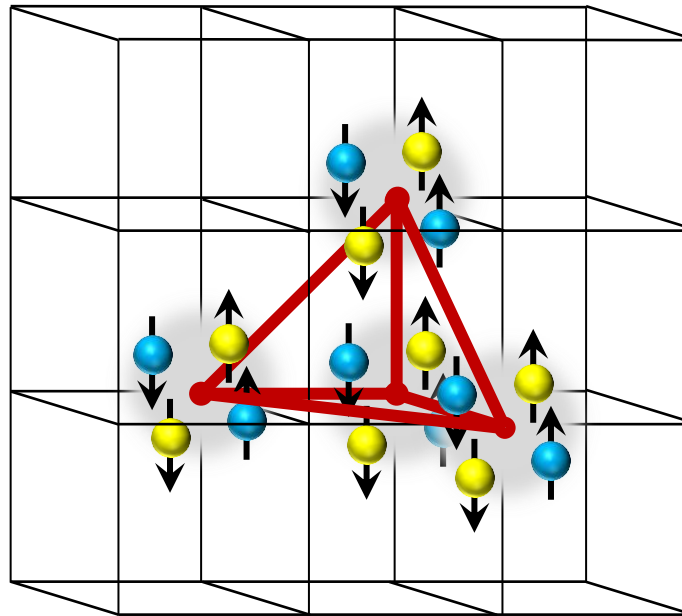




## Preliminary: Oxygen-16 structure and spectrum



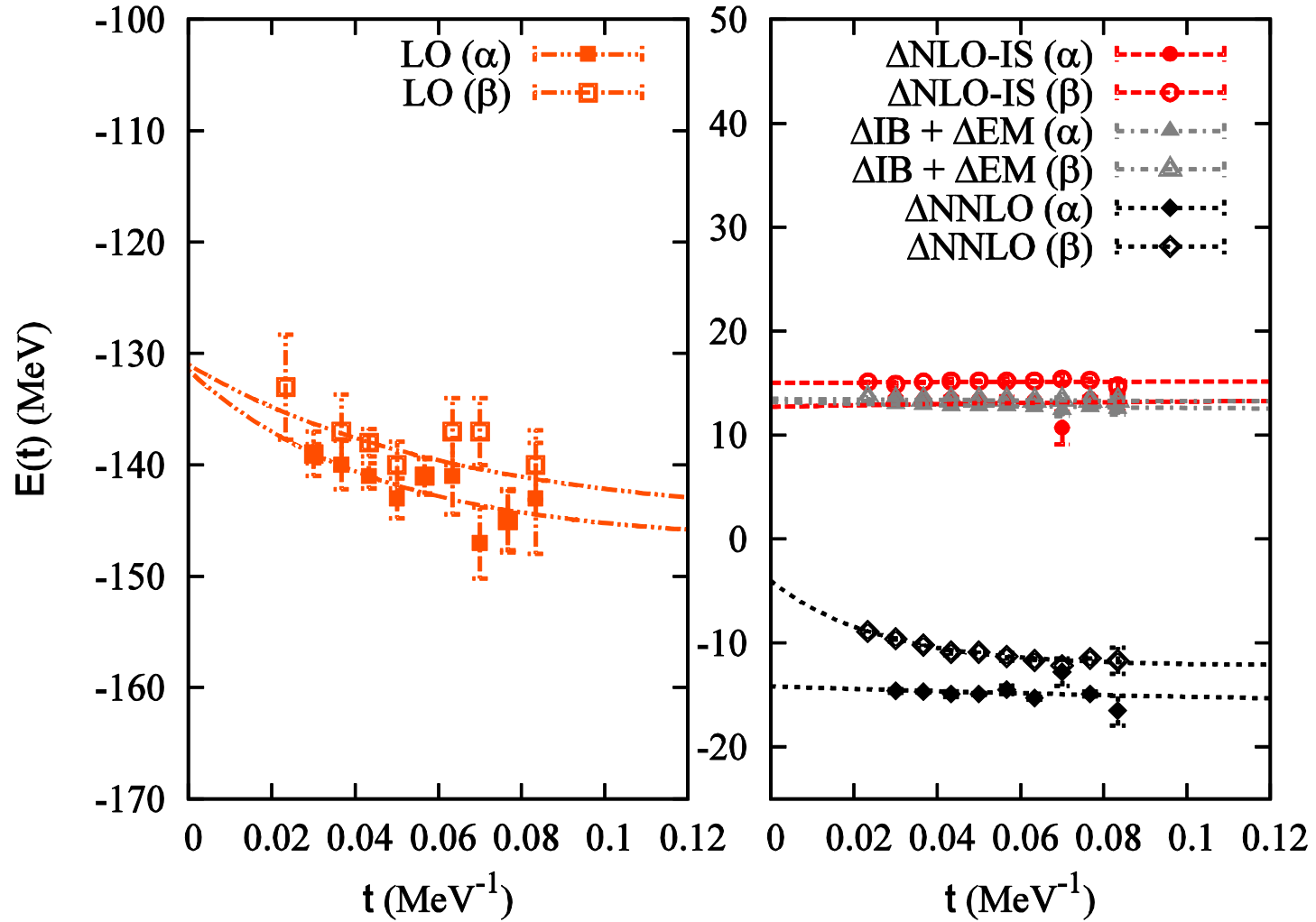
Tetrahedral cluster structure of first  $0^+$  and  $3^-$



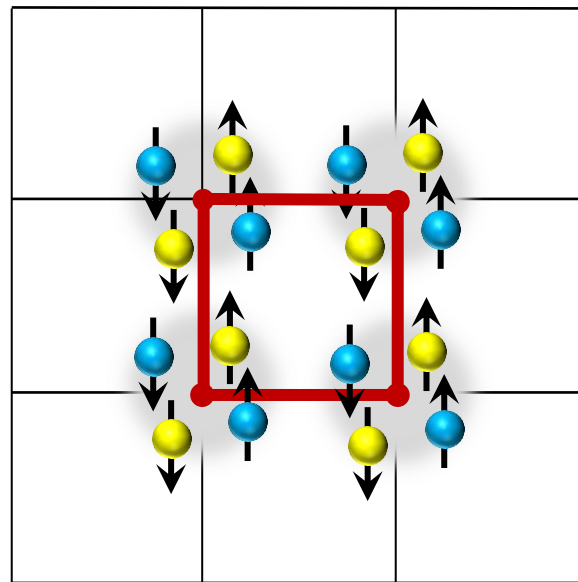
**8 rotational orientations**

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

## Finding the second $0^+$ state



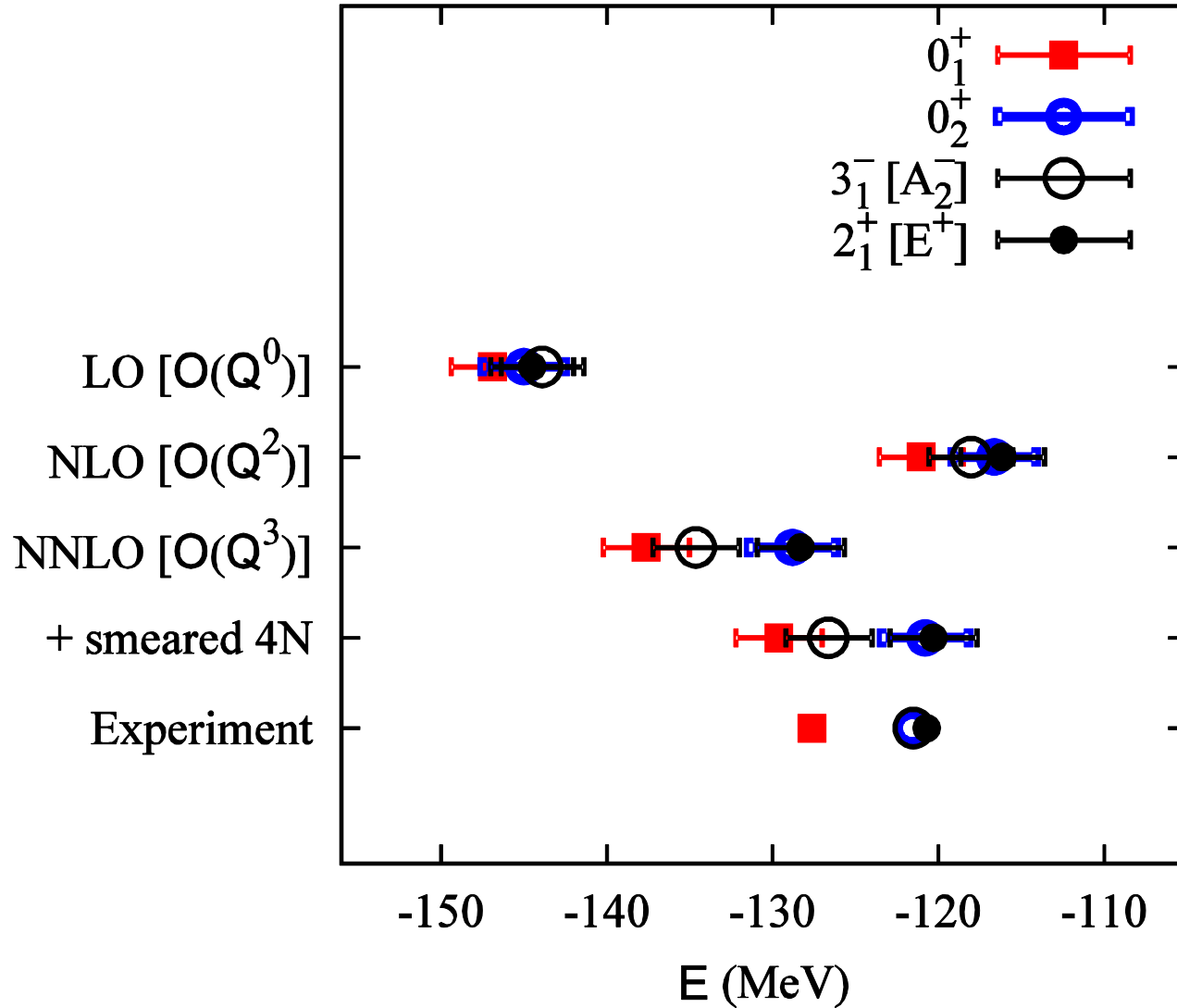
Cluster structure of second  $0^+$  state and first  $2^+$  state



**6 rotational orientations**

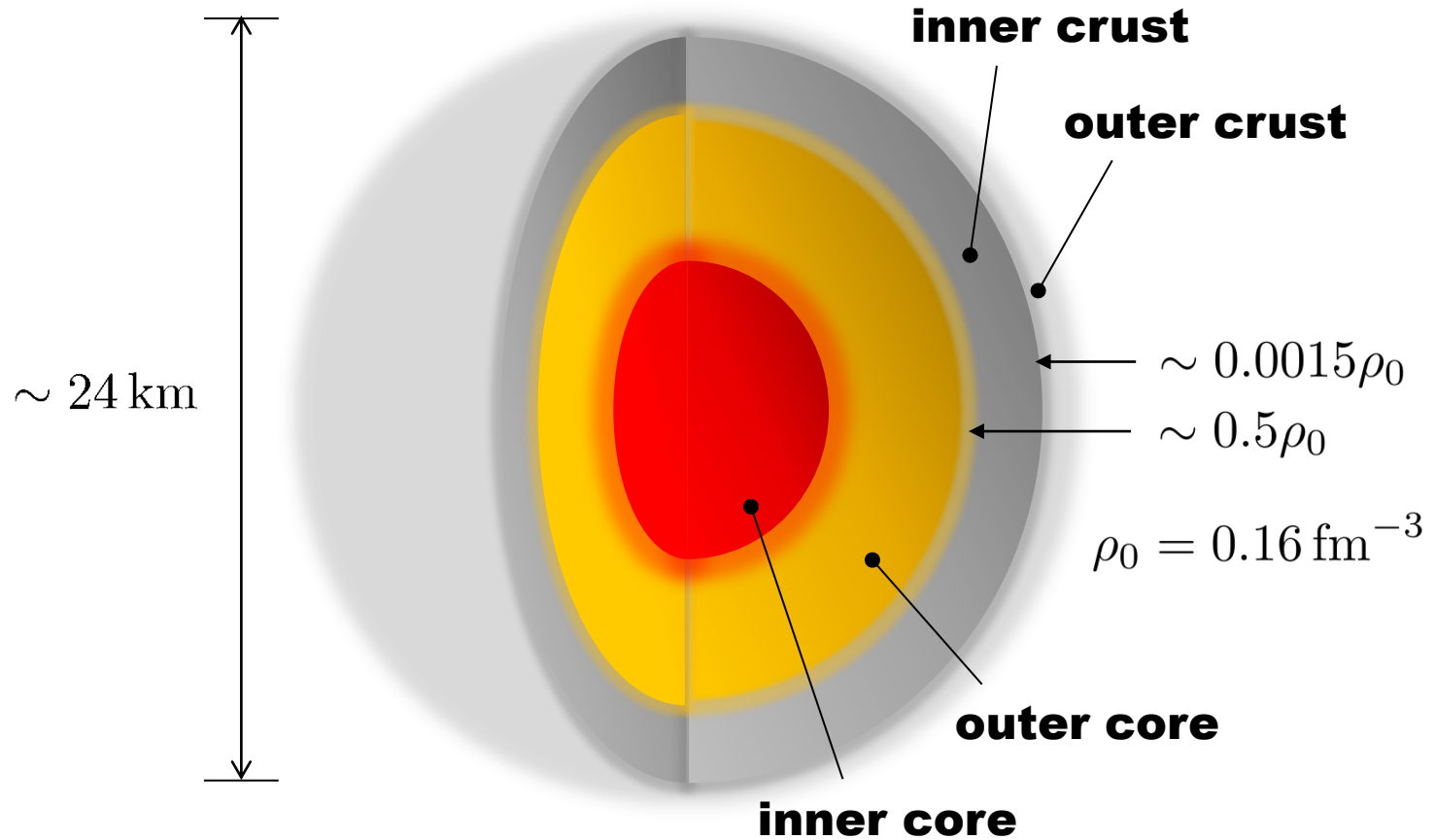
$$b = 1.97 \text{ fm}$$

# Low-lying spectrum of Oxygen-16

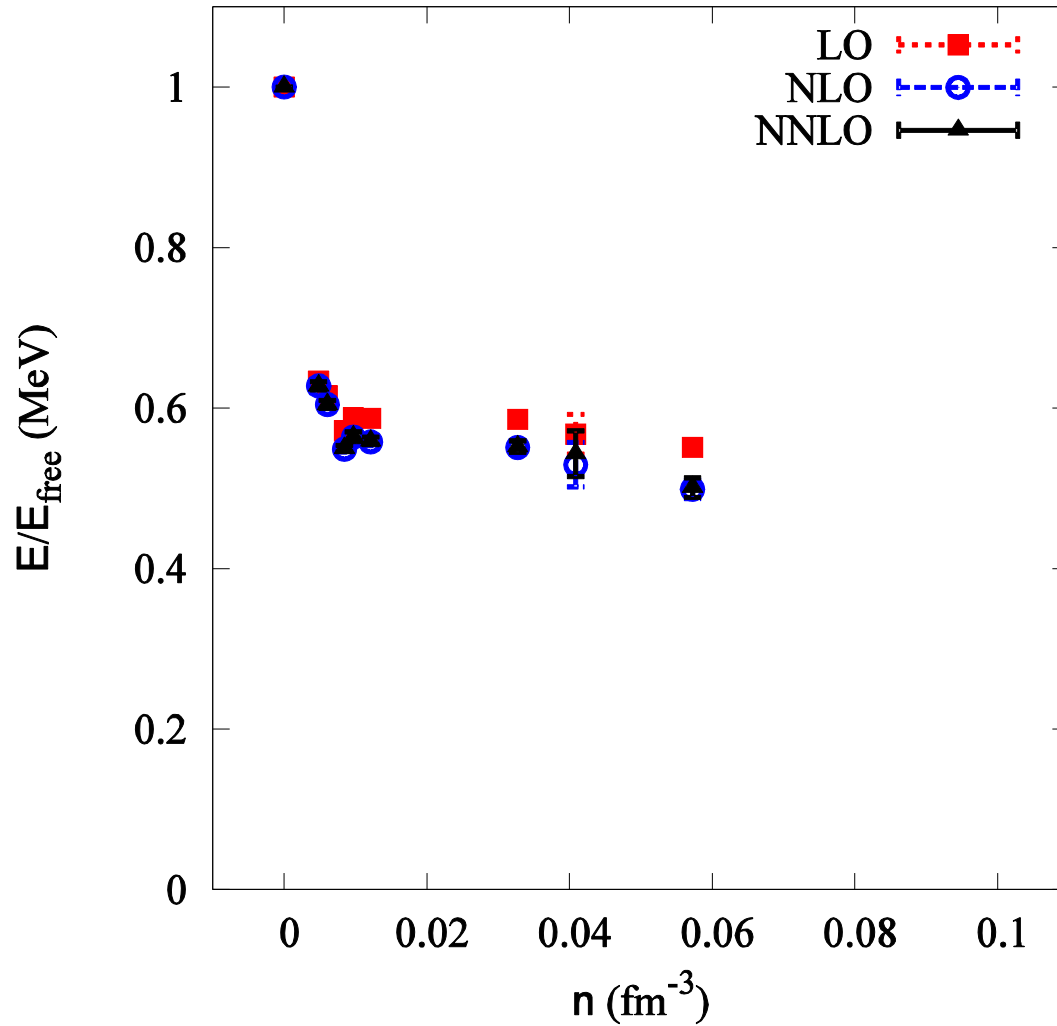


## Preliminary: Properties of neutron matter

### Neutron Star



## Energy of the ground state as fraction of free Fermi gas



See talks by  
Achim and Kai  
at this workshop

## Energy per neutron in the ground state

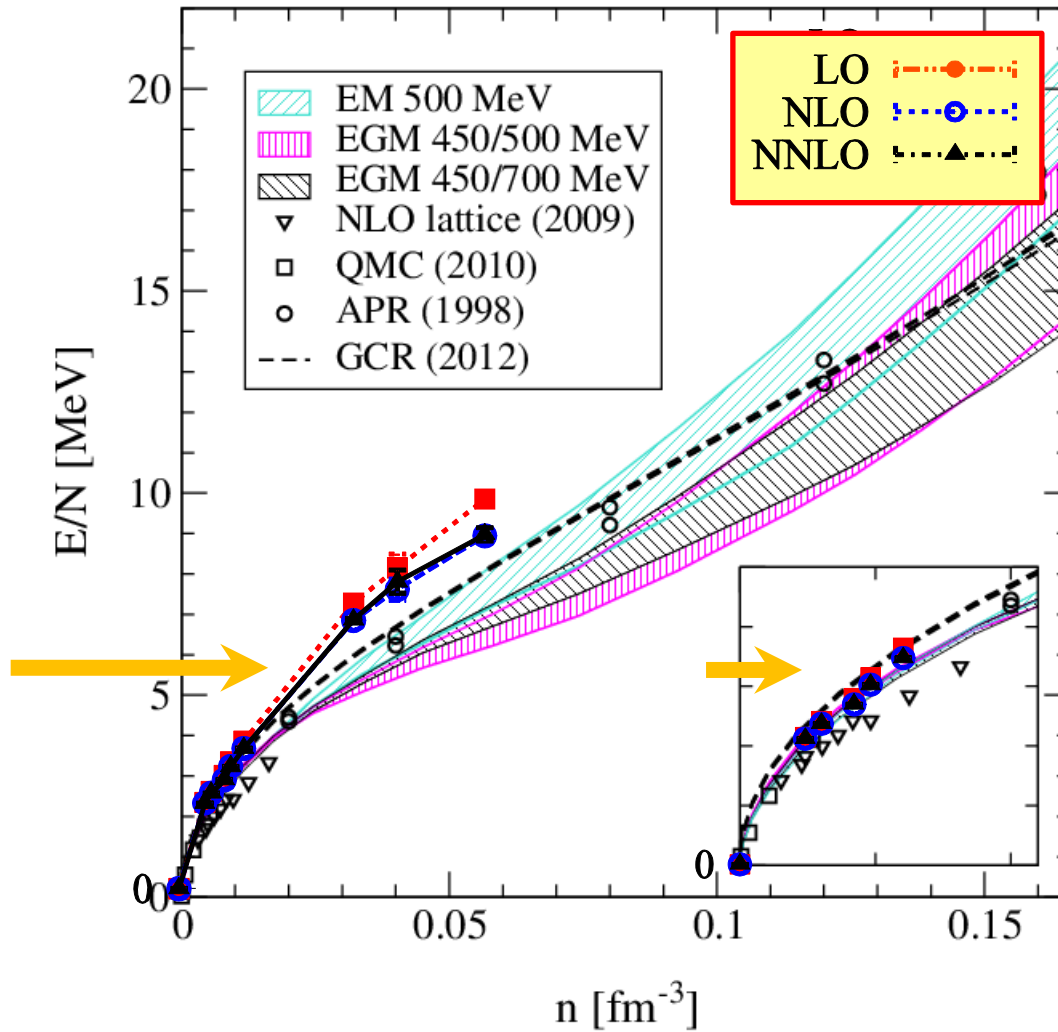


Figure adapted from Tews, et al., PRL 110 (2013) 032504



## Energy per neutron in the ground state

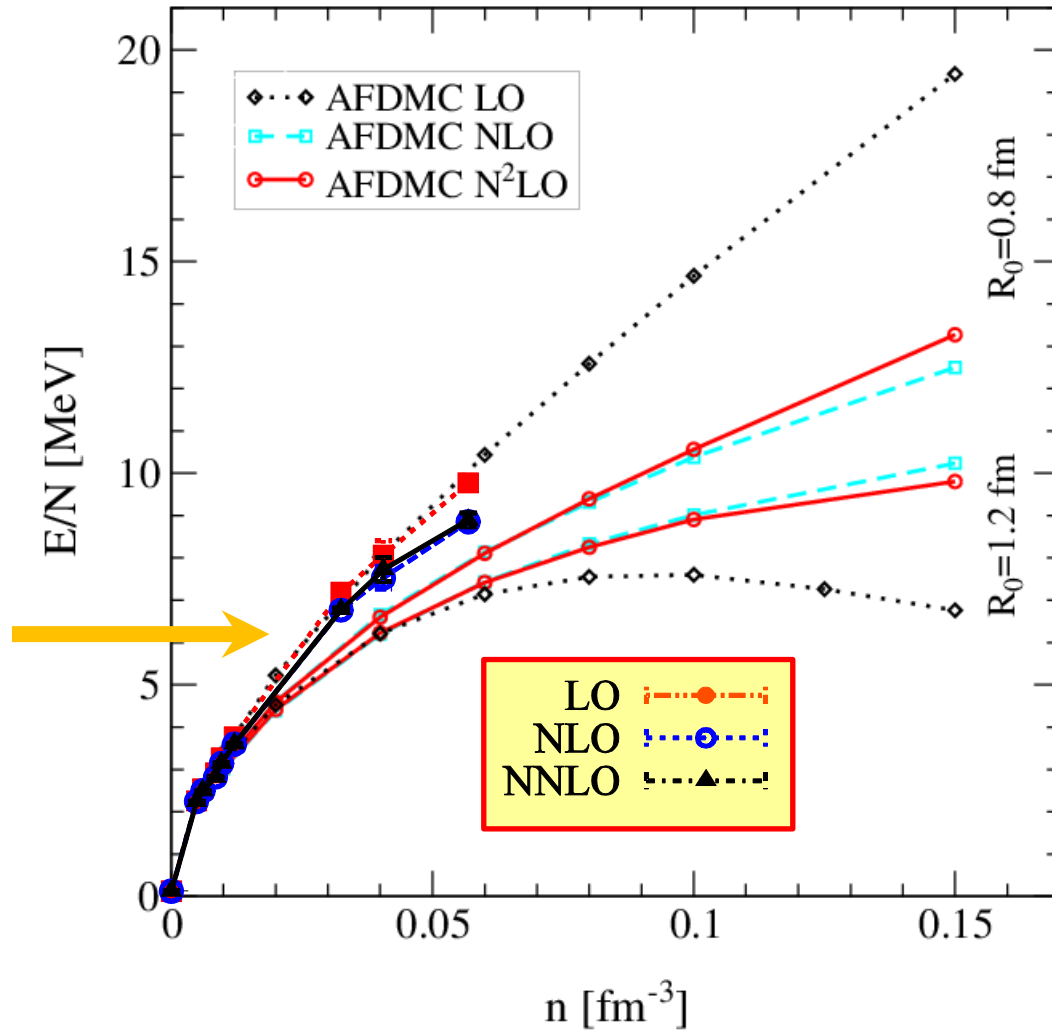
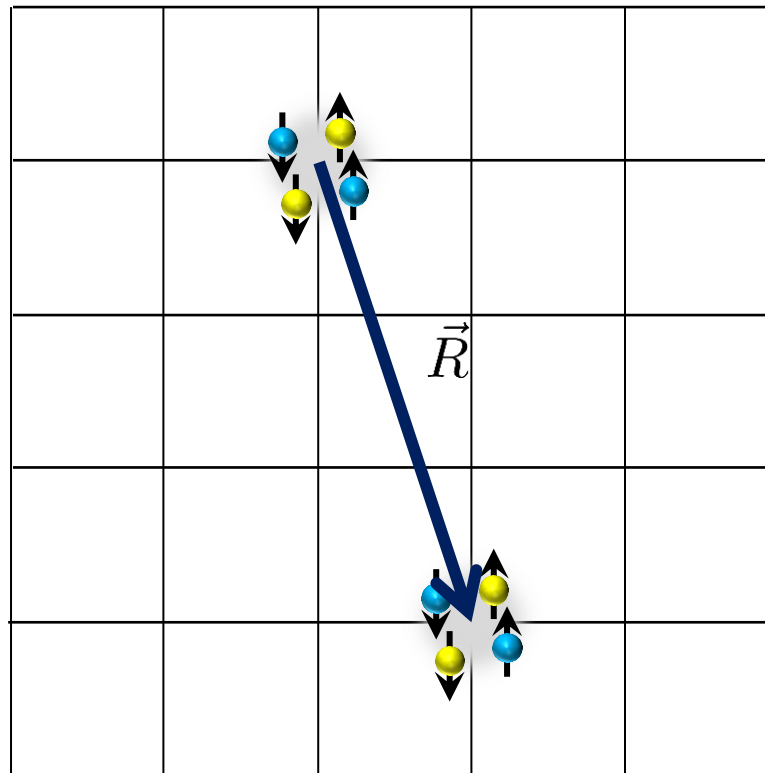


Figure adapted from Gezerlis, et al., arXiv: 1303.6243

# Preliminary: Scattering and reactions on the lattice

## Projected adiabatic matrix method



Using cluster  
wavefunctions  
for initial  
continuum  
scattering states

$$|\vec{R}\rangle$$

Use projection Monte Carlo to propagate cluster wavefunctions in Euclidean time

$$|\vec{R}\rangle_t = e^{-Ht} |\vec{R}\rangle$$

$$|\vec{R}\rangle_t = \left[ \text{blue grid} \right] \left[ \text{black grid} \right] |\vec{R}\rangle$$

Construct a norm matrix and matrix of expectation values

$$\langle N \rangle_t = {}_t \langle \vec{R}' | \vec{R} \rangle_t =$$

$$\langle \vec{R}' | \left[ \text{black grid} \right] \left[ \text{blue grid} \right] \left[ \text{black grid} \right] | \vec{R} \rangle$$

$$\langle O \rangle_t = {}_t \langle \vec{R}' | O | \vec{R} \rangle_t =$$

$$\langle \vec{R}' | \left[ \text{black grid} \right] \left[ \text{blue grid} \right] \left[ \text{yellow bar} \right] \left[ \text{blue grid} \right] \left[ \text{black grid} \right] | \vec{R} \rangle$$

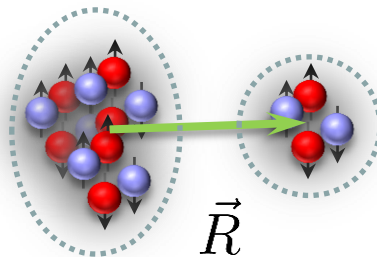
Compute the projected adiabatic matrix

$$\langle O \rangle_{\text{adiab}} = \langle N \rangle_t^{-1/2} \langle O \rangle_t \langle N \rangle_t^{-1/2}$$

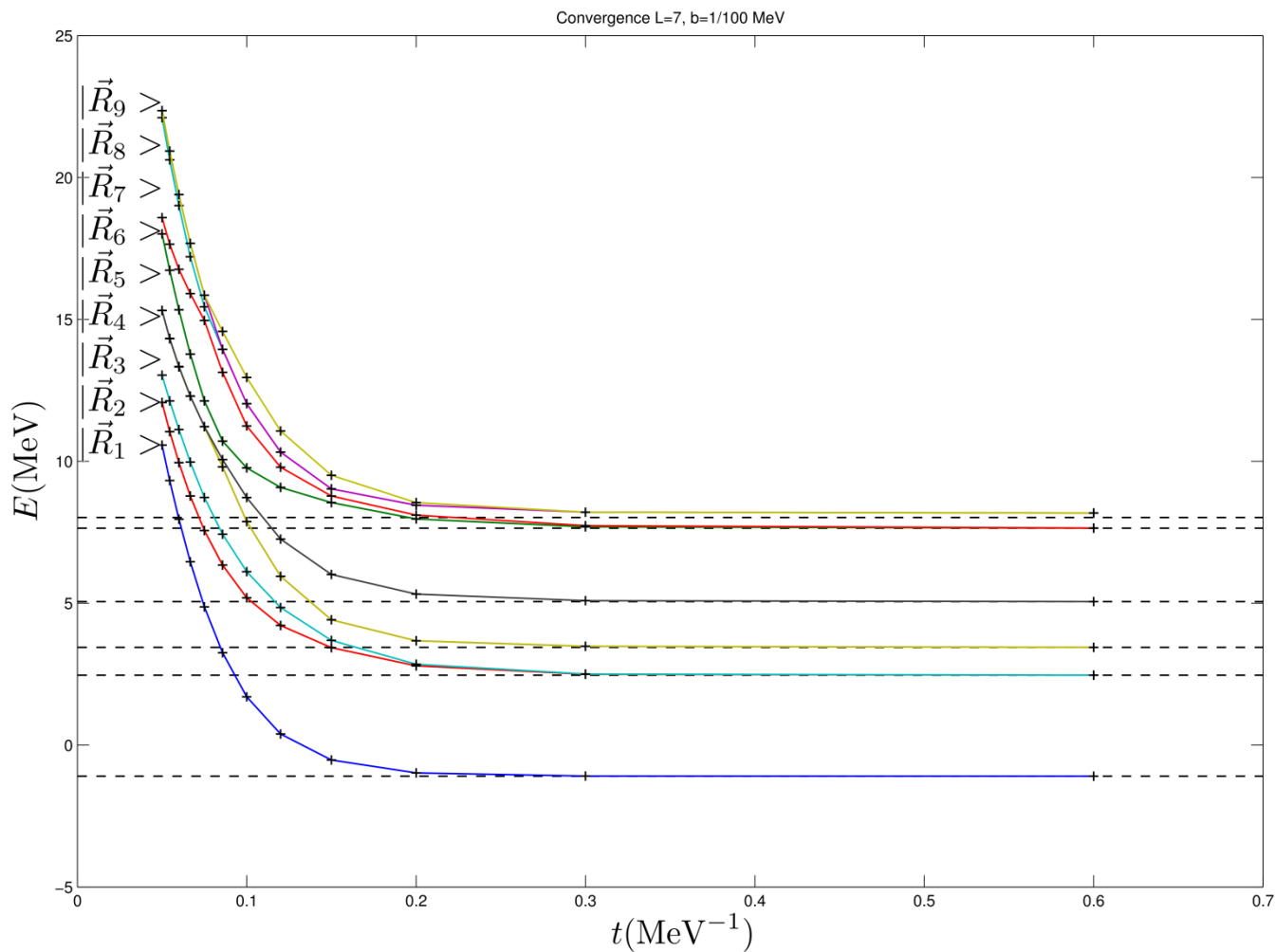
Projected adiabatic Hamiltonian is now an effective two-body Hamiltonian. Similar in spirit to no-core shell model with resonating group method.

See talk by Petr  
at this workshop

But some differences. Distortion of the nucleus wavefunctions is automatic due to projection in Euclidean time.

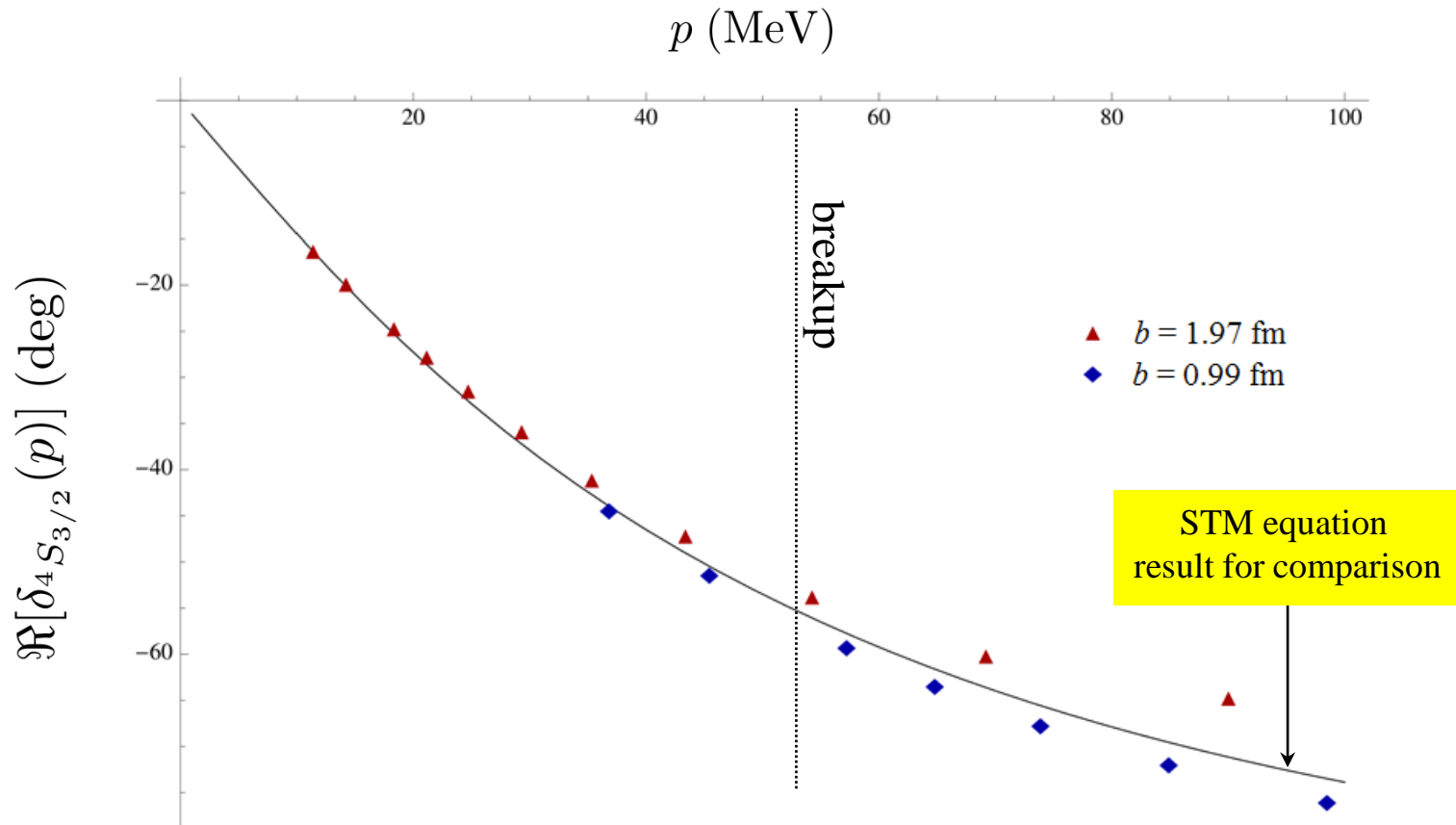


# Example: Quartet neutron-deuteron scattering



*Pine, D.L., Rupak, work in progress*

# Quartet neutron-deuteron scattering (pionless EFT at LO)



*Pine, D.L., Rupak, work in progress*

Use coupled channels for capture reactions and break up processes.

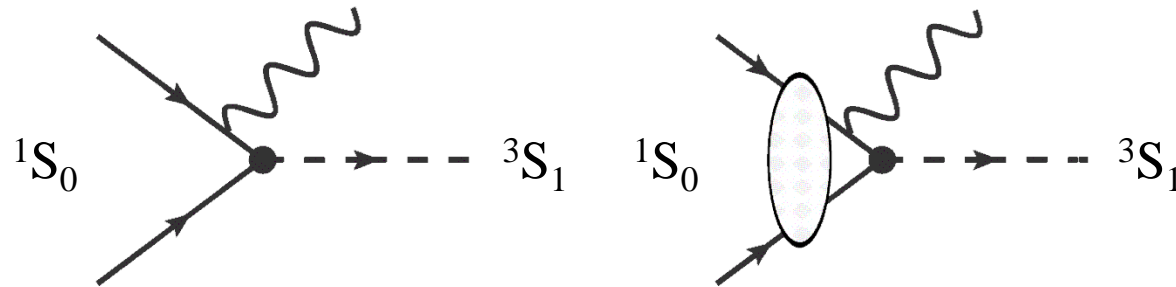
Lattice Green's function methods for radiative capture tested for  $n + p \rightarrow d + \gamma$  in pionless effective field theory at leading order.

Elastic scattering amplitude ( $^1S_0$  and  $^3S_1$ )

$$i\mathcal{A}_a(p) = \text{Diagram 1} + \text{Diagram 2} + \dots$$

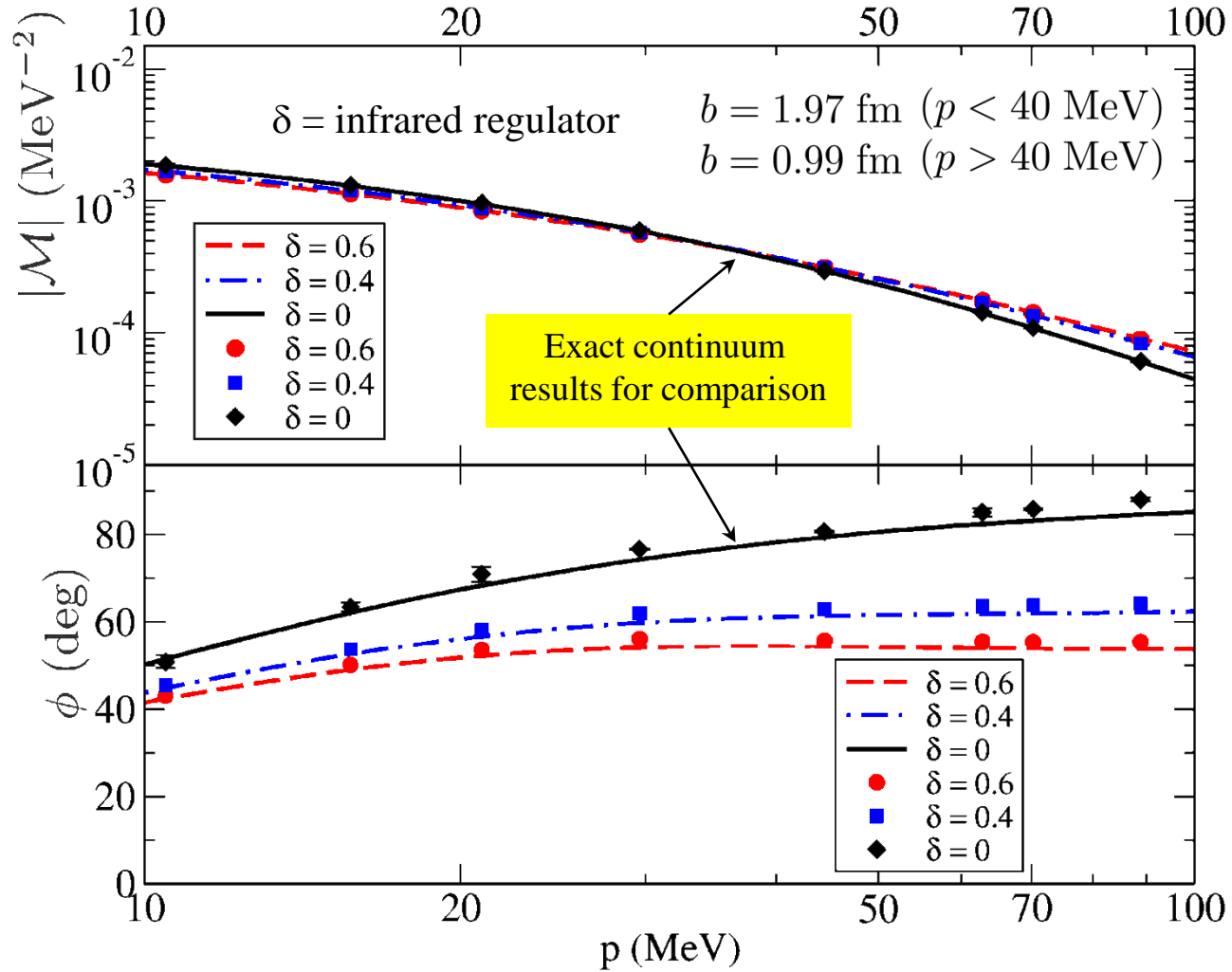
The equation shows the expansion of the elastic scattering amplitude  $i\mathcal{A}_a(p)$ . The first term is a contact interaction represented by a black dot with four external lines (two incoming, two outgoing) and a label  $-iC_a$  below it. The second term is a loop diagram with two such vertices connected by two internal lines forming a loop, also labeled  $-iC_a$  for each vertex. The series continues with  $+\dots$ .

M1 radiative capture amplitude



Rupak, D.L., arXiv:1302.4158 [nucl-th]

# M1 transition amplitude $n + p \rightarrow d + \gamma$



Rupak, D.L., arXiv:1302.4158 [nucl-th]



## Summary

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.

*Additional topics to be addressed in the near future...*

Different lattice spacings,  $N \neq Z$  nuclei, transition from S-wave to P-wave pairing in superfluid neutron matter, etc.