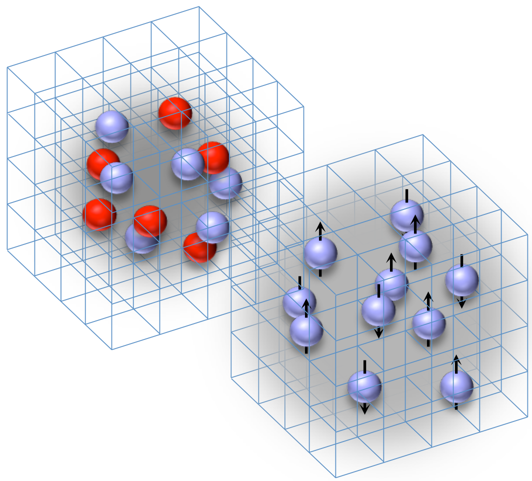
Ab initio nuclear structure from lattice effective field theory



Nuclear Lattice EFT Collaboration

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Computational Challenges in Nuclear and Many-Body Physics

Nordita, Stockholm

October 6, 2014

Outline

What is lattice effective field theory?

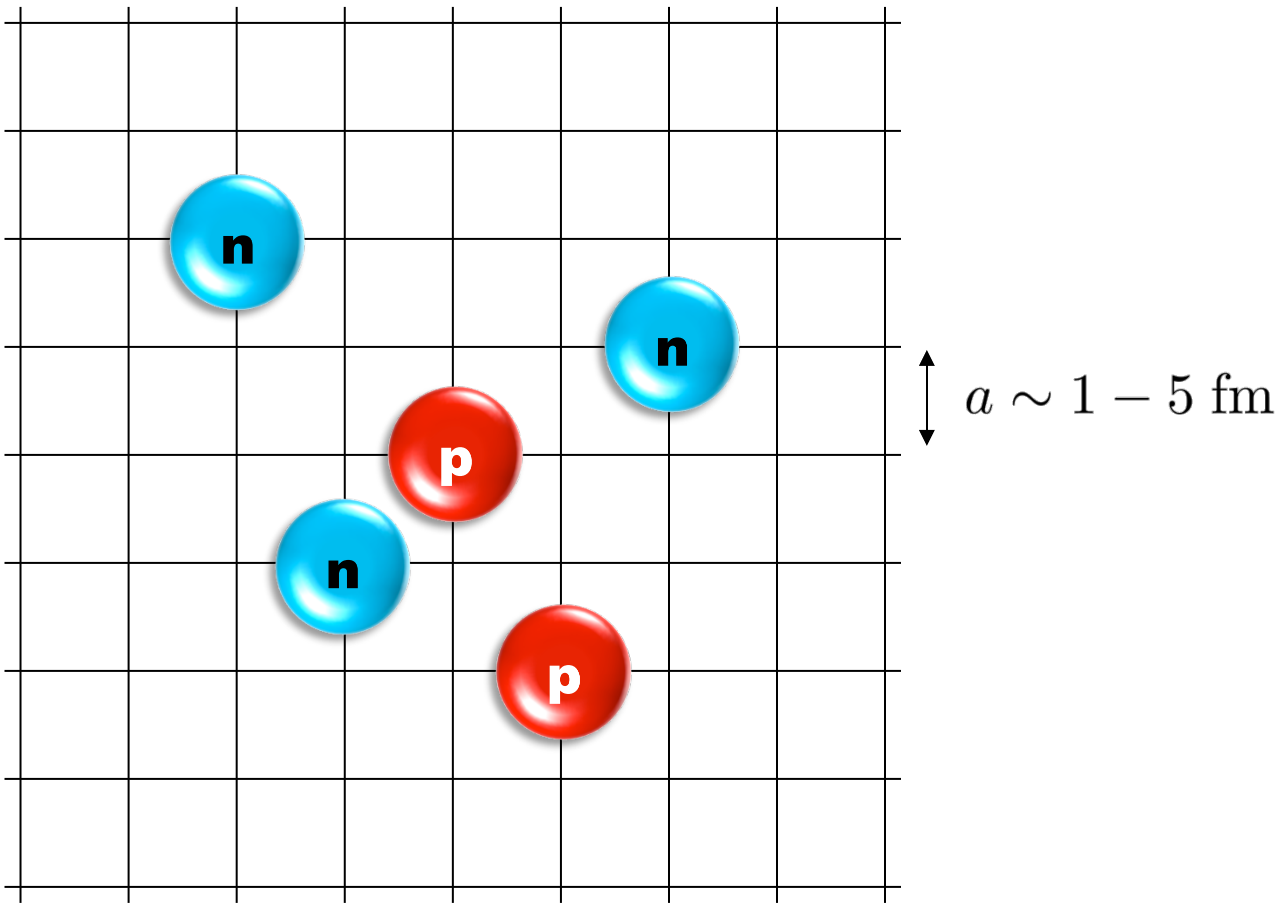
Carbon-12 spectrum and the Hoyle state

Oxygen-16 structure and spectrum

Light quark mass dependence of helium burning

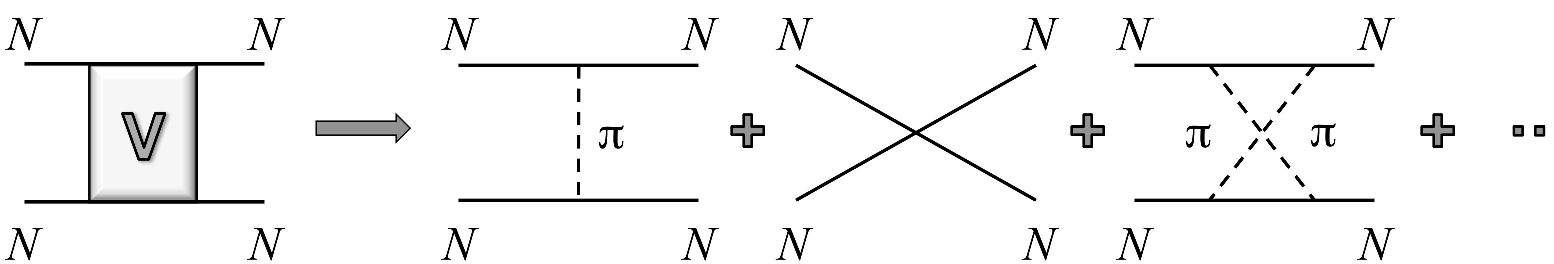
Summary and future directions

Lattice effective field theory



Low energy nucleons: Chiral effective field theory

Construct the effective potential order by order



V^{OPEP} Contact interactions V^{TPEP}

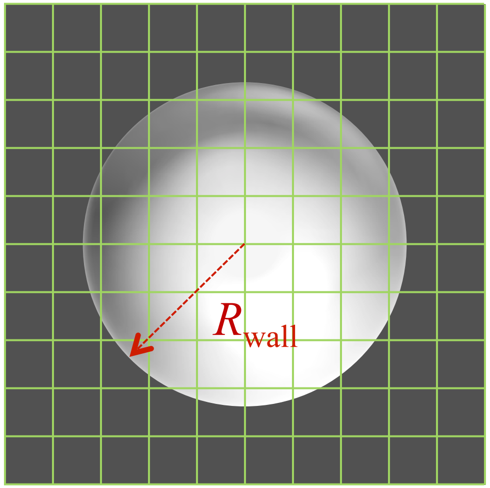
$\underbrace{V^{\mathrm{OPEP}} \quad \text{Contact interactions}}_{\text{Leading order (LO)}} \quad \underbrace{V^{\mathrm{TPEP}}}_{\text{Next-to-leading order (NLO)}}$

Physical scattering data → Unknown operator coefficients

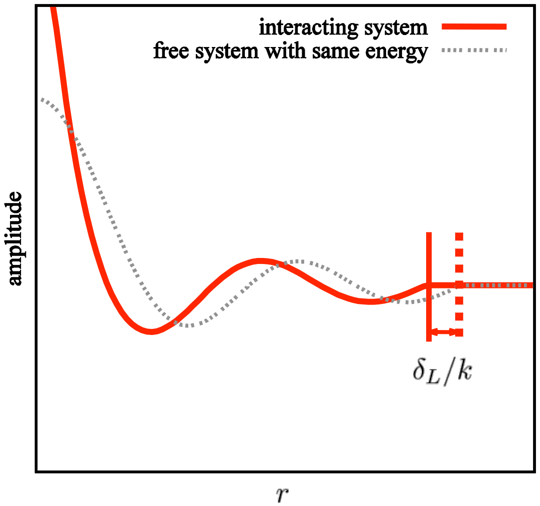
<u>Spherical wall method</u>

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

Spherical wall imposed in the center of mass frame

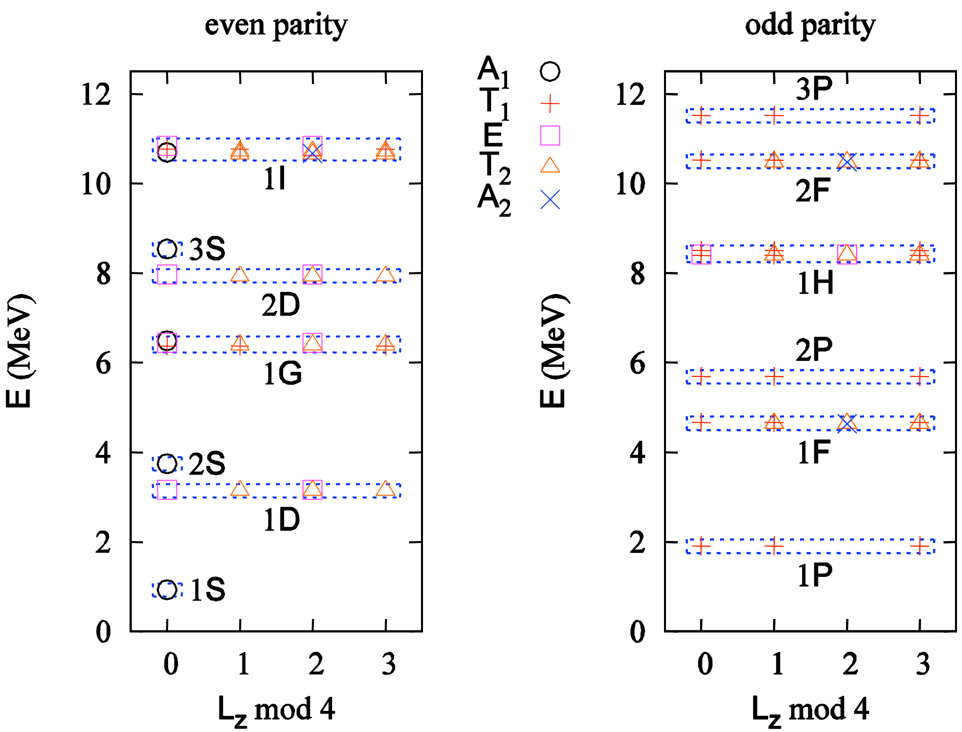


Representation	J_z	Example
A_1	$0 \bmod 4$	$Y_{0,0}$
T_1	$0, 1, 3 \bmod 4$	$\{Y_{1,0}, Y_{1,1}, Y_{1,-1}\}$
E	$0, 2 \bmod 4$	$\left\{Y_{2,0}, \frac{Y_{2,-2}+Y_{2,2}}{\sqrt{2}}\right\}$
T_2	$1, 2, 3 \bmod 4$	$\left\{Y_{2,1}, \frac{Y_{2,-2}-Y_{2,2}}{\sqrt{2}}, Y_{2,-1}\right\}$
A_2	$2 \bmod 4$	$\frac{Y_{3,2}-Y_{3,-2}}{\sqrt{2}}$



Energy levels with spherical wall

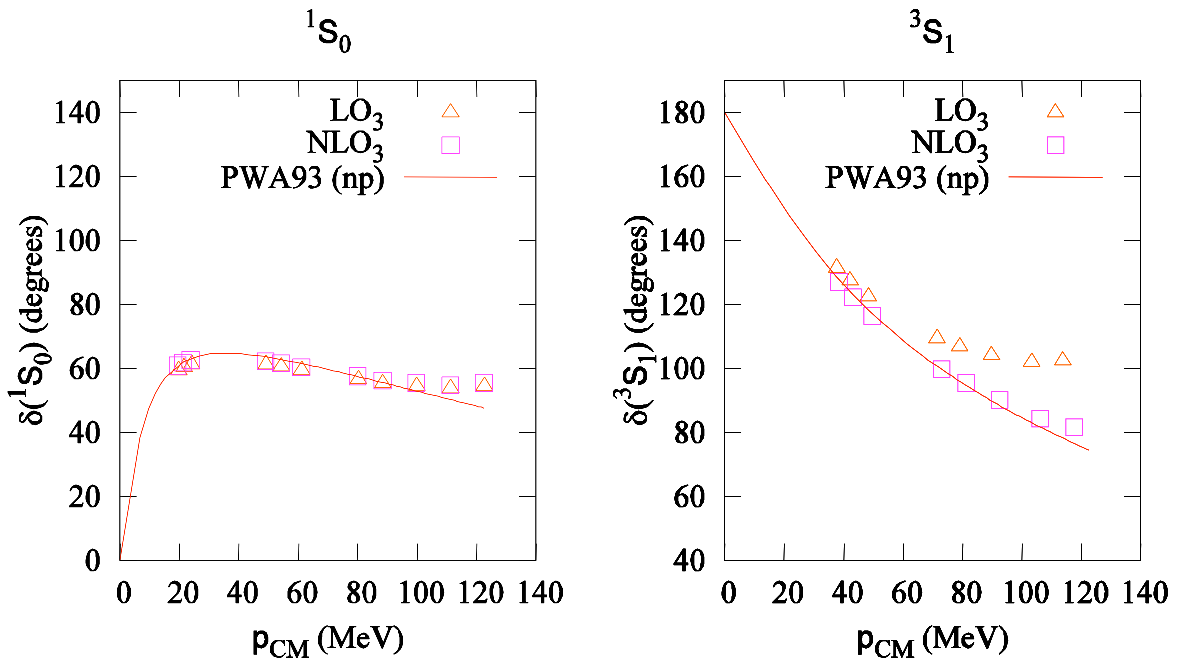
$$R_{\text{wall}} = 10a$$
$$a = 1.97 \text{ fm}$$



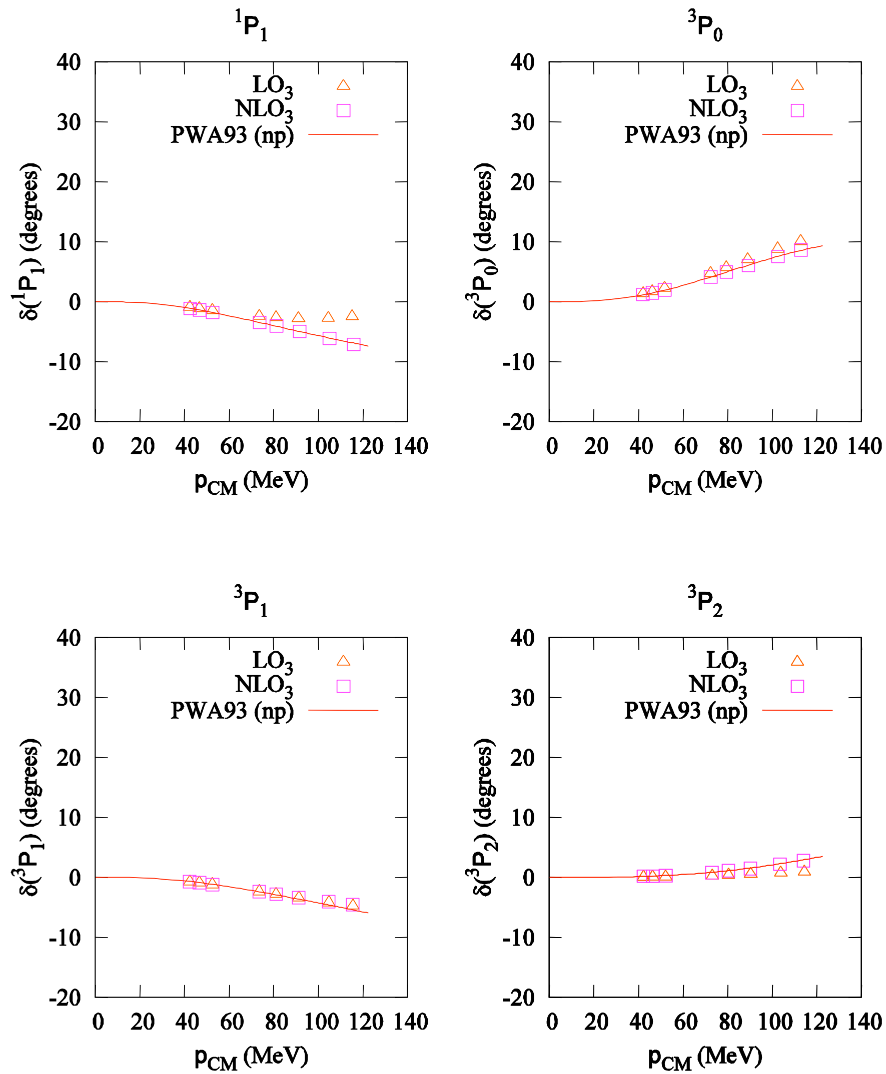
Energy shift from free-particle values gives the phase shift

Nucleon-nucleon phase shifts

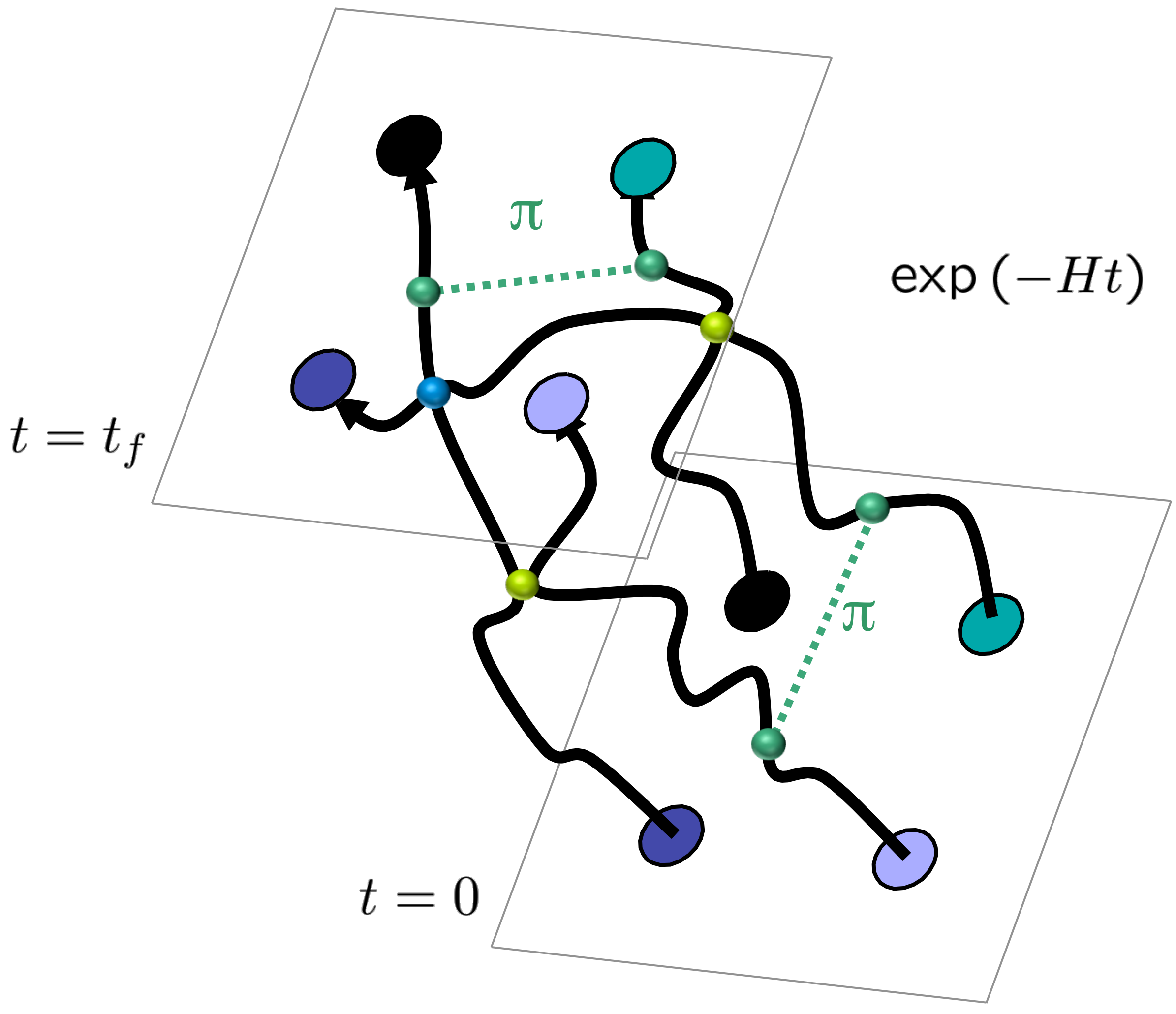
S waves $a = 1.97$ fm



P waves $a = 1.97$ fm



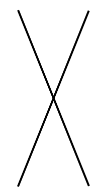
Euclidean time projection



Auxiliary field method

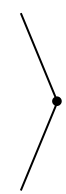
We can write exponentials of the interaction using a Gaussian integral identity

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



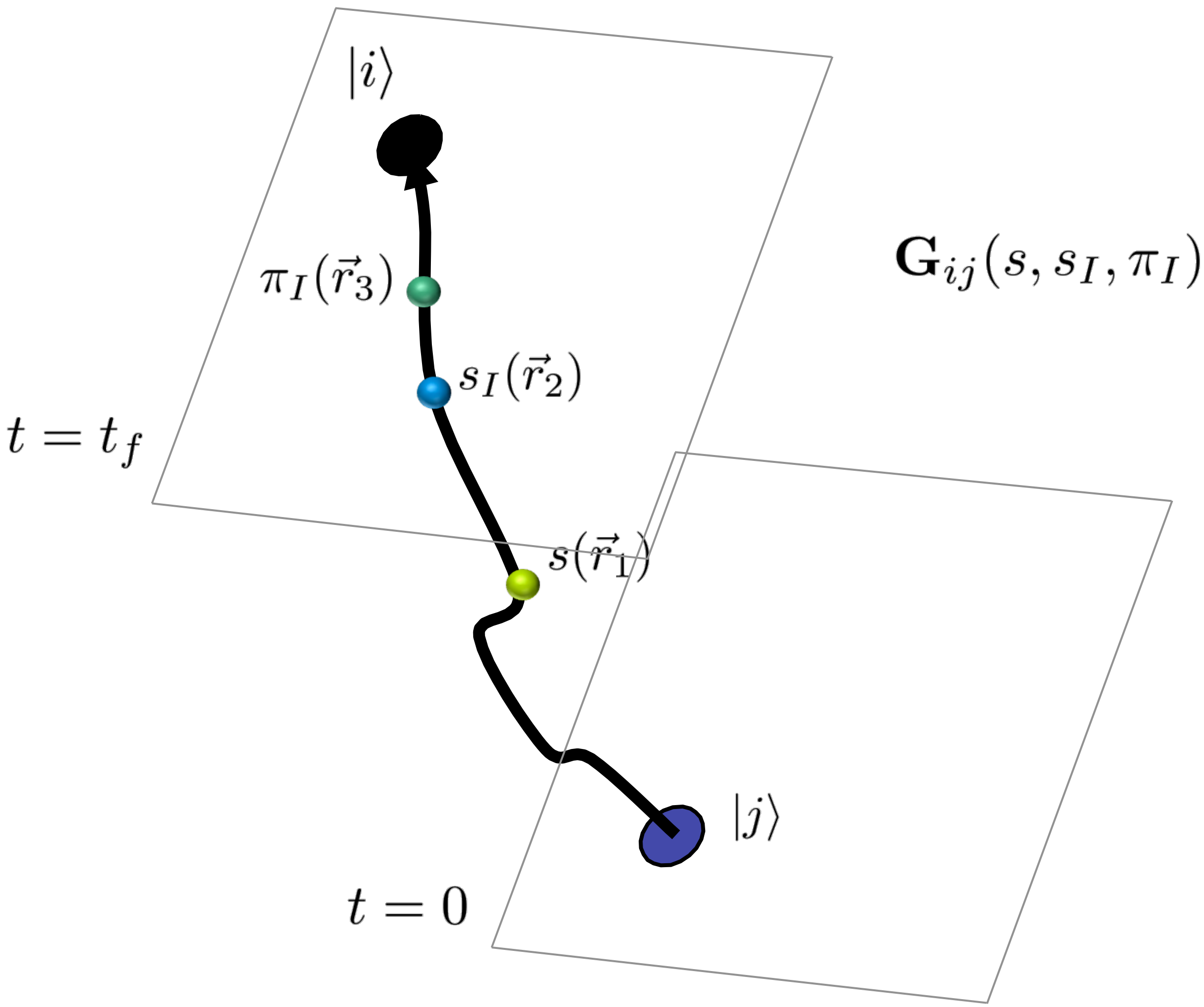
$(N^\dagger N)^2$

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

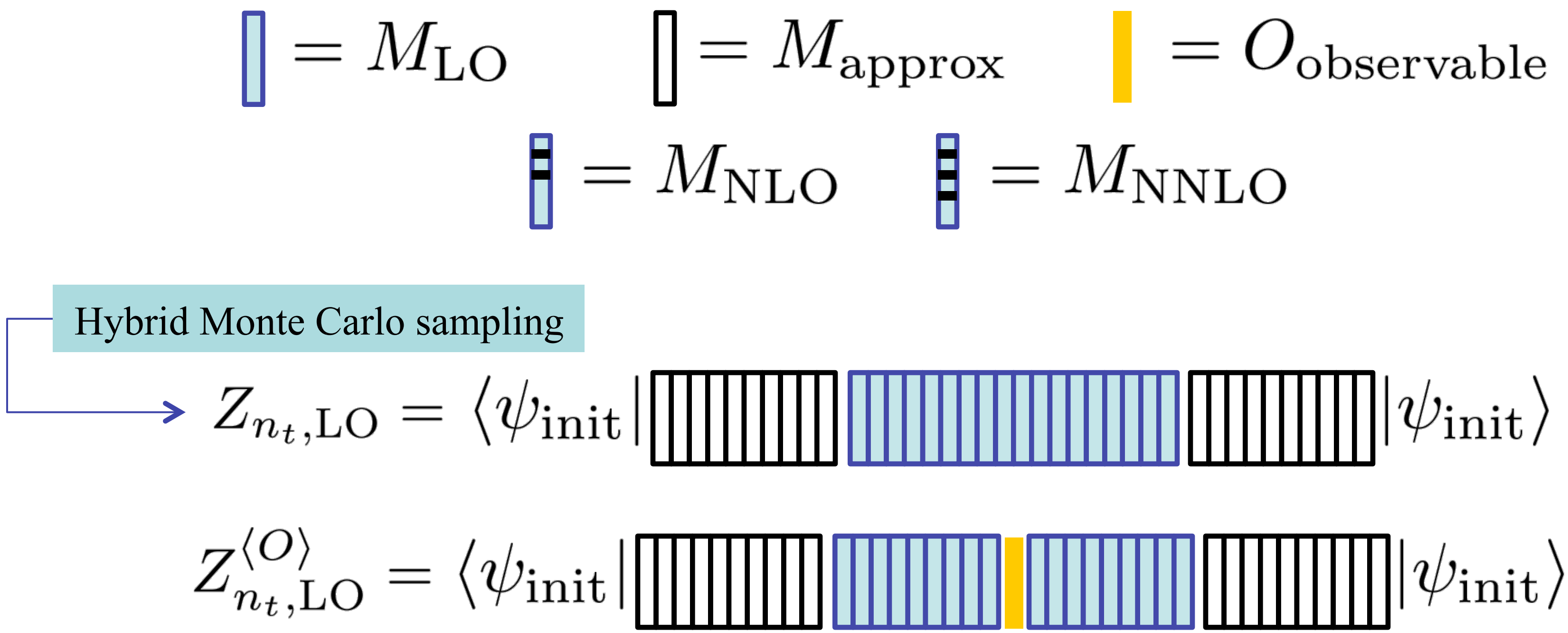


$sN^\dagger N$

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

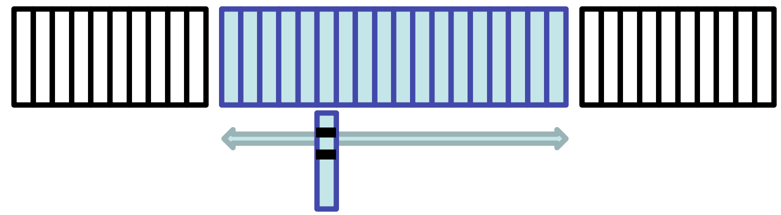

$|i\rangle$
$\mathbf{G}_{ij}(s, s_I, \pi_I)$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$t = t_f$
$s(\vec{r}_1)$
$|j\rangle$
$t = 0$

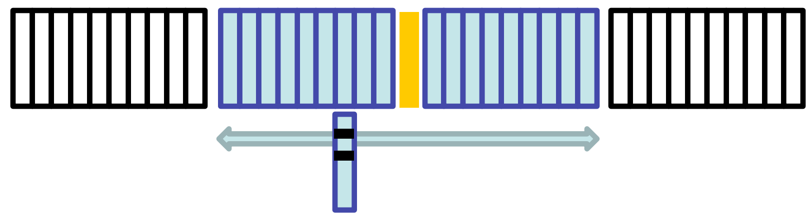
Schematic of lattice Monte Carlo calculation



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

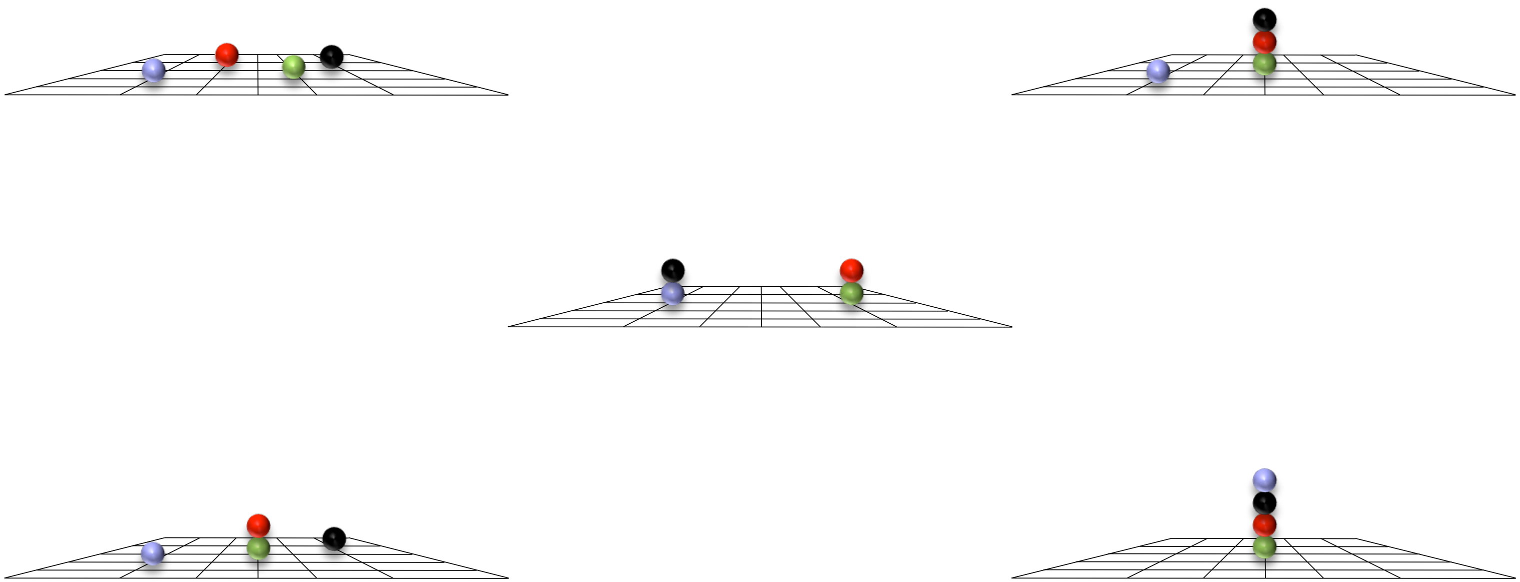
$$\langle O \rangle_{0,\mathrm{LO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

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

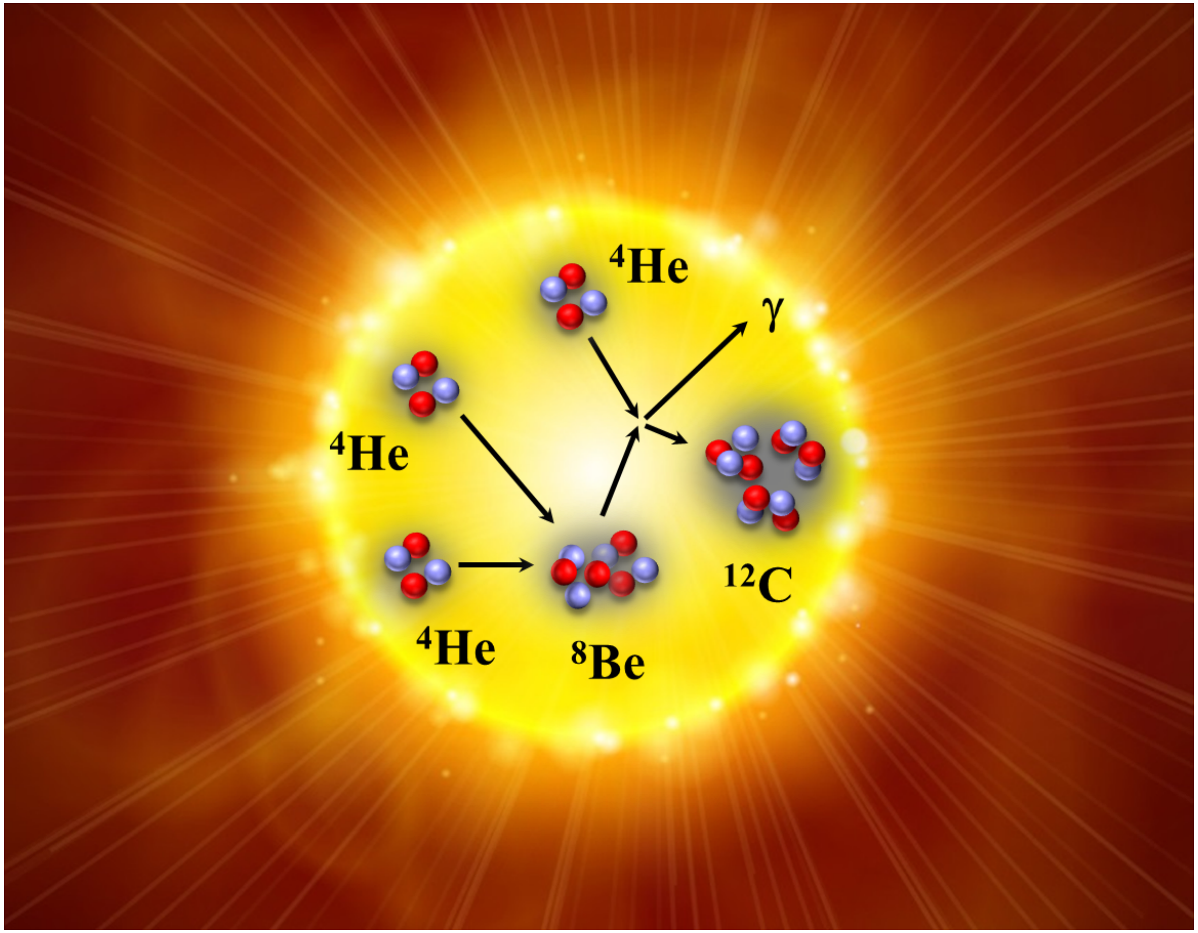
$Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$  $| \psi_{\mathrm{init}} \rangle$

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

<u>Particle clustering included automatically</u>

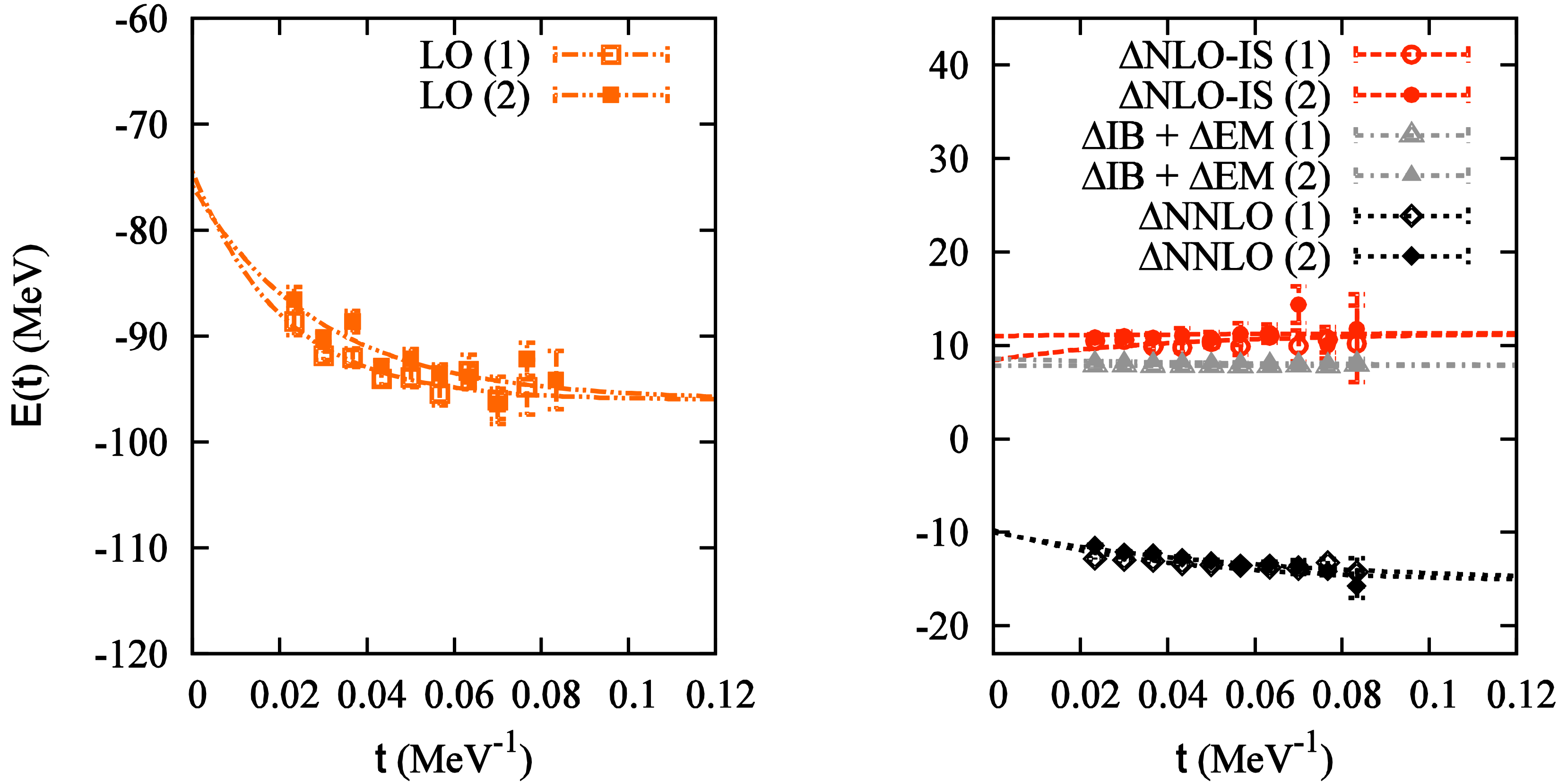


Carbon-12 spectrum and the Hoyle state



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

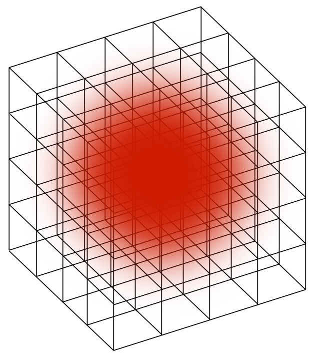
Ground state of Carbon-12

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

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

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

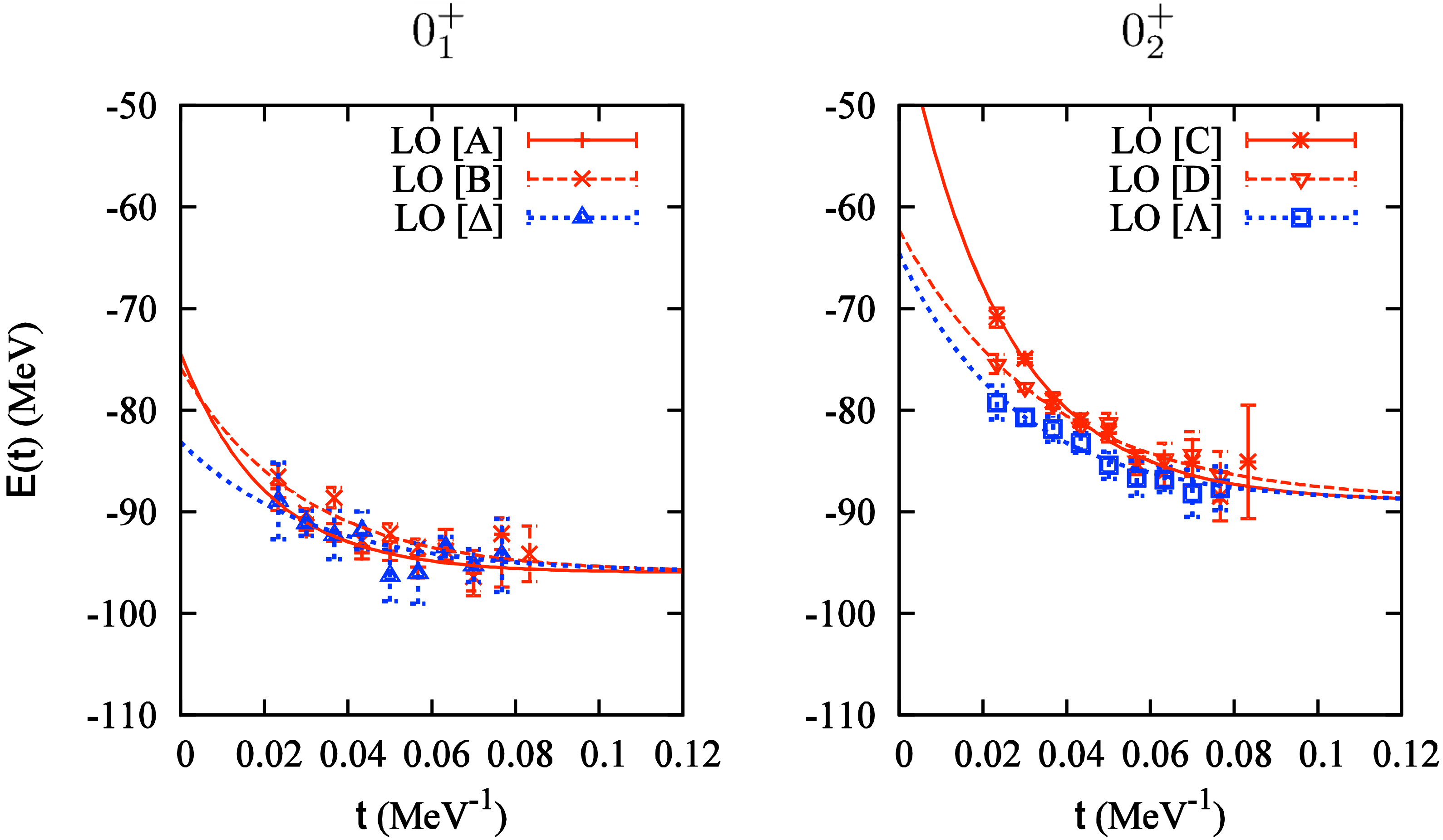
$$\psi_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m})^2]$$
$$\psi_j'(\vec{n}) = \exp[-c(\vec{n} - \vec{m}')^2]$$
$$\psi_j''(\vec{n}) = \exp[-c(\vec{n} - \vec{m}'')^2]$$
$$\vdots$$

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.

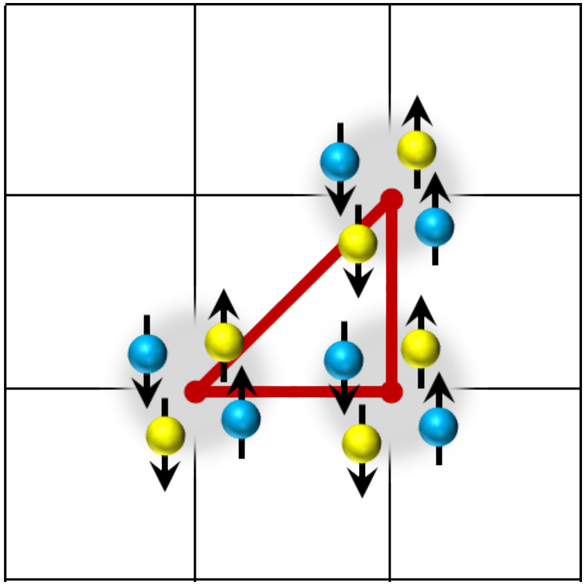
But can reproduce same results starting directly from alpha cluster wavefunctions [Δ and Λ in plots on next slide].



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

Structure of ground state and first 2^+

Strong overlap with compact triangle configuration

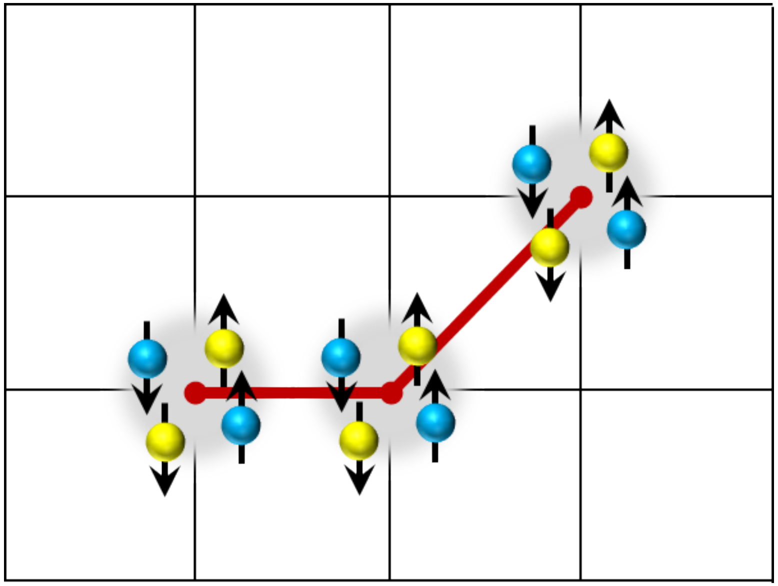


12 rotational orientations

$b = 1.97$ fm

Structure of Hoyle state and second 2+

Strong overlap with bent arm configuration



24 rotational orientations

$b = 1.97$ 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

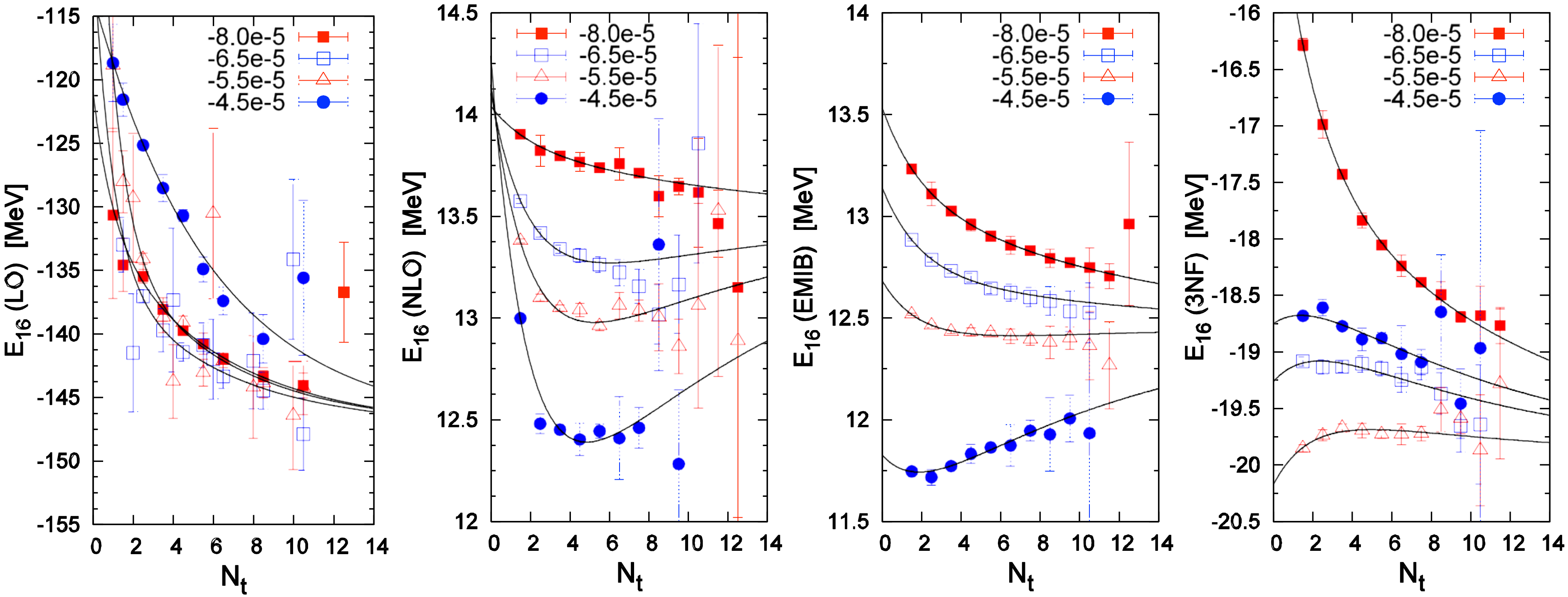
D – Itoh et al., PRC 84 (2011) 054308

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

Oxygen-16

Oxygen-16 ground state

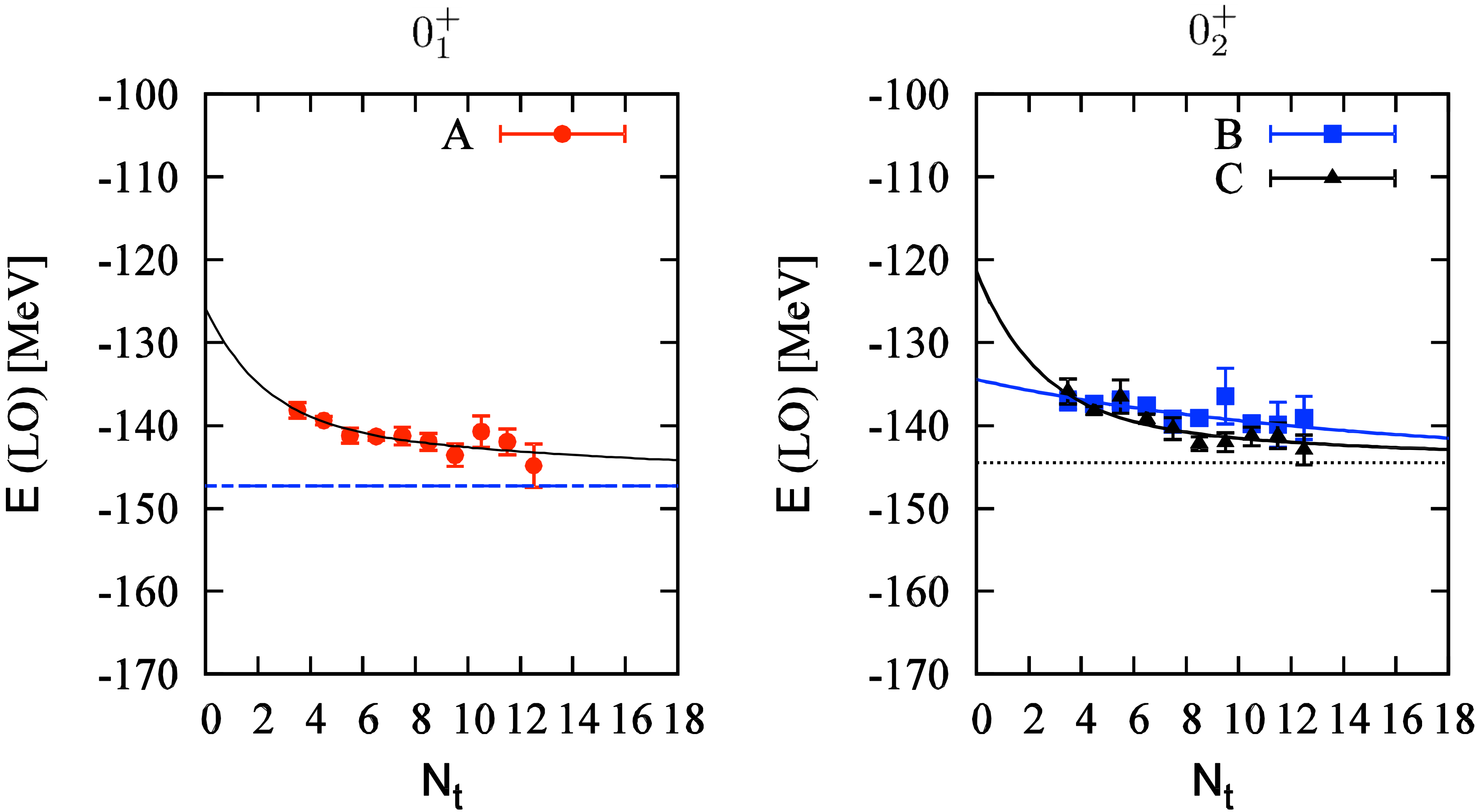
LO NLO EM & IB 3NF



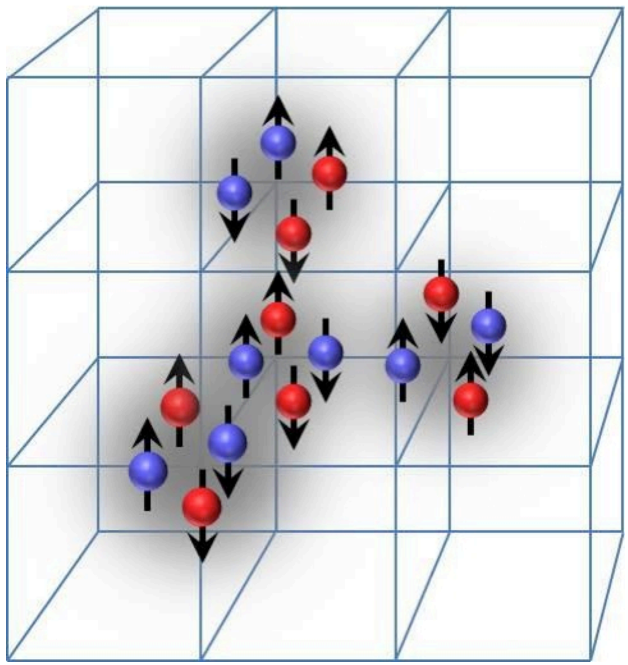
$$a = 1.97\,\mathrm{fm}$$

Epelbaum, Krebs, Lähde, D.L, Meißner, Rupak, PRL112, 102501 (2014)

Oxygen-16 spectrum and structure

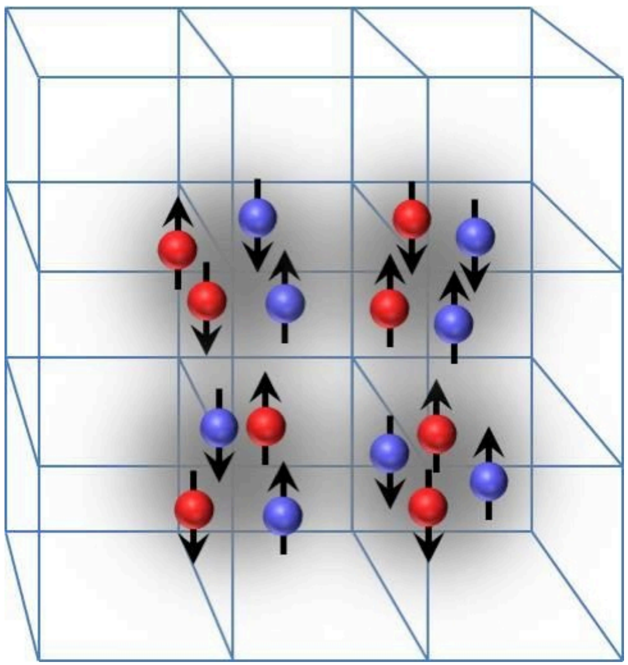


0_1^+

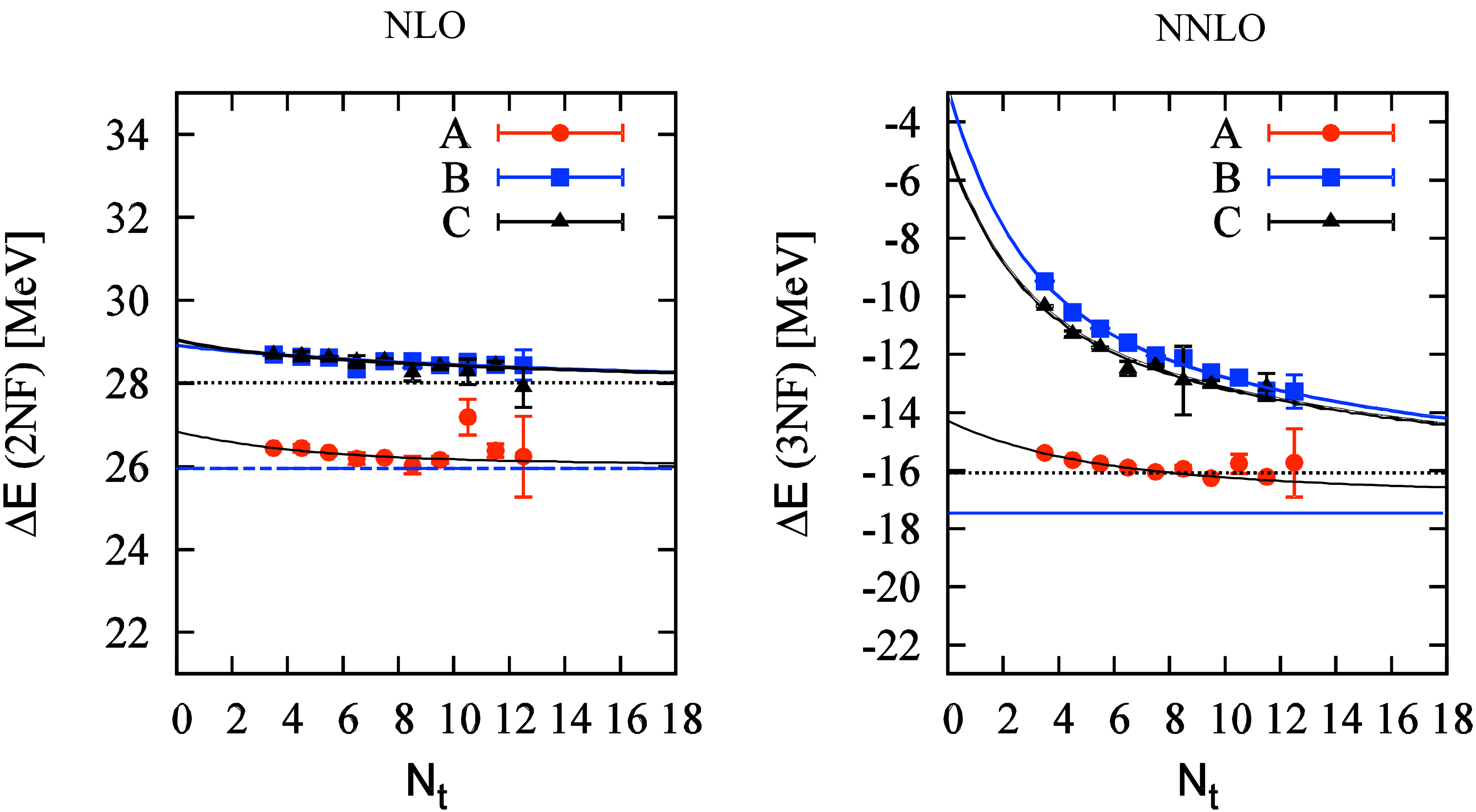


A - Tetrahedral structure

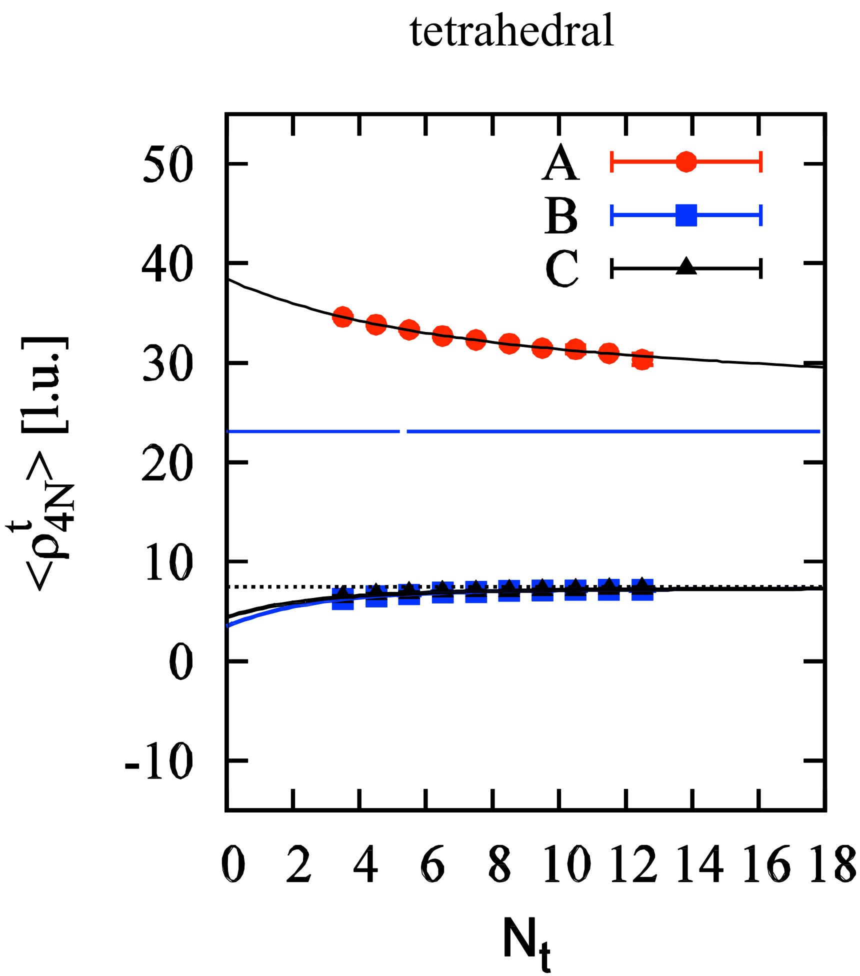
0_2^+

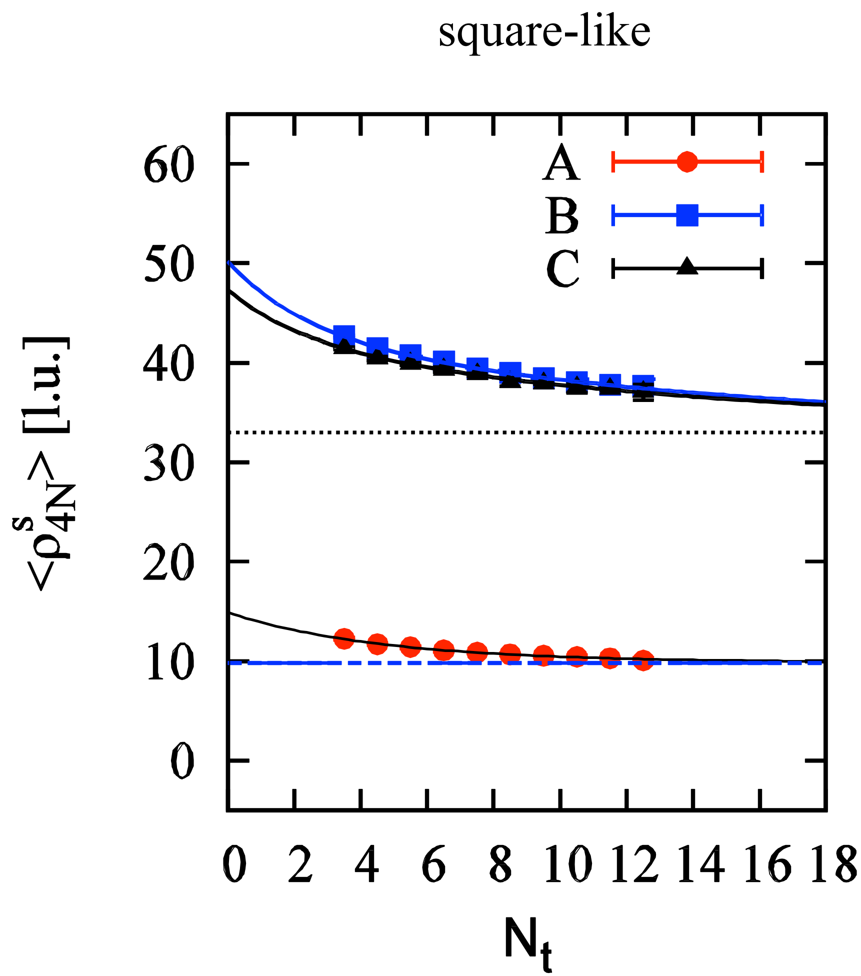


B,C - Square-like structure



NLO
NNLO
A
B
C
ΔE (2NF) [MeV]
ΔE (3NF) [MeV]
N_t
N_t


tetrahedral
A
B
C
$<\rho^t_{4N}>$ [l.u.]
N_t

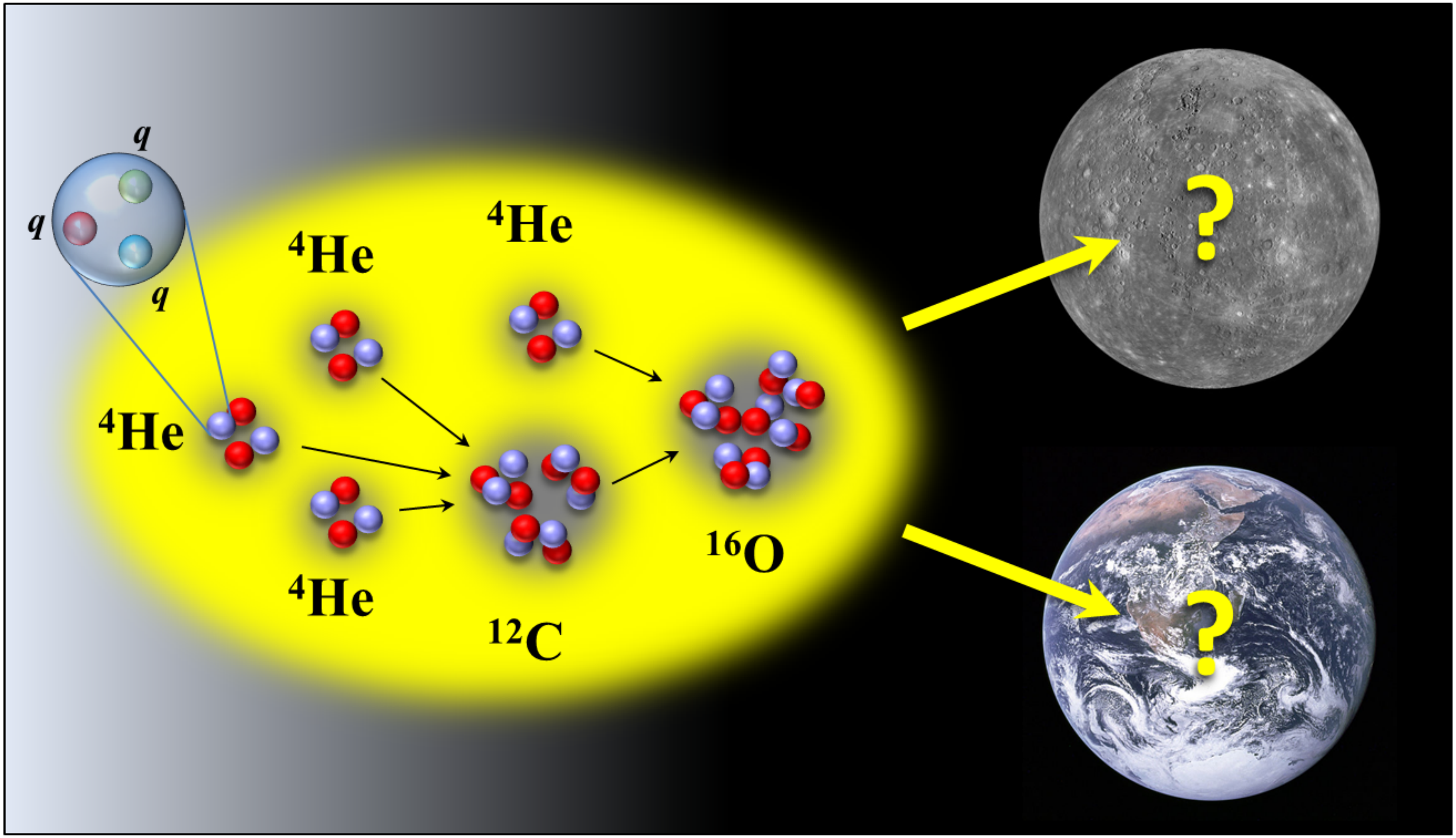

square-like
A
B
C
$<\rho^s_{4N}>$ [l.u.]
N_t

	LO	NLO	NNLO	Exp.
0_1^+	-147.3(5)	-121.4(5)	-138.8(5)	-127.62
0_2^+	-145(2)	-116(2)	-136(2)	-121.57
2_1^+	-145(2)	-116(2)	-136(2)	-120.70

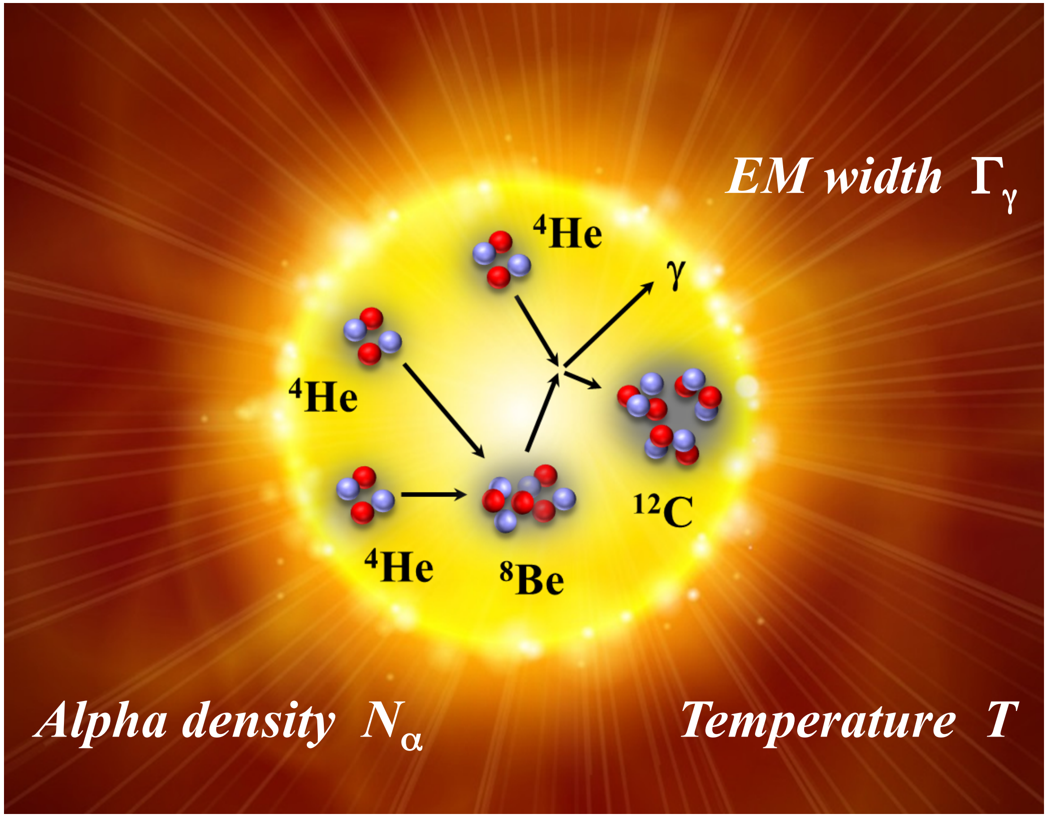
Overbinding is eliminated with a better NLO lattice action
that fits the nuclear phase shifts to higher momenta
(work in progress)

Epelbaum, Krebs, Lähde, D.L, Meißner, Rupak, PRL112, 102501 (2014)

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?

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

$\varepsilon > 480\,\mathrm{keV}$

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

$\varepsilon < 280\,\mathrm{keV}$

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.

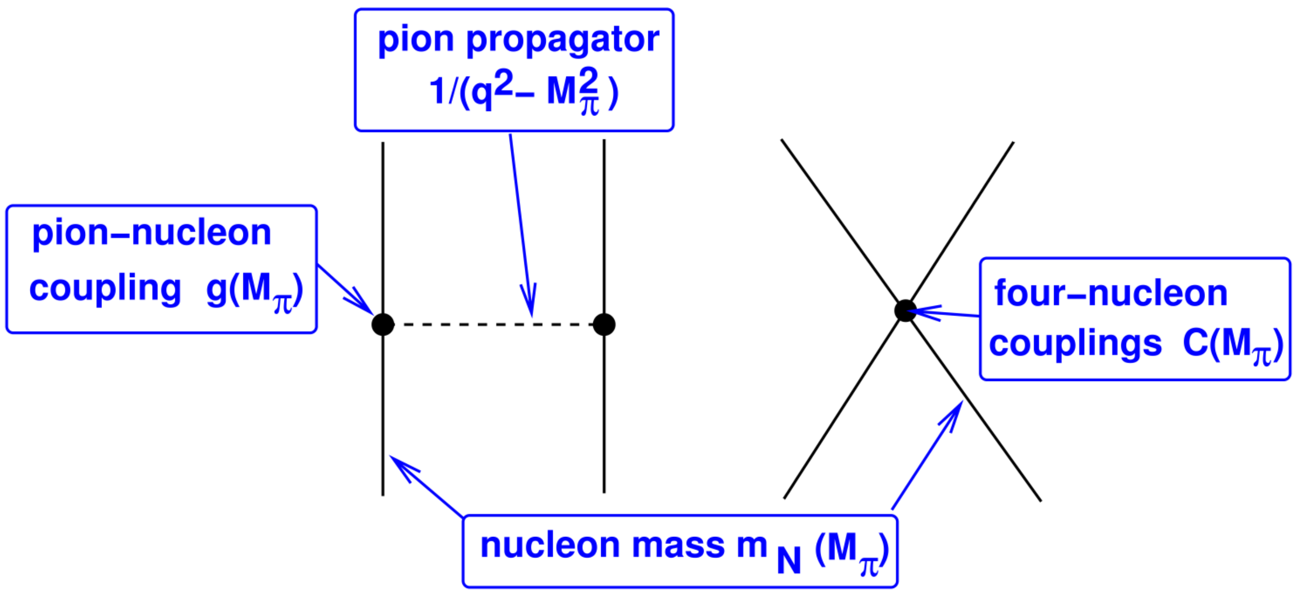
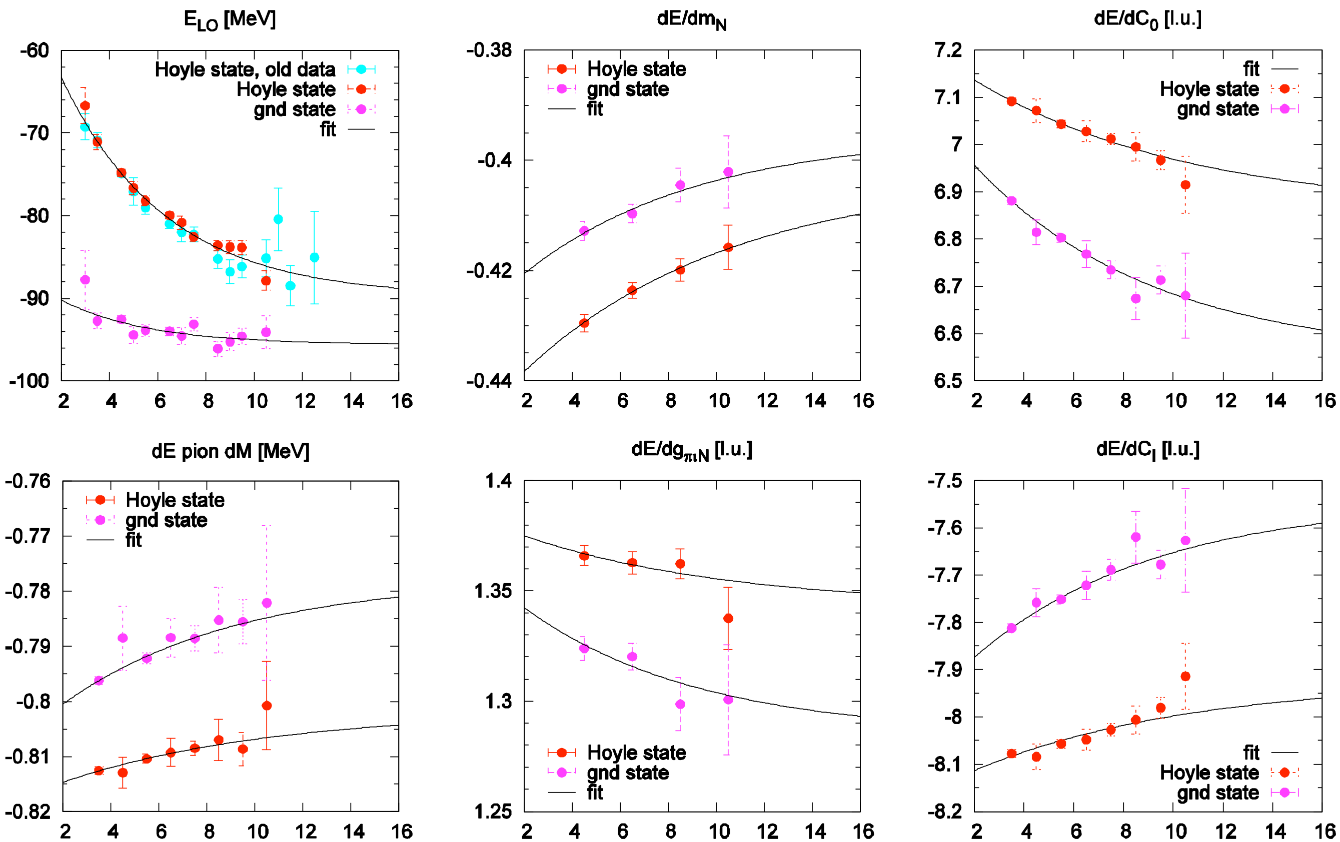


Figure courtesy of U.-G. Meißner

Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 110 (2013) 112502; ibid., EPJA 49 (2013) 82
Berengut et al., Phys. Rev. D 87 (2013) 085018

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

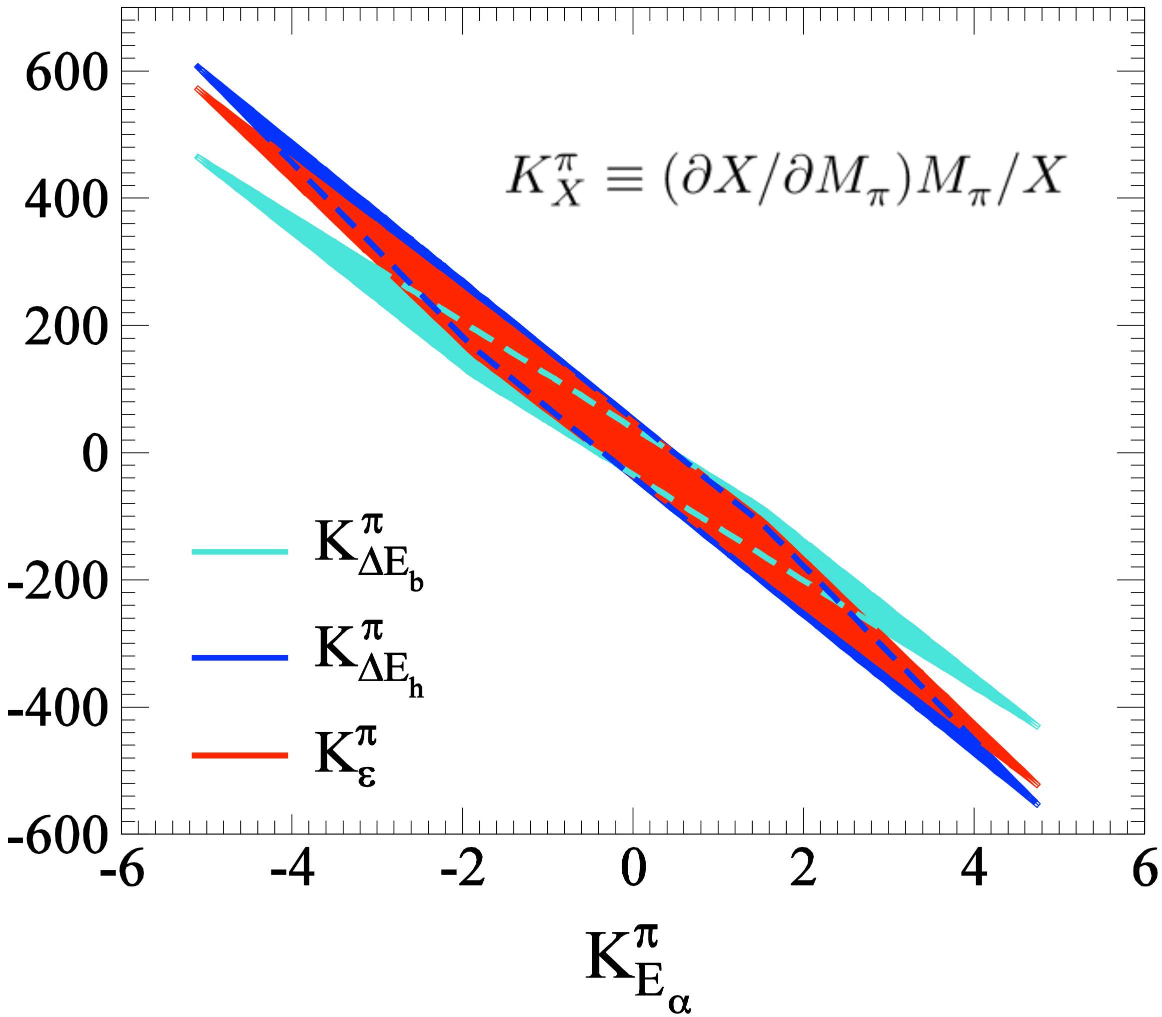
$$\left.\frac{\partial \Delta E_h}{\partial M_\pi}\right|_{M_\pi^{\rm ph}} = -0.455(35)\bar{A}_s - 0.744(24)\bar{A}_t + 0.051(19)$$

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

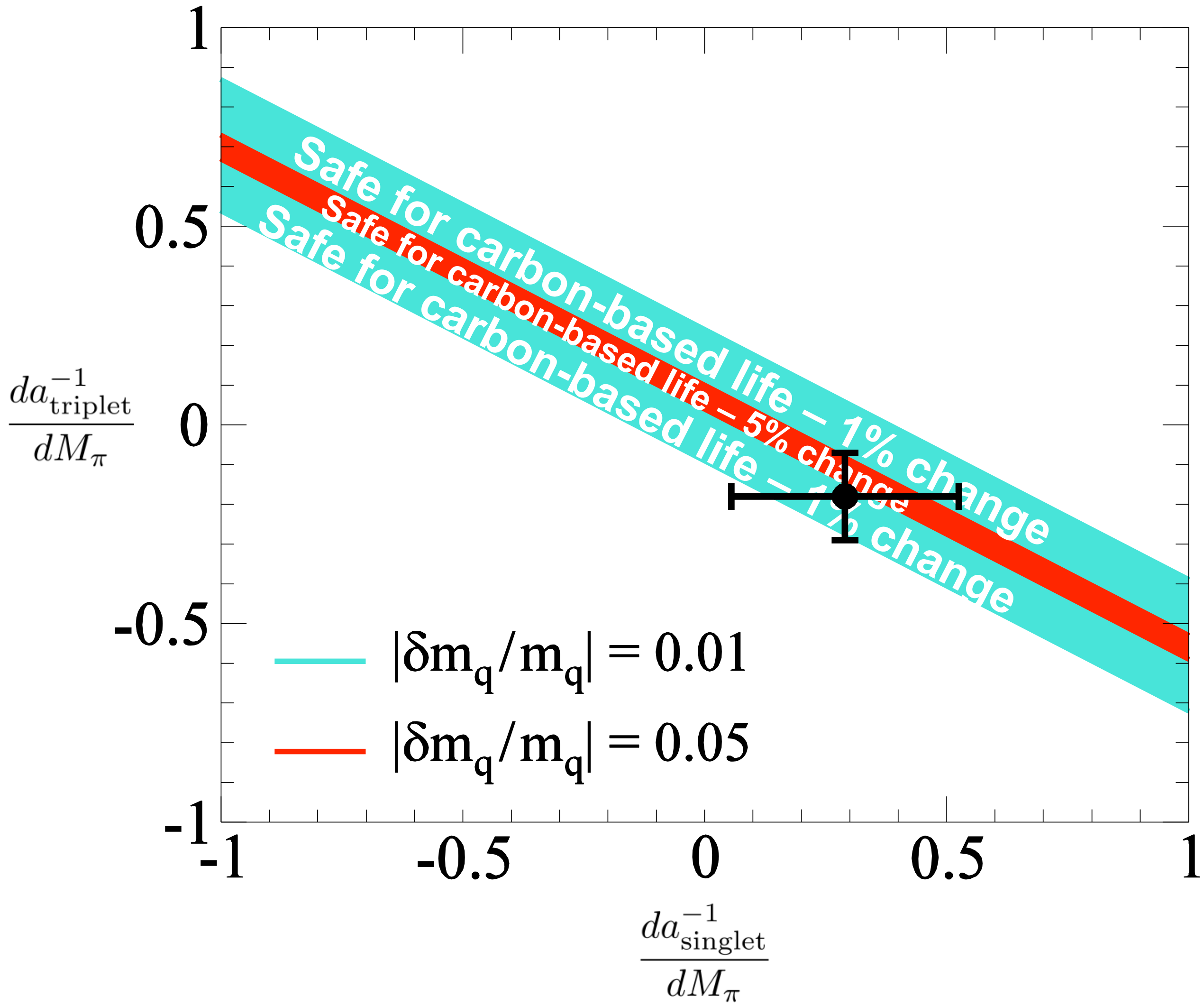
$$\left.\frac{\partial \varepsilon}{\partial M_\pi}\right|_{M_\pi^{\rm ph}} = -0.572(19)\bar{A}_s - 0.933(15)\bar{A}_t + 0.064(16)$$

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

Evidence for correlation with alpha binding energy



“End of the world” plot



Epelbaum, Krebs, Lähde, D.L, Meißner, PRL 110 (2013) 112502; ibid., EPJA 49 (2013) 82

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. Hopefully can play a significant role in the future of *ab initio* nuclear theory.

Additional topics to be addressed in the near future…

$N \neq Z$ nuclei, asymmetric nuclear matter, different lattice spacings, chiral EFT interactions at N3LO, scattering and reactions using adiabatic projection method, etc.