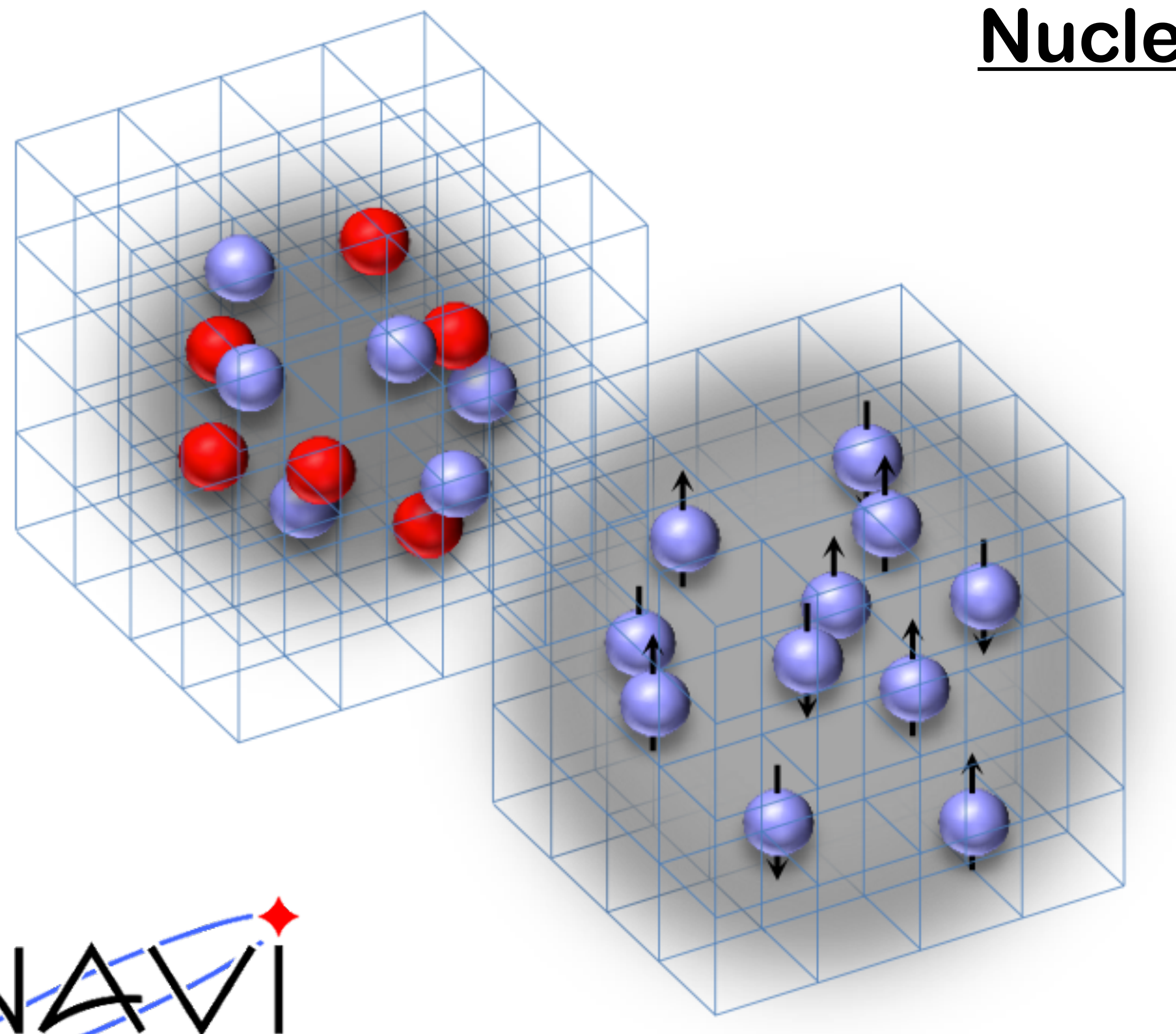
Nuclear Lattice Simulations
Progress report



Nuclear Lattice EFT Collaboration

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Dean Lee (NC State)
Thomas Luu (Jülich)
Ulf-G. Meißner (Bonn/Jülich)
Gautam Rupak (MS State)
…

NAVI Physics Days
KBW Lecture Hall, GSI Darmstadt
February 26, 2015, 12:15

Outline

Chiral EFT for nuclei on the lattice
extension to N3LO

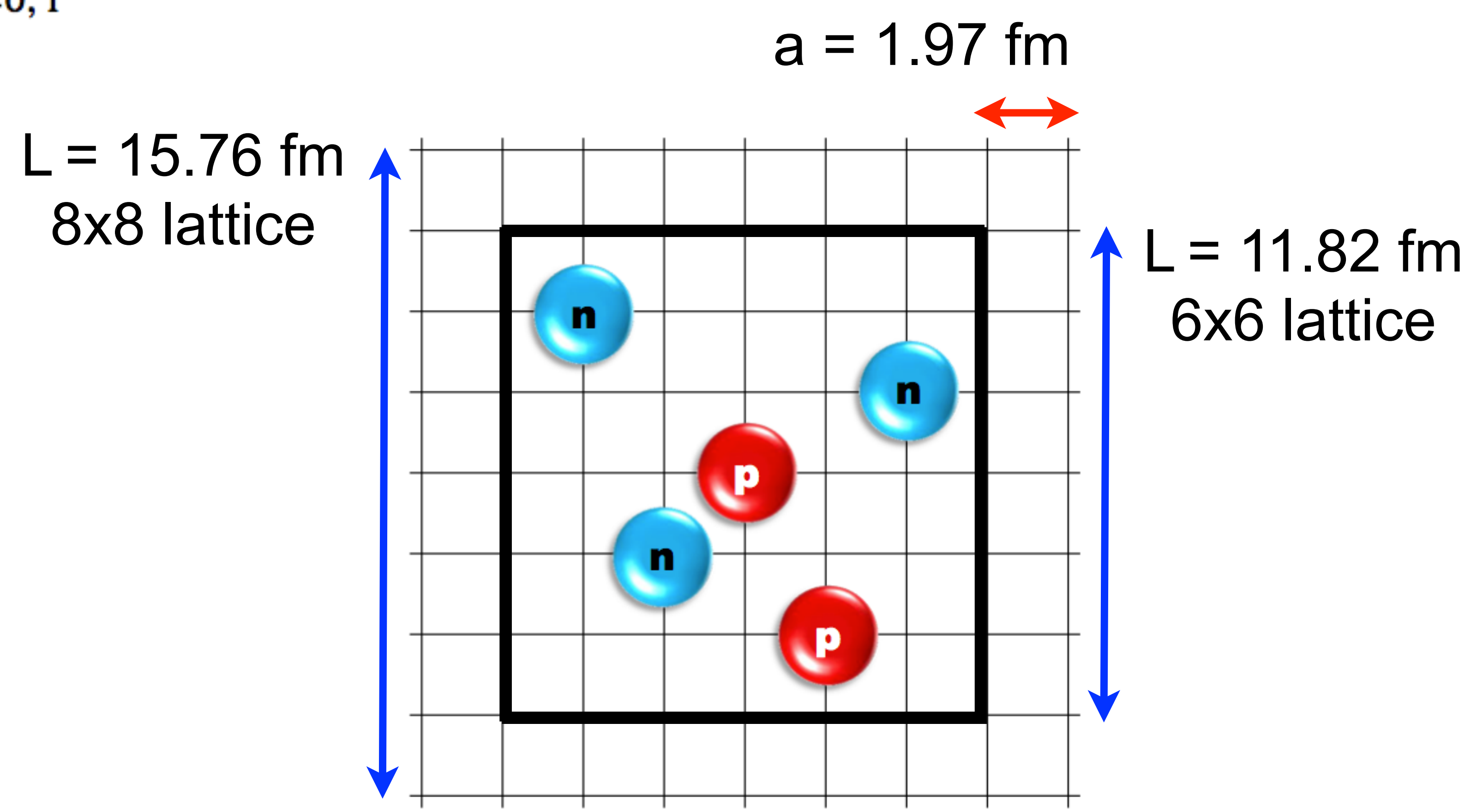
Solving the two-nucleon problem on the lattice
improved determination of low-energy constants

Projection Monte Carlo for medium-mass nuclei
working around the sign problem

Some recent highlights
for ^{12}C and ^{16}O

Lattice theory of pointlike protons and neutrons
we do not resolve the quarks and gluons!

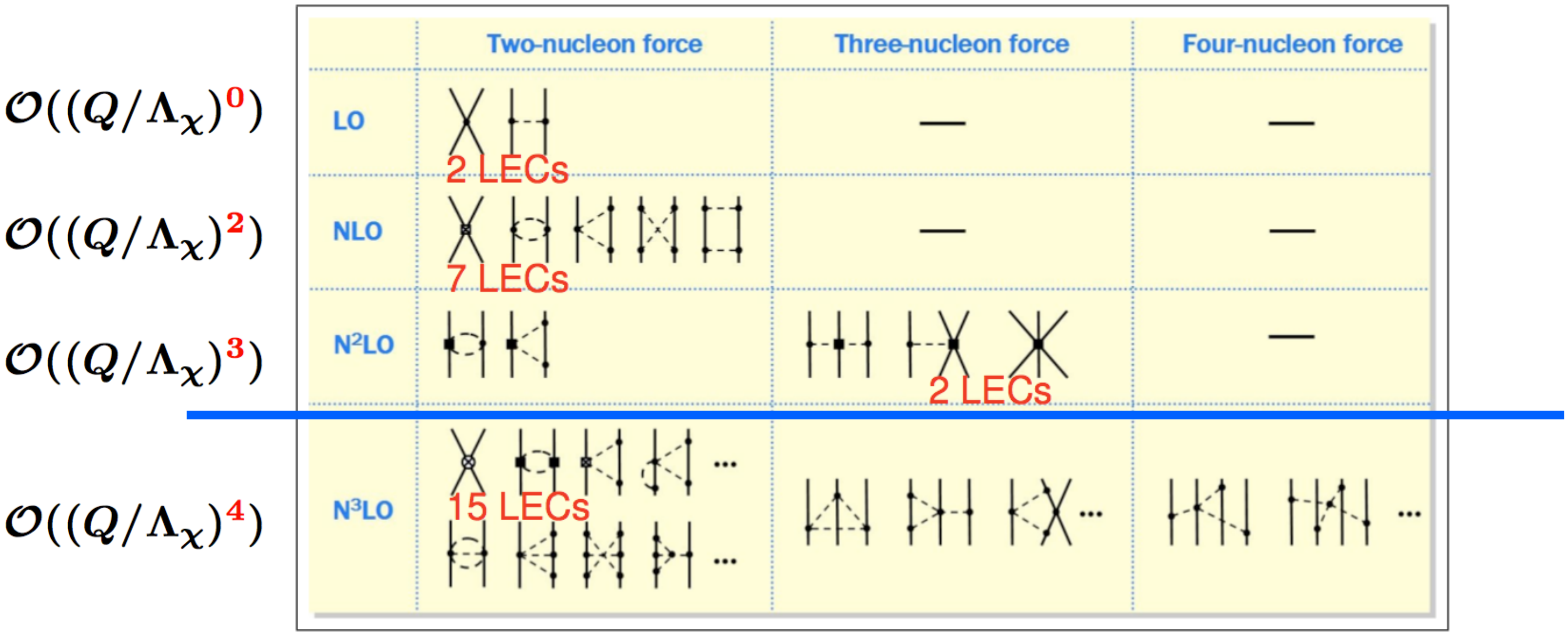
$$H_{\text{free}} = \frac{1}{2m} \sum_{i,j=0,1} \int \mathrm{d}^3\vec{r}\ \vec{\nabla} a^\dagger_{i,j}(\vec{r}) \cdot \vec{\nabla} a_{i,j}(\vec{r})$$



Work on smaller lattice spacings underway,
a = 1.4 - 1.6 fm ...
also: larger volumes, antiperiodic boundary conditions
(Christopher Körber, Jülich)

Order-by-order expansion of the nucleon-nucleon potential:

Epelbaum, Hammer, Meißner: Rev. Mod. Phys. 81, 1773 (2009)



Also EM and pion mass difference effects ...

Currently implemented to NNLO (without TPEP)

Extension to N^3LO + TPEP (at smaller lattice spacings):

Dechuan Du, Ning Li (FZ Jülich) ...

At NLO, we need to determine several unknown constants
—> fix these from nucleon-nucleon phase shifts!

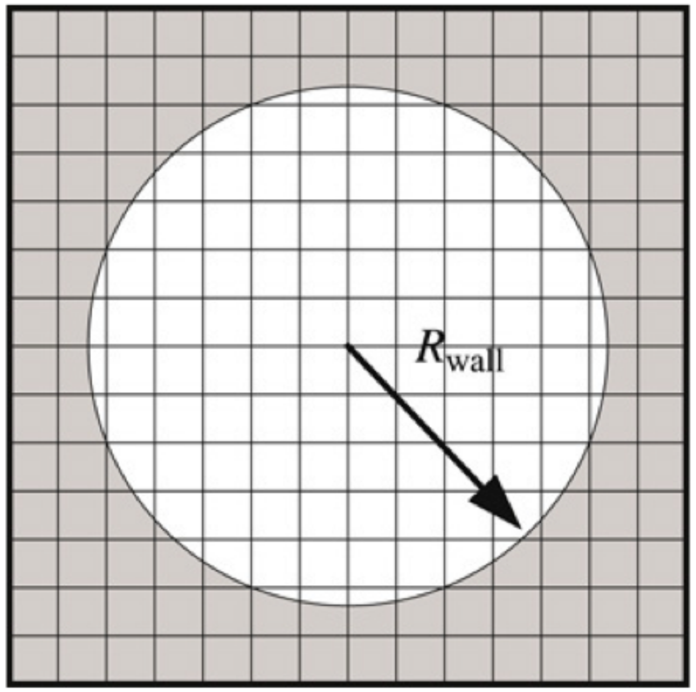
Asymptotically, beyond the range of the interaction:

$$[\cos\delta_L \cdot j_L(kr) - \sin\delta_L \cdot y_L(kr)]\, Y_{L,L_z}(\theta,\phi)$$

Introduce a "spherical wall" in the asymptotic region:

$$\cos\delta_L \cdot j_L(kR_{\text{wall}}) = \sin\delta_L \cdot y_L(kR_{\text{wall}}),$$

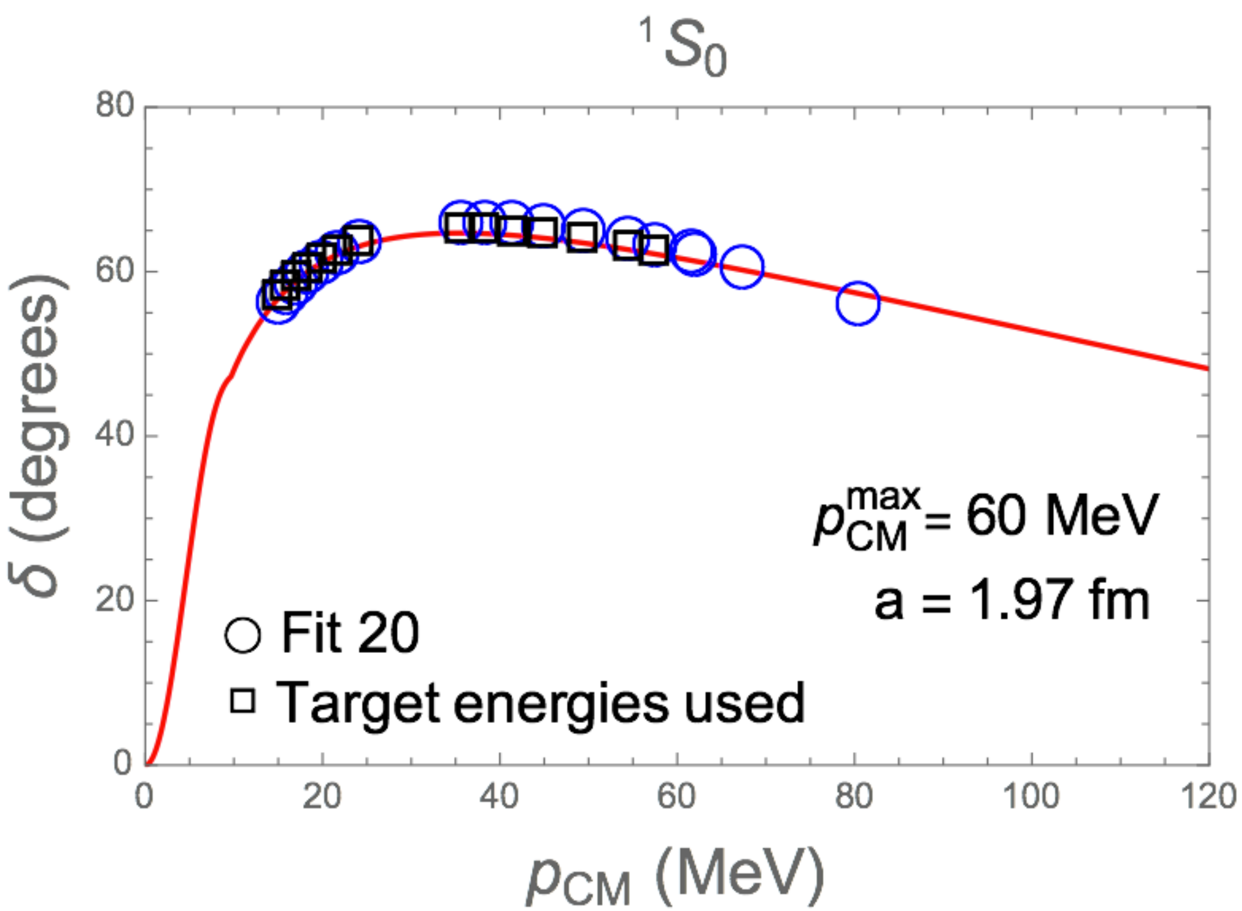
$$\delta_L = \tan^{-1}\left[\frac{j_L(kR_{\text{wall}})}{y_L(kR_{\text{wall}})}\right].$$

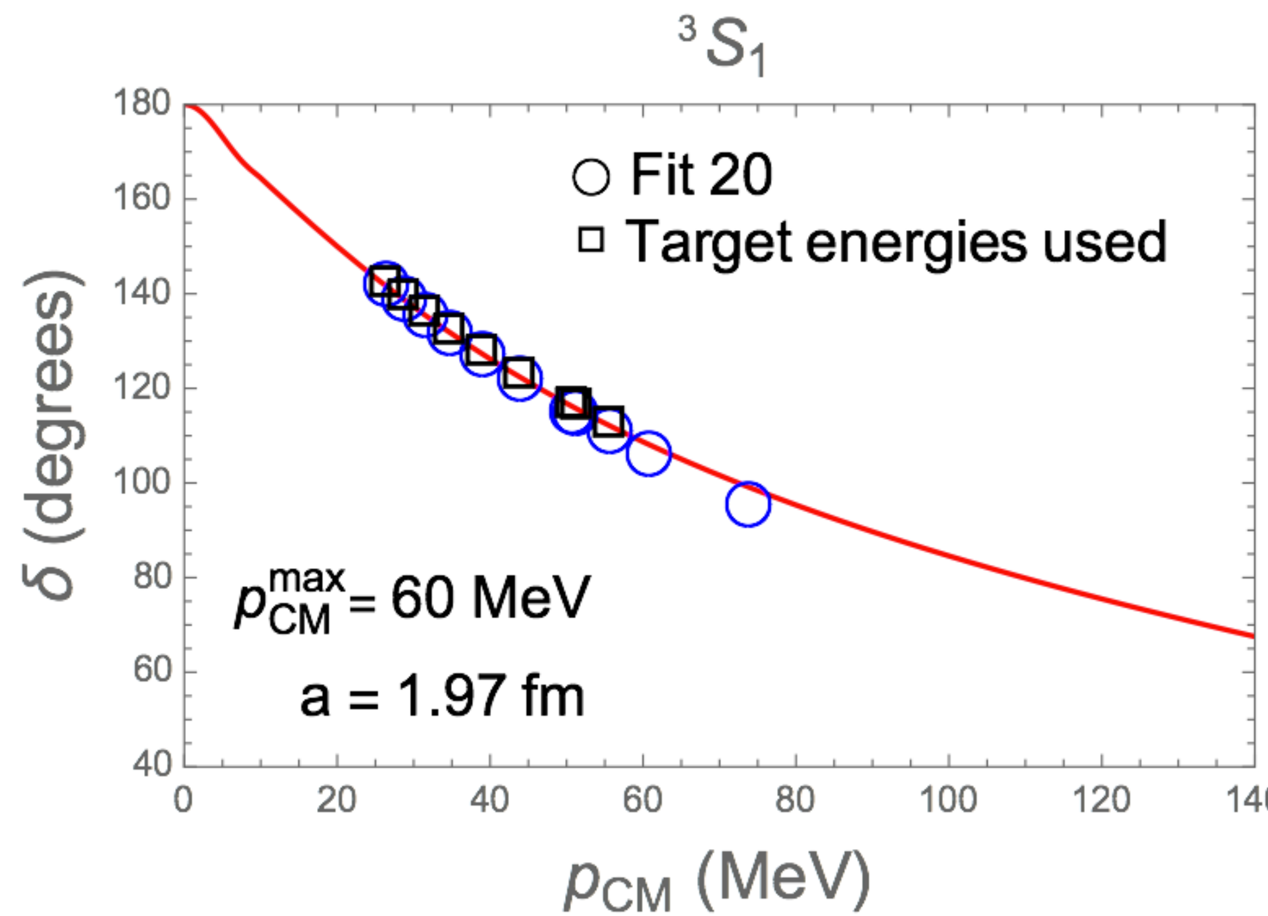


Lanczos diagonalization of the Hamiltonian
(computationally feasible up to A = 3)

More accurate and systematical determination of 2NF constants at LO and NLO

José Alarcon (Bonn), Ning Li (Jülich) ...





Preliminary LO fits by José Alarcon (Bonn)

Extension to higher orders underway ...

Transfer matrix formalism for NLEFT

Exponential of the Hamiltonian over a small Euclidean time interval

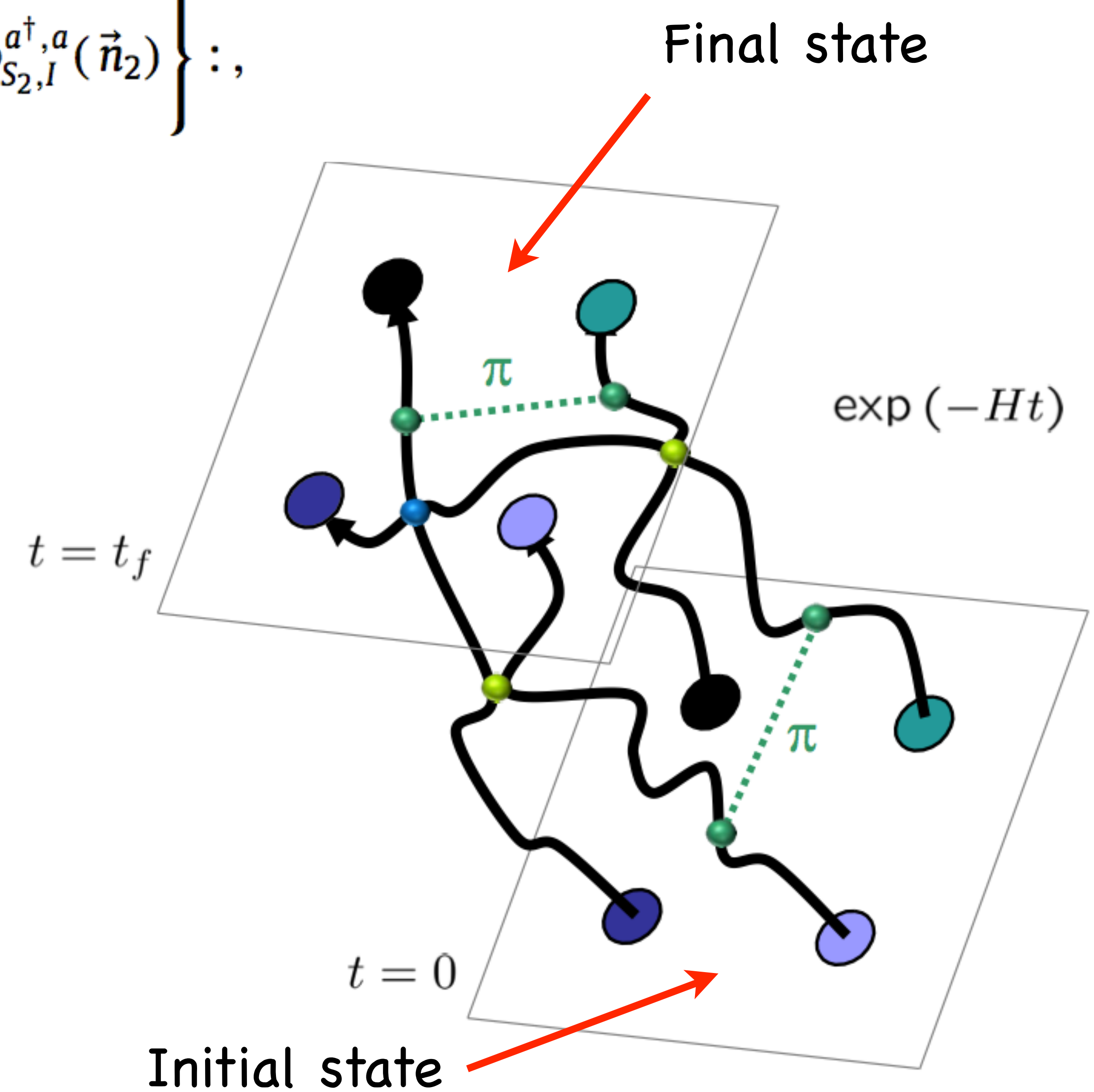
$$M_{\mathrm{LO}_1} = :\exp\left\{-H_{\mathrm{free}}\alpha_t - \frac{1}{2}C\alpha_t\sum_{\vec{n}}\left[\rho^{a^\dagger,a}(\vec{n})\right]^2 - \frac{1}{2}C_{I^2}\alpha_t\sum_{\vec{n},I}\left[\rho_I^{a^\dagger,a}(\vec{n})\right]^2 + \frac{g_A^2\alpha_t^2}{8f_\pi^2 q_\pi}\sum_{S_1,S_2,I}\sum_{\vec{n}_1,\vec{n}_2} G_{S_1S_2}(\vec{n}_1-\vec{n}_2)\rho_{S_1,I}^{a^\dagger,a}(\vec{n}_1)\rho_{S_2,I}^{a^\dagger,a}(\vec{n}_2)\right\}:,$$

$$\mathcal{Z}_{\mathrm{LO}_1} = \mathrm{Tr}\left[\left(M_{\mathrm{LO}_1}\right)^{L_t}\right]$$

Discrete Euclidean time evolution

Low-lying spectrum via Projection Monte Carlo

Initial states: Plane waves, alpha clusters, shell model wavefunctions ...



Allocations of supercomputing time (example for 2014-2015)
Resources provided by Forschungszentrum Jülich and RWTH Aachen
(deadline for 2015-2016 extension tomorrow at 17:00 :)

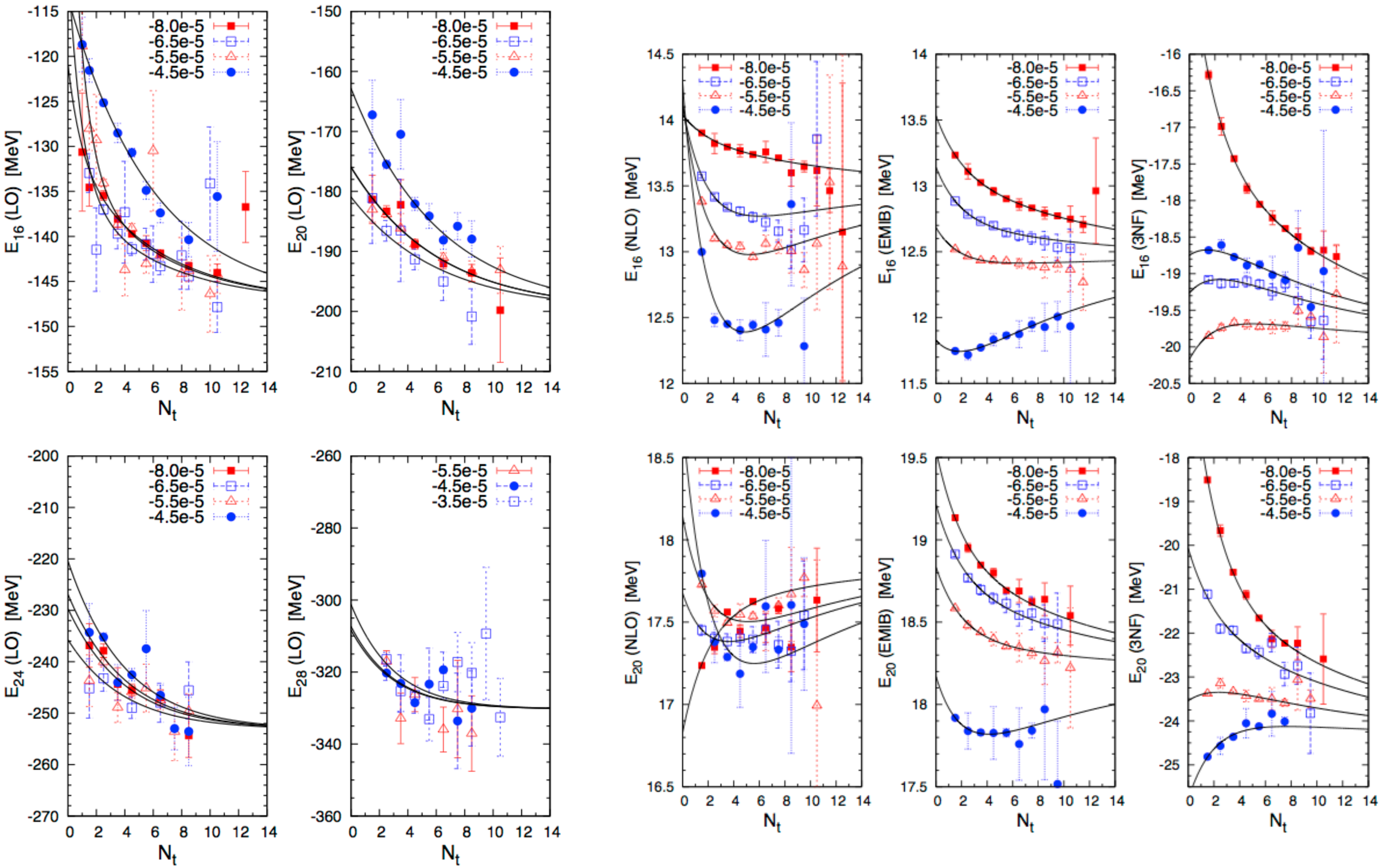
- JUQUEEN (BG/Q, Jülich), 47 Mcore-h (project) + > 100 Mcore-h (institutional)
- RWTH cluster (Intel, Aachen), 1.3 Mcore-h (project)

Figure courtesy of Jülich Supercomputer Centre (JSC)

Projection Monte Carlo NLEFT calculations

Limited by sign problem —> constrained extrapolations

Lähde, Epelbaum, Krebs, Lee, Meißner, Rupak: Phys. Lett. B732, 110 (2014)



What has been achieved (a = 1.97 fm) so far?

Overview of the present status for alpha nuclei from ^{4}He to ^{28}Si:

Lähde, Epelbaum, Krebs, Lee, Meißner, Rupak: Phys. Lett. B732, 110 (2014)

+ contact 4N interaction, see: EPJA 45, 335 (2010)

+ nearest-neighbor 4N interaction (relevant for A = 16 and larger)

A	LO (2N)	NNLO (2N)	+3N	+4N$_{\text{eff}}$	Exp
4	−28.87(6)	−25.60(6)	−28.93(7)	−28.93(7)	−28.30
8	−57.9(1)	−48.6(1)	−56.4(2)	−56.3(2)	−56.35
12	−96.9(2)	−78.7(2)	−91.7(2)	−90.3(2)	−92.16
16	−147.3(5)	−121.4(5)	−138.8(5)	−131.3(5)	−127.62
20	−199.7(9)	−163.6(9)	−184.3(9)	−165.9(9)	−160.64
24	−253(2)	−208(2)	−232(2)	−198(2)	−198.26
28	−330(3)	−275(3)	−308(3)	−233(3)	−236.54

Adjusted

Smaller lattice spacing, improved NLO amplitude, extension to N3LO ...

(Dechuan Du, Ning Li, José Alarcon ...)

also: finite volume effects, antiperiodic boundary conditions

(Christopher Körber, Jülich)

Working around the sign problem in NLEFT

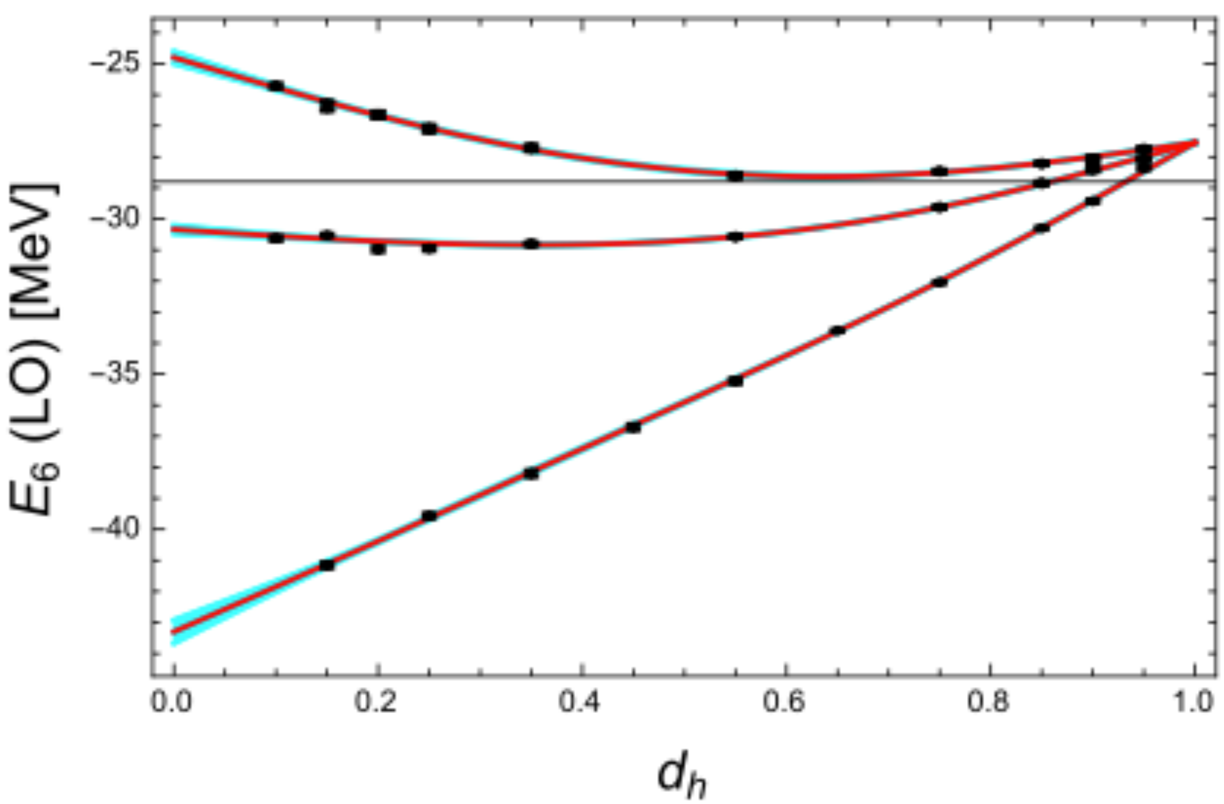
Lähde, Luu, Lee, Meißner, Epelbaum, Krebs, Rupak, arXiv:1502.06787

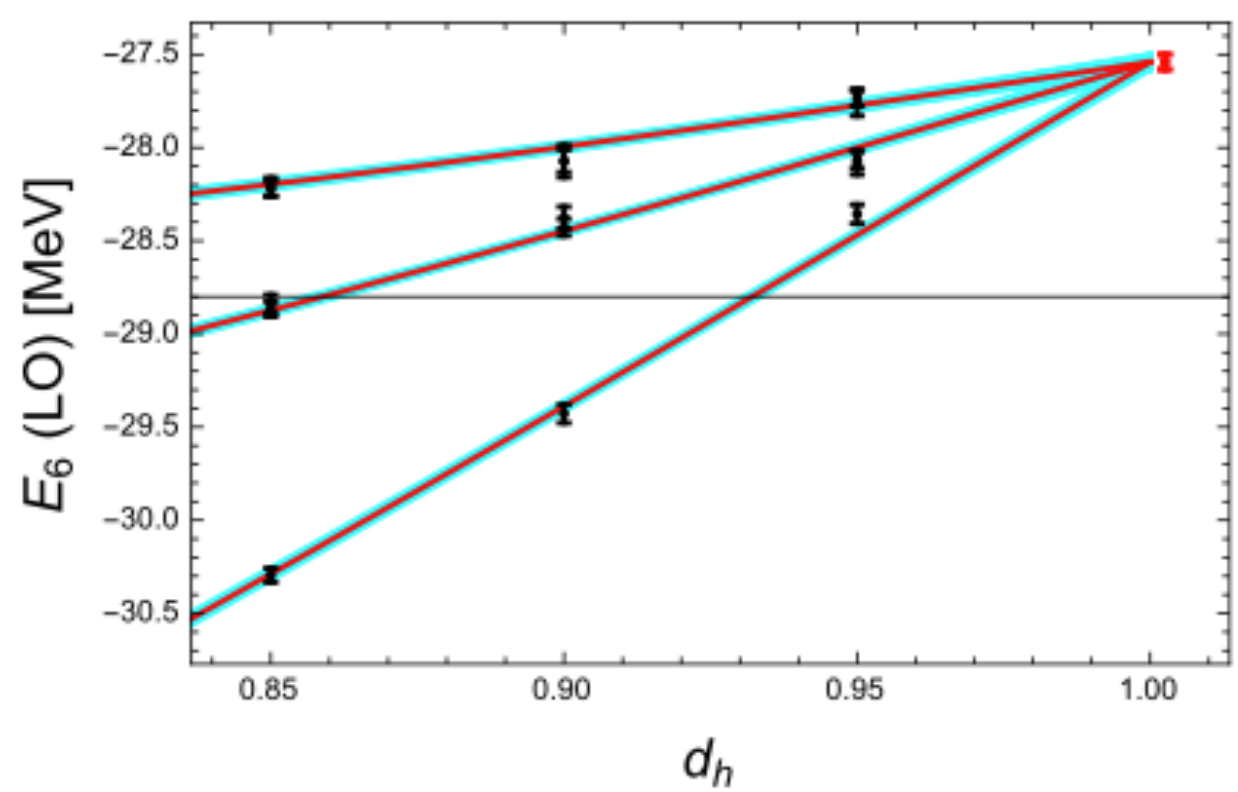
first NLEFT calculation of ^{6}He

$$H \equiv d_h H_{\rm LO} + (1 - d_h) H_4$$

full LO NLEFT Hamiltonian

Wigner SU(4) symmetric Hamiltonian





Perform calculations where the sign problem is more favorable

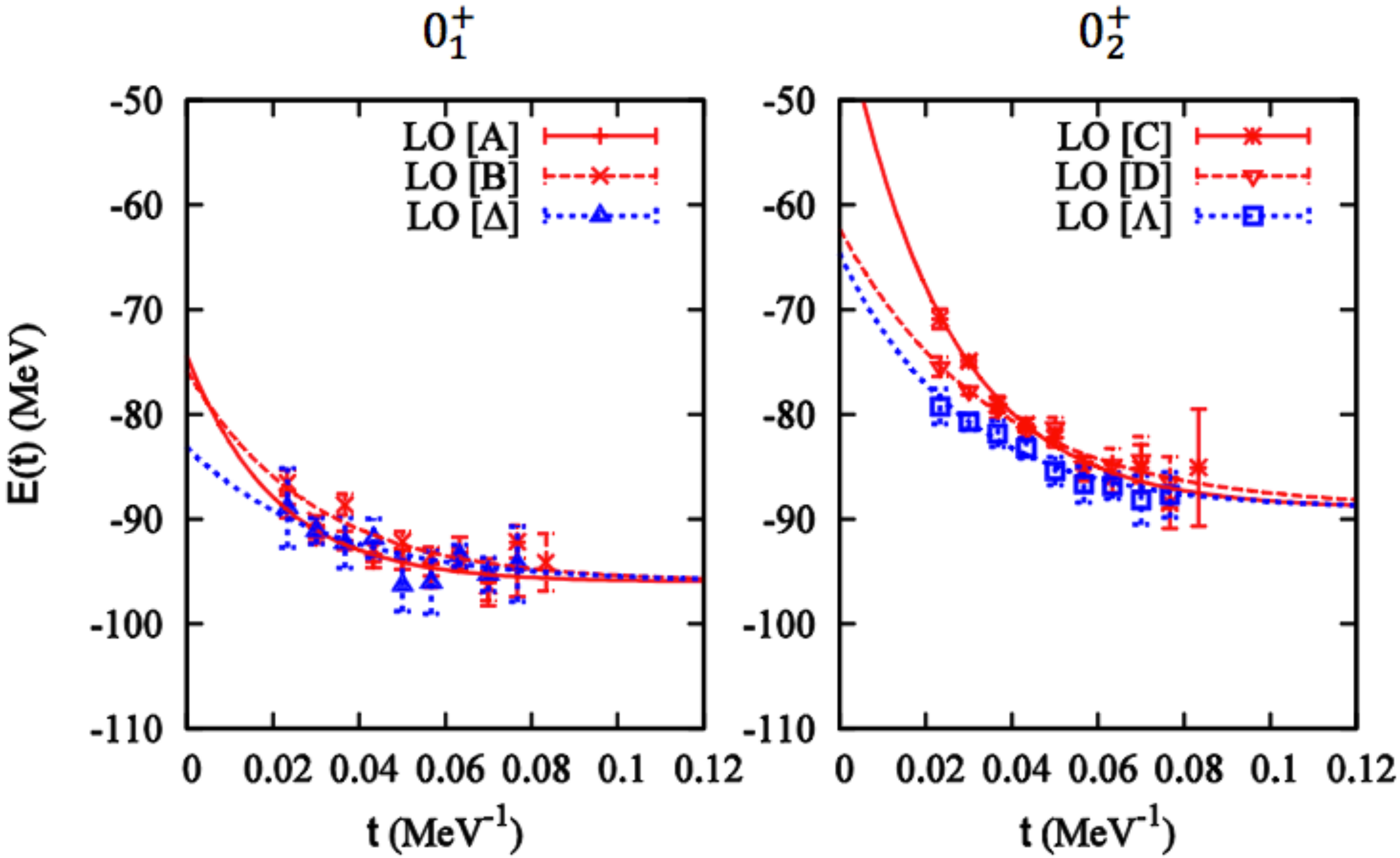
-> Extrapolate to the physical point!

Makes smaller lattice spacings and neutron-rich nuclei accessible

^{12}C and ^{16}O in NLEFT
some highlights

NLEFT results for ^{12}C —> Ground state and "Hoyle State"

Epelbaum, Krebs, Lähde, Lee, Meißner: Phys. Rev. Lett. 109, 252501 (2012)



Red —> Plane wave trial wave functions

Blue —> Alpha cluster trial wave functions

NNLO NLEFT results for the low-energy spectrum of ^{12}C

Epelbaum, Krebs, Lähde, Lee, Meißner: Phys. Rev. Lett. 109, 252501 (2012)

	Ground		Hoyle	
	0_1^+	$2_1^+(E^+)$	0_2^+	$2_2^+(E^+)$
LO	−96(2)	−94(2)	−89(2)	−88(2)
NLO	−77(3)	−74(3)	−72(3)	−70(3)
NNLO	−92(3)	−89(3)	−85(3)	−83(3)
Expt.	−92.16	−87.72	−84.51	−82.6(1) [8,10] −81.1(3) [9] −82.32(6) [11]

[8] M. Freer *et al.*, Phys. Rev. C **80**, 041303 (2009).

[9] S. Hyldegaard *et al.*, Phys. Rev. C **81**, 024303 (2010).

[10] W. R. Zimmerman, N. E. Destefano, M. Freer, M. Gai, and F. D. Smit, Phys. Rev. C **84**, 027304 (2011).

[11] M. Itoh *et al.*, Phys. Rev. C **84**, 054308 (2011).

Effects of rotational symmetry breaking on the lattice

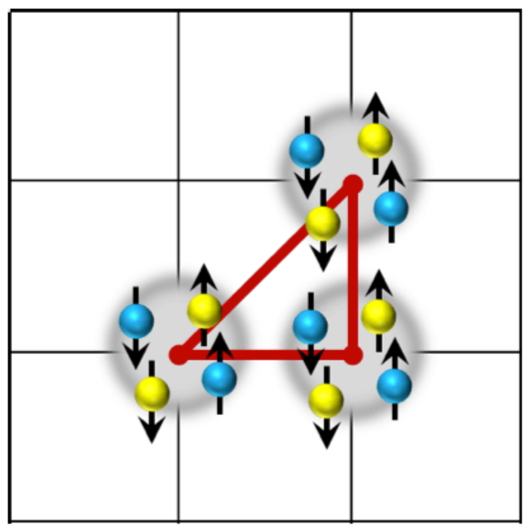
(Bing-Nan Lu, Jülich)

Alpha cluster structure of ^{12}C and ^{16}O emerges naturally

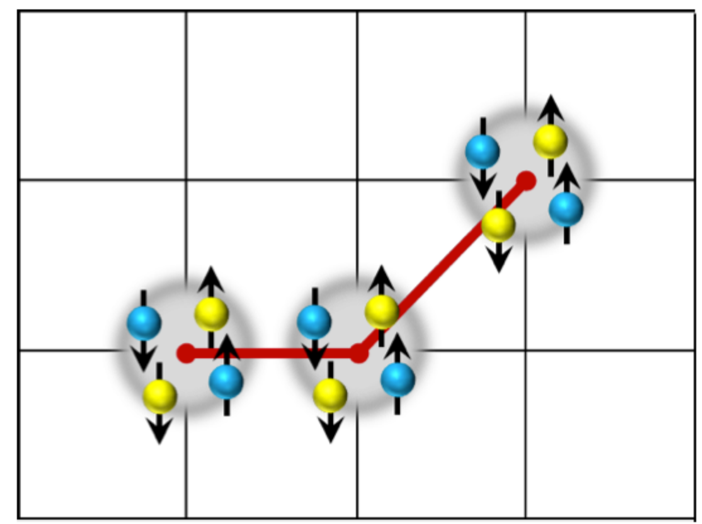
Epelbaum, Krebs, Lähde, Lee, Meißner: Phys. Rev. Lett. 109, 252501 (2012)

Epelbaum, Krebs, Lähde, Lee, Meißner, Rupak: Phys. Rev. Lett. 112, 102501 (2014)

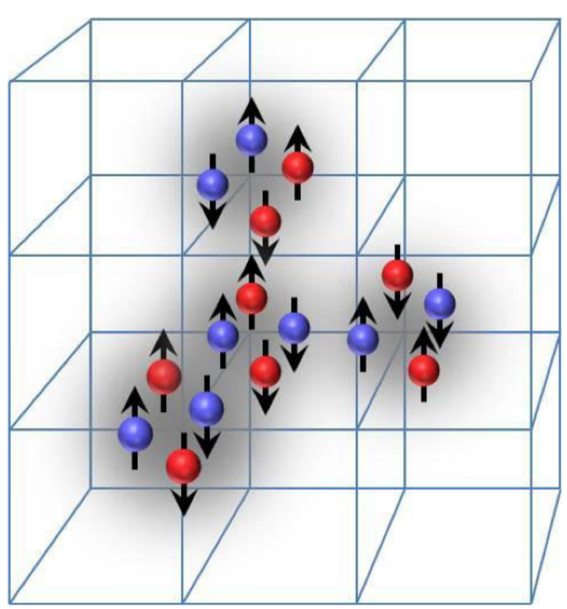
Ground state of ^{12}C, 0_1^+



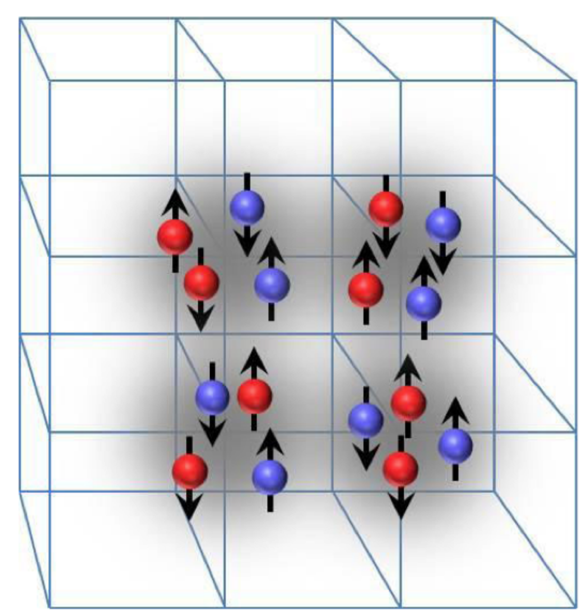
"Hoyle state" of ^{12}C, 0_2^+



Ground state of ^{16}O, 0_1^+



First excited state of ^{16}O, 0_2^+



LO NLEFT results for charge radii and quadrupole moments in ^{12}C

Epelbaum, Krebs, Lähde, Lee, Meißner: Phys. Rev. Lett. 109, 252501 (2012)

	LO	Expt.
$r(0_1^+)$ [fm]	2.2(2)	2.47(2) [26]
$r(2_1^+)$ [fm]	2.2(2)	...
$Q(2_1^+)$ [e fm^2]	6(2)	6(3) [27]
$r(0_2^+)$ [fm]	2.4(2)	...
$r(2_2^+)$ [fm]	2.4(2)	...
$Q(2_2^+)$ [e fm^2]	−7(2)	...

[26] L. A. Schaller, L. Schellenberg, T. Q. Phan, G. Piller, A. Ruetschi, and H. Schneuwly, Nucl. Phys. **A379**, 523 (1982).

[27] W. J. Vermeer, M. T. Esat, J. A. Kuehner, R. H. Spear, A. M. Baxter, and S. Hinds, Phys. Lett. **122B**, 23 (1983).

LO NLEFT results for transition matrix elements in ^{12}C

Epelbaum, Krebs, Lähde, Lee, Meißner: Phys. Rev. Lett. 109, 252501 (2012)

	LO	Expt.
$B(E2, 2_1^+ \to 0_1^+)$ $[e^2\,\mathrm{fm}^4]$	5(2)	7.6(4) [28]
$B(E2, 2_1^+ \to 0_2^+)$ $[e^2\,\mathrm{fm}^4]$	1.5(7)	2.6(4) [28]
$B(E2, 2_2^+ \to 0_1^+)$ $[e^2\,\mathrm{fm}^4]$	2(1)	...
$B(E2, 2_2^+ \to 0_2^+)$ $[e^2\,\mathrm{fm}^4]$	6(2)	...
$m(E0, 0_2^+ \to 0_1^+)$ $[e\,\mathrm{fm}^2]$	3(1)	5.5(1) [17]

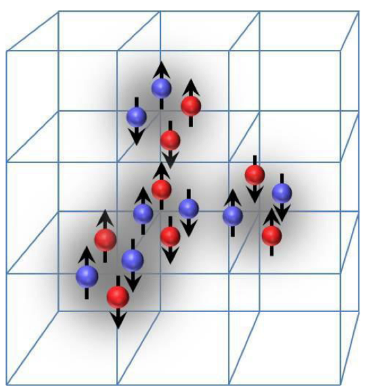
[17] M. Chernykh, H. Feldmeier, T. Neff, P. von Neumann-Cosel, and A. Richter, Phys. Rev. Lett. **105**, 022501 (2010).

[28] F. Ajzenberg-Selove, Nucl. Phys. **A506**, 1 (1990).

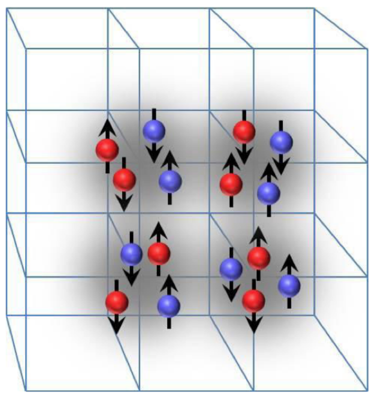
Extension to NNLO in the near future

LO NLEFT results for the EM properties of ^{16}O

Epelbaum, Krebs, Lähde, Lee, Meißner, Rupak: Phys. Rev. Lett. 112, 102501 (2014)



	LO	Rescaled	Expt.
$r(0_1^+)$ [fm]	2.3(1)	⋯	2.710(15) [26]
$r(0_2^+)$ [fm]	2.3(1)	⋯	⋯
$r(2_1^+)$ [fm]	2.3(1)	⋯	⋯
$Q(2_1^+)$ [e fm^2]	10(2)	15(3)	⋯
$B(E2, 2_1^+ \to 0_2^+)$ [e^2 fm^4]	22(4)	46(8)	65(7) [27]
$B(E2, 2_1^+ \to 0_1^+)$ [e^2 fm^4]	3.0(7)	6.2(1.6)	7.4(2) [28]
$M(E0, 0_2^+ \to 0_1^+)$ [e fm^2]	2.1(7)	3.0(1.4)	3.6(2) [29]



[26] J. C. Kim, R. S. Hicks, R. Yen, I. P. Auer, H. S. Caplan, and J. C. Bergstrom, Nucl. Phys. **A297**, 301 (1978).

[27] F. Ajzenberg-Selove, Nucl. Phys. **B166**, 1 (1971).

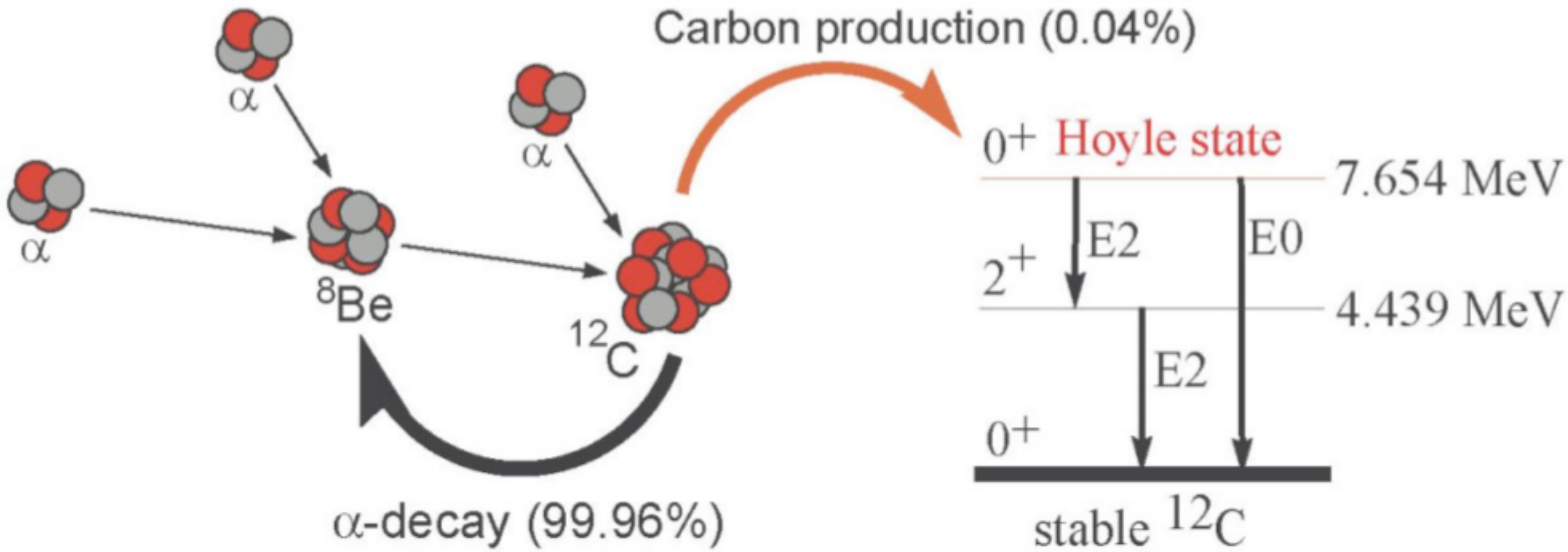
[28] R. Moreh, W. C. Sellyey, D. Sutton, and R. Vodhanel, Phys. Rev. C **31**, 2314 (1985).

[29] H. Miska, H. D. Gräf, A. Richter, R. Schneider, D. Schüll, E. Spamer, H. Theissen, O. Titze, and Th. Walcher, Phys. Lett. **58B**, 155 (1975).

"Rescaled" —> Approximate correction of overbinding effects at LO

How is ^{12}C produced in red giant stars? The "triple alpha" process:

Epelbaum, Krebs, Lähde, Lee, Meißner: PRL 110, 112502 (2013); EPJA 49, 82 (2010)



$$r_{3\alpha} = 3^{\frac{3}{2}} N_\alpha^3 \left(\frac{2\pi\hbar^2}{M_\alpha k_B T} \right)^3 \frac{\Gamma_\gamma}{\hbar} \exp\left(-\frac{\Delta E_{h+b}}{k_B T} \right)$$

What happens if we shift the Hoyle state slightly relative to the triple alpha threshold?

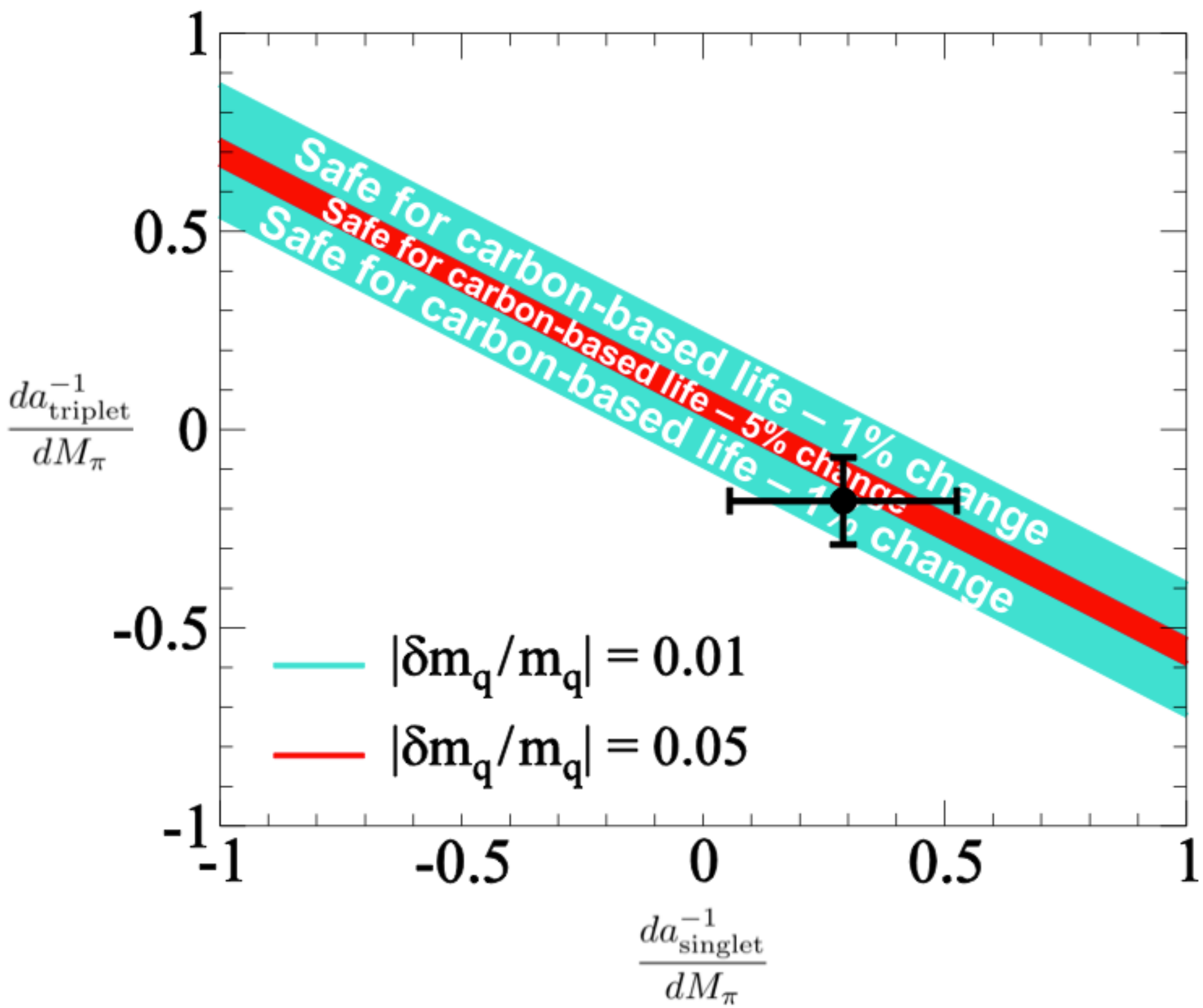
$$\Delta E_{h+b} \equiv \Delta E_h + \Delta E_b = E_{12}^\star - 3E_4$$
$$\Delta E_h \equiv E_{12}^\star - E_8 - E_4$$
$$\Delta E_b \equiv E_8 - 2E_4$$

Experiment: 379.47 ± 0.18 keV

The "end of the world" plot :)

Epelbaum, Krebs, Lähde, Lee, Meißner: Phys. Rev. Lett. 110, 112502 (2013); EPJA 49, 82 (2013)

$$\left|\left[0.572(19)\bar{A}_s + 0.933(15)\bar{A}_t - 0.064(6)\right] \times \left(\frac{\delta m_q}{m_q}\right)\right| < 0.15\%$$



Datapoint with errorbars —> current knowledge of pion mass dependence of scattering lengths

Berengut et al.: Phys. Rev. D 87, 085018 (2013)

Lattice QCD may offer further insight in the near future

Thank you for your attention!