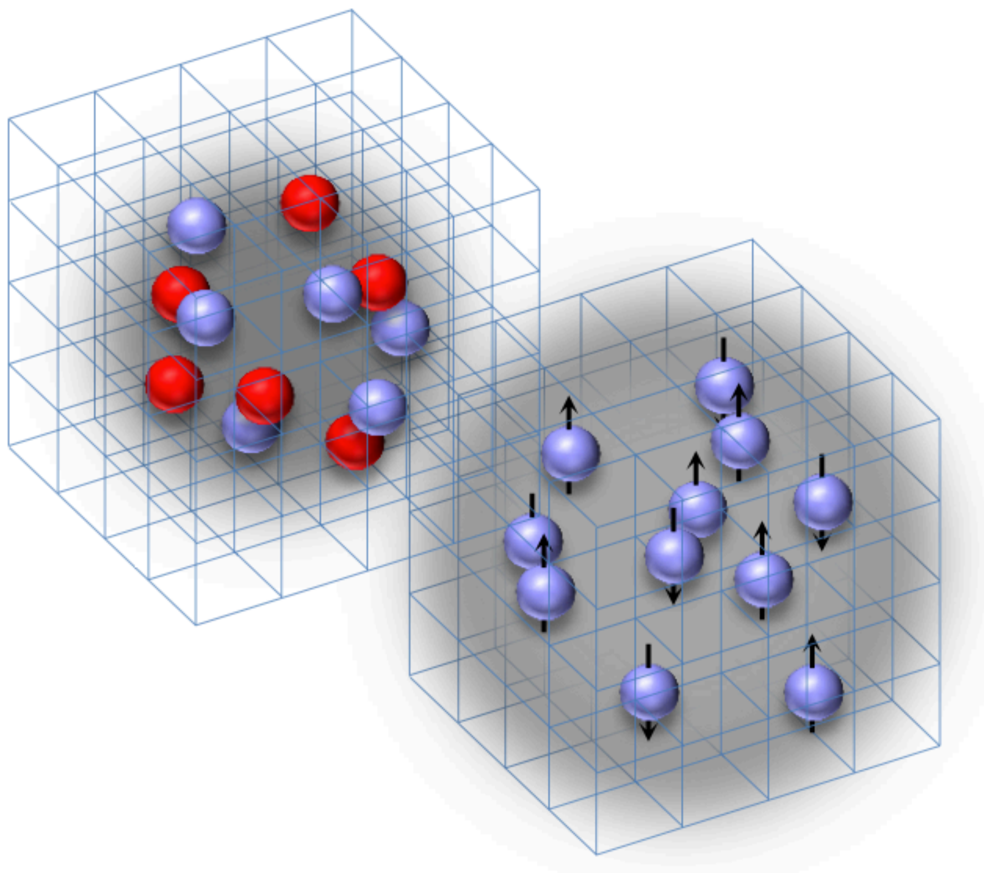
Lattice Effective Field Theory for Nuclei from A = 4 to A = 28



Nuclear Lattice EFT Collaboration

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Advances in Quantum Monte Carlo Techniques for Non-Relativistic Many-Body Systems
INT-13-2a Workshop, Seattle
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Deutsche Forschungsgemeinschaft DFG
HELMHOLTZ GEMEINSCHAFT
Study of Strongly Interacting Matter HadronPhysics3
erc
JÜLICH FORSCHUNGSZENTRUM

Outline

Brief introduction to Lattice EFT for nuclei

Carbon-12 and the Hoyle state

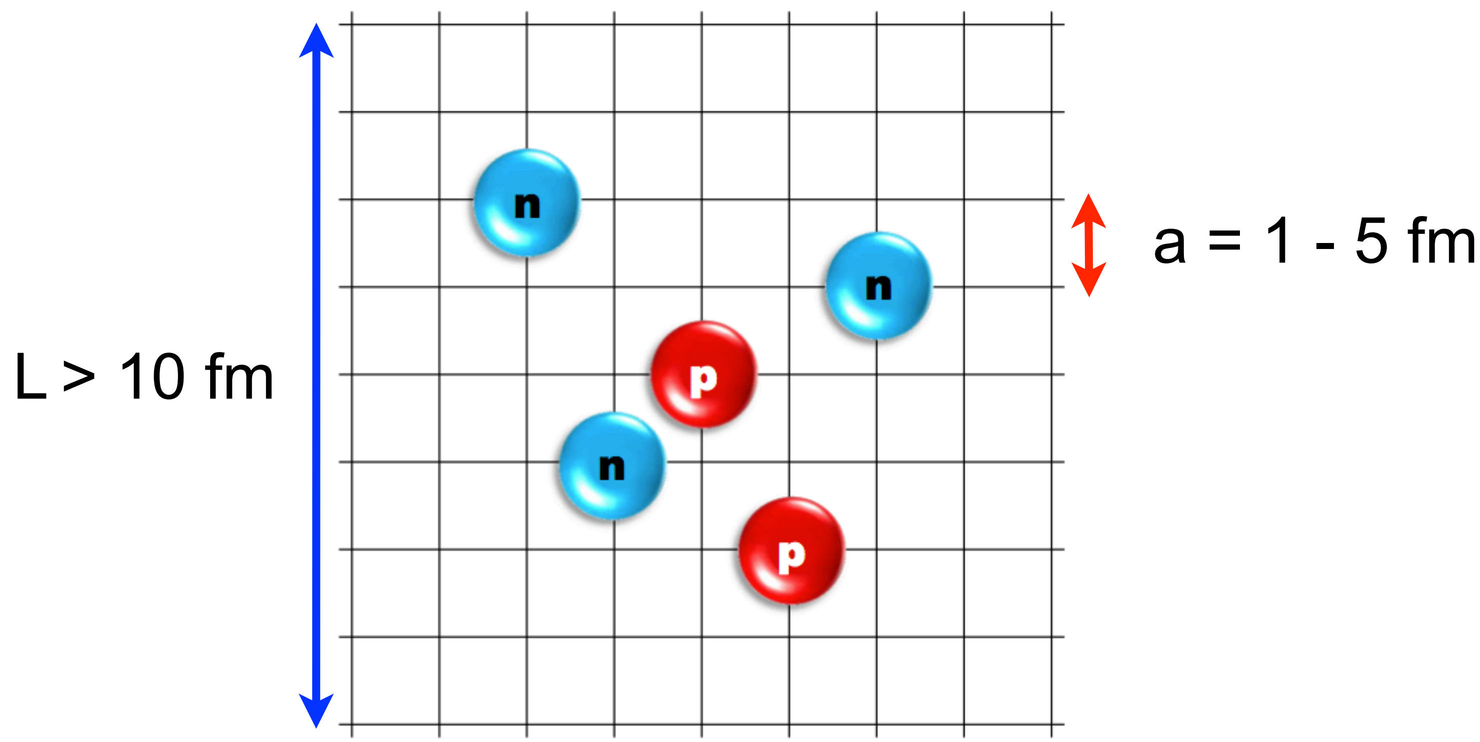
Production of Carbon-12 in red giant stars

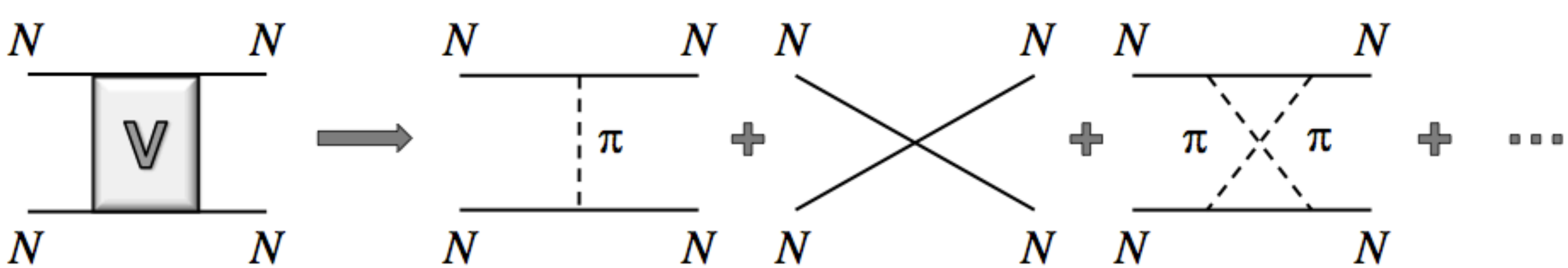
Bounds on the anthropic scenario

Preliminary results up to A = 28

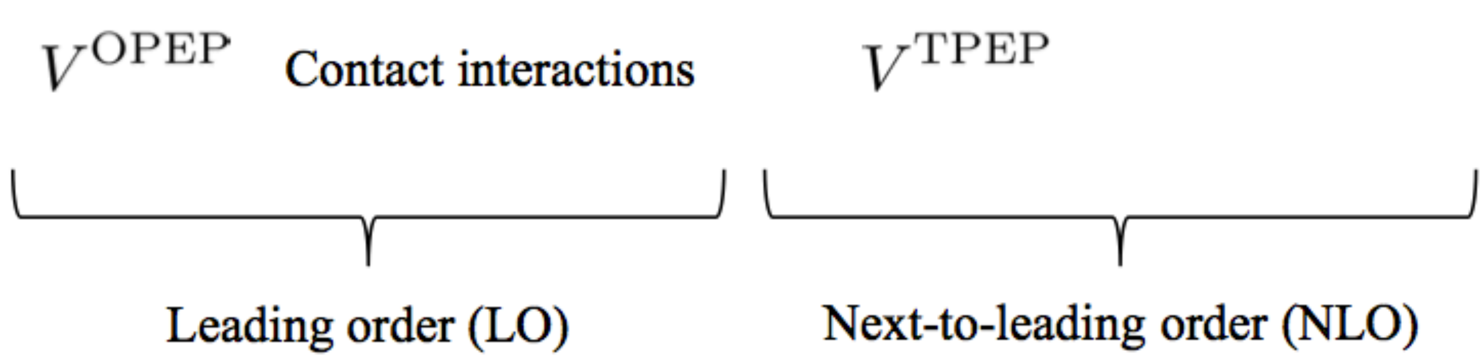
Low-energy nucleons

Chiral effective field theory on the lattice ...





Order-by-order construction of the effective NN potential



Current status of lattice chiral EFT

Improved NNLO interaction ...

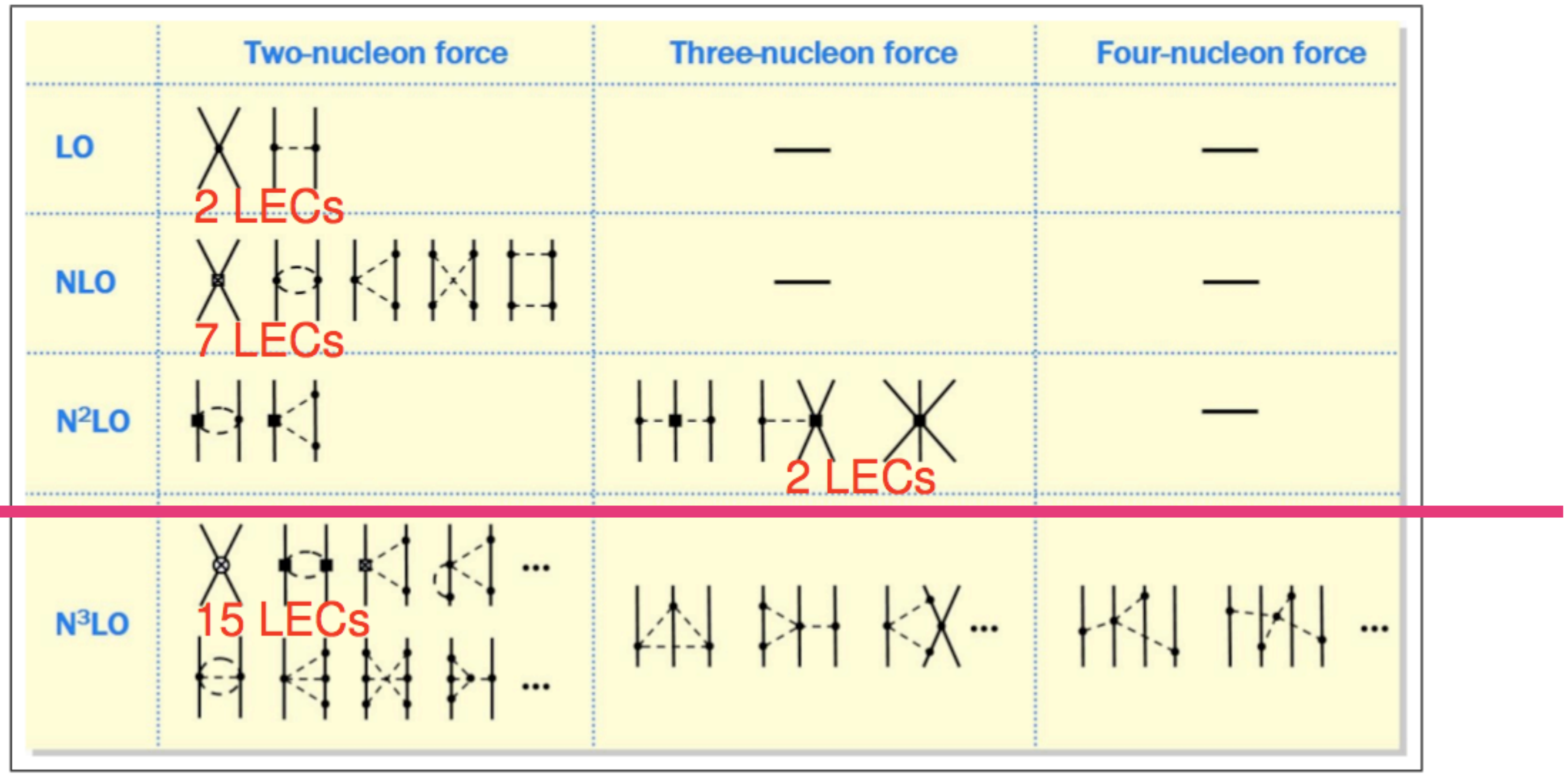
Epelbaum, Hammer, Meißner, Rev. Mod. Phys. 81 (2009) 1773

$\mathcal{O}((Q/\Lambda_\chi)^0)$

$\mathcal{O}((Q/\Lambda_\chi)^2)$

$\mathcal{O}((Q/\Lambda_\chi)^3)$

$\mathcal{O}((Q/\Lambda_\chi)^4)$



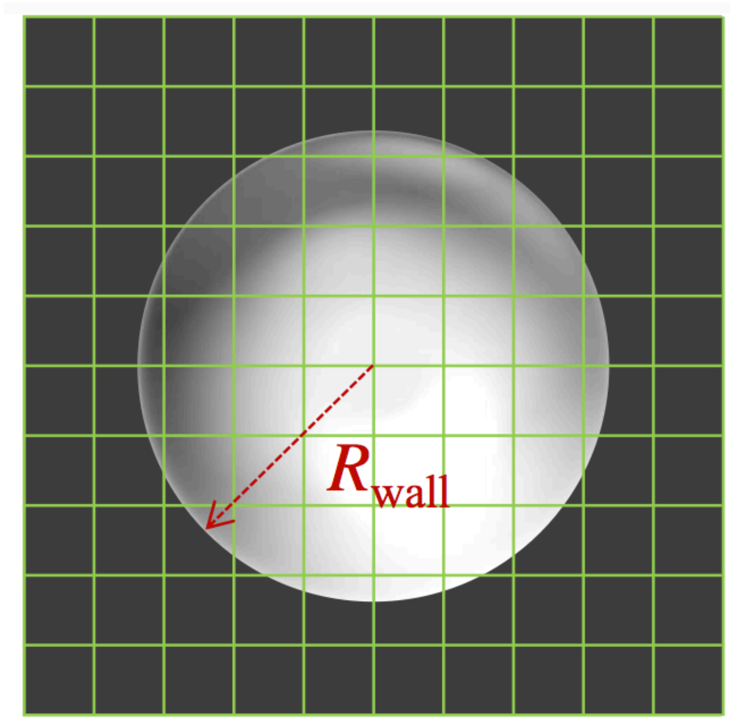
$$\mathcal{A}_{\rm LO} = C_{S=0,I=1}\, f(\boldsymbol{q}) \left(\frac{1}{4} - \frac{1}{4}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\right)\left(\frac{3}{4} + \frac{1}{4}\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j\right)$$
$$+ C_{S=1,I=0}\, f(\boldsymbol{q}) \left(\frac{3}{4} + \frac{1}{4}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\right)\left(\frac{1}{4} - \frac{1}{4}\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j\right)$$
$$- \tilde{g}_{\pi N}^2 \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \frac{\boldsymbol{\sigma}_i \cdot \boldsymbol{q}\, \boldsymbol{\sigma}_j \cdot \boldsymbol{q}}{\boldsymbol{q}^2 + M_\pi^2},$$

Smearing of LO contact interactions

$$C_0 = \frac{3}{4} C_{S=0,I=1} + \frac{1}{4} C_{S=1,I=0}$$
$$C_I = \frac{1}{4} C_{S=0,I=1} - \frac{1}{4} C_{S=1,I=0}$$

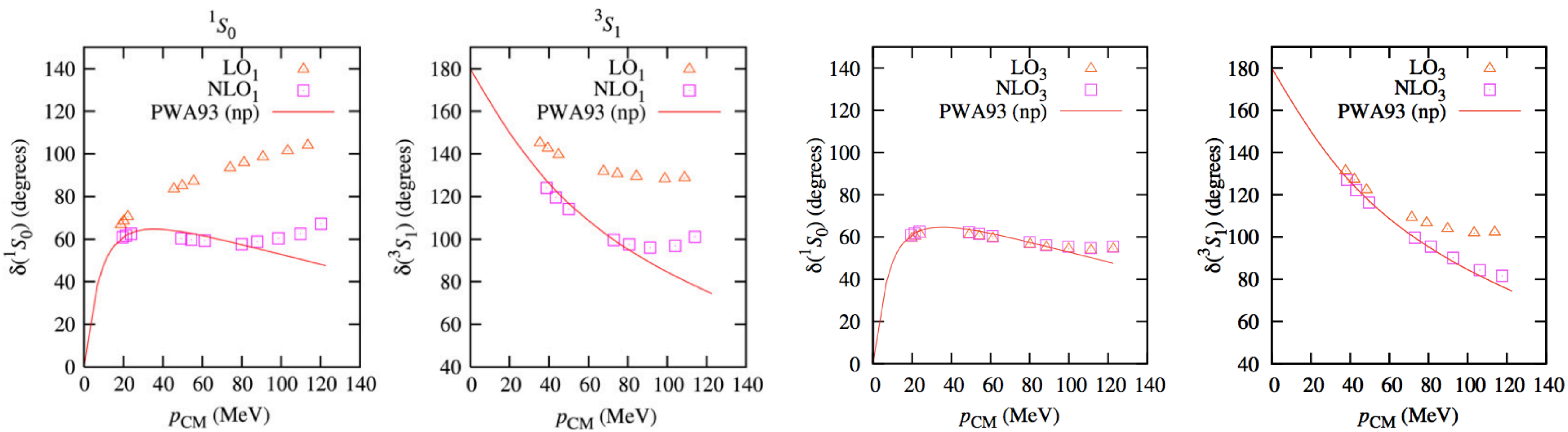
Fix constants from the two-nucleon sector

Lattice EFT is predictive for A > 2 ...



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

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



Gaussian smearing of contact terms

Borasoy, Krebs, Lee, Meißner,
Nucl. Phys. A768 (2006) 179; Eur. Phys. J. A31 (2007) 105;
Lee, Prog. Part. Nucl. Phys. 63 (2009) 179

Euclidean time projection

Ground state energy ...

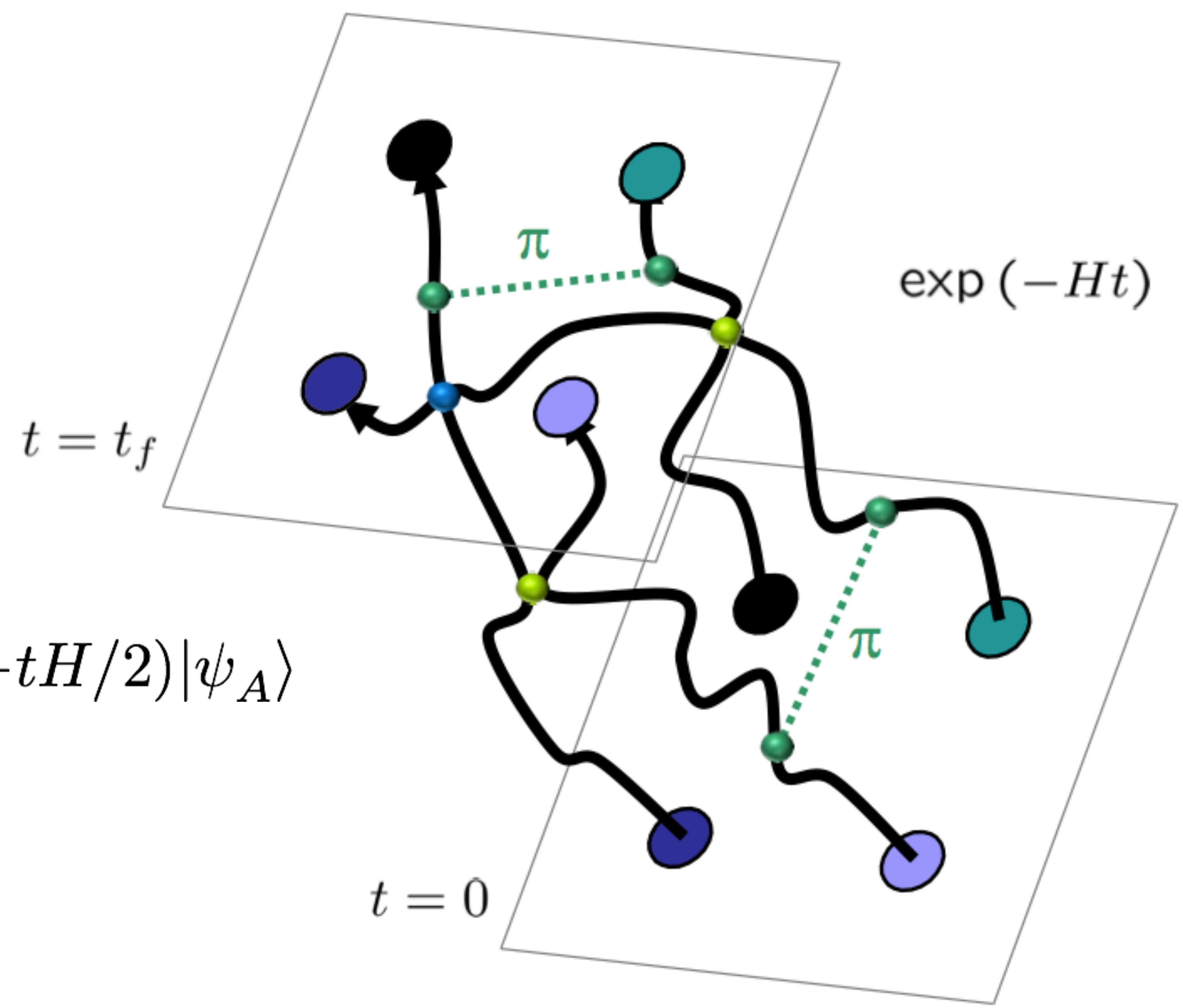
$$Z_A(t) = \langle \psi_A | \exp(-tH) | \psi_A \rangle$$

Lattice Hamiltonian
(discretized)

$$E_A = -\lim_{t \to \infty} \frac{d(\ln Z_A)}{dt}$$

Extrapolation
(from finite time)

Choice of trial wavefunction:
- Standing waves
- Alpha clusters
- Shell model wavefunctions



Operator expectation values ...

$$Z_A^{\mathcal{O}}(t) = \langle \psi_A | \exp(-tH/2) \mathcal{O} \exp(-tH/2) | \psi_A \rangle$$

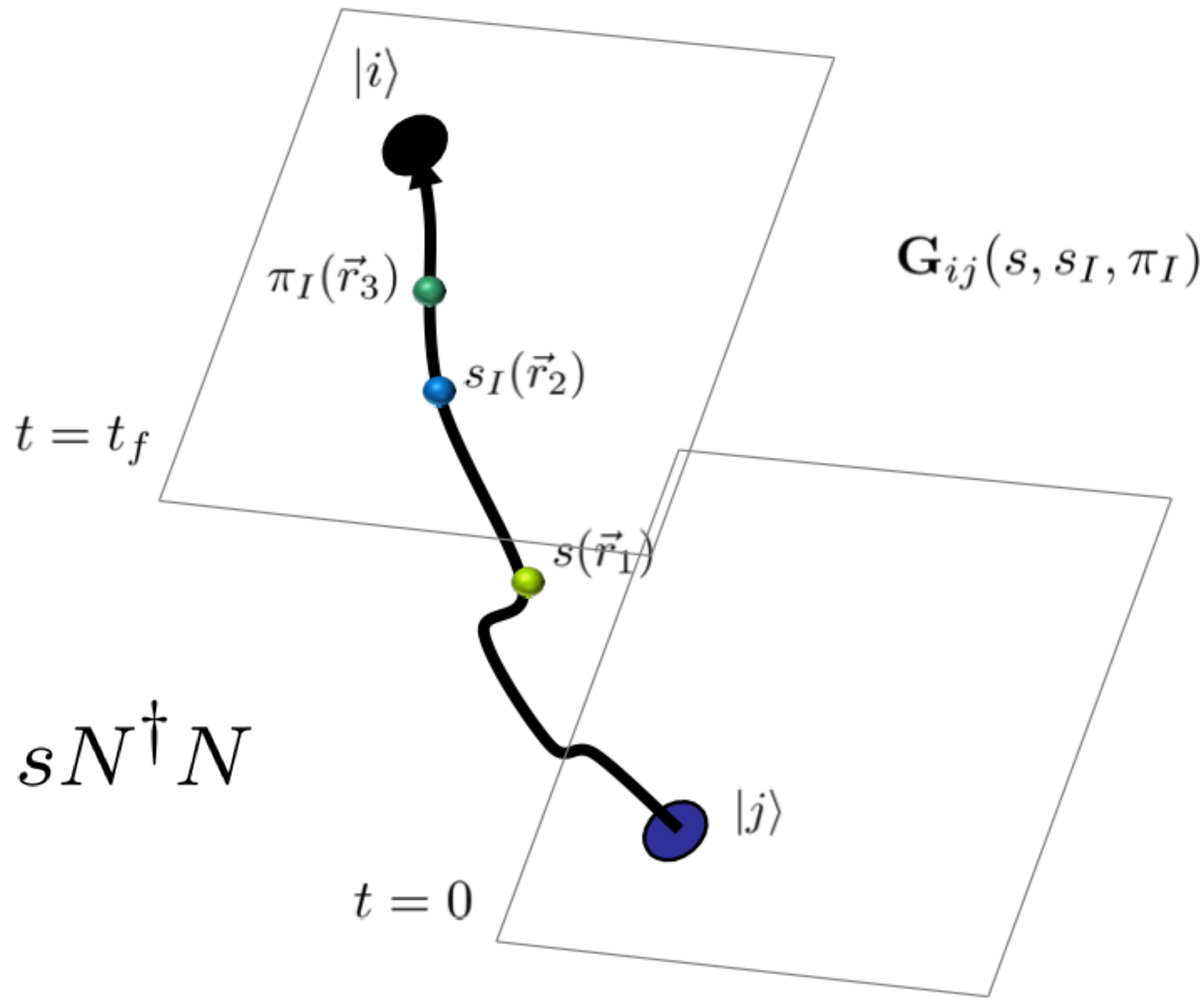
$$\lim_{t \to \infty} \frac{Z_A^{\mathcal{O}}(t)}{Z_A(t)} = \langle \psi_A | \mathcal{O} | \psi_A \rangle$$

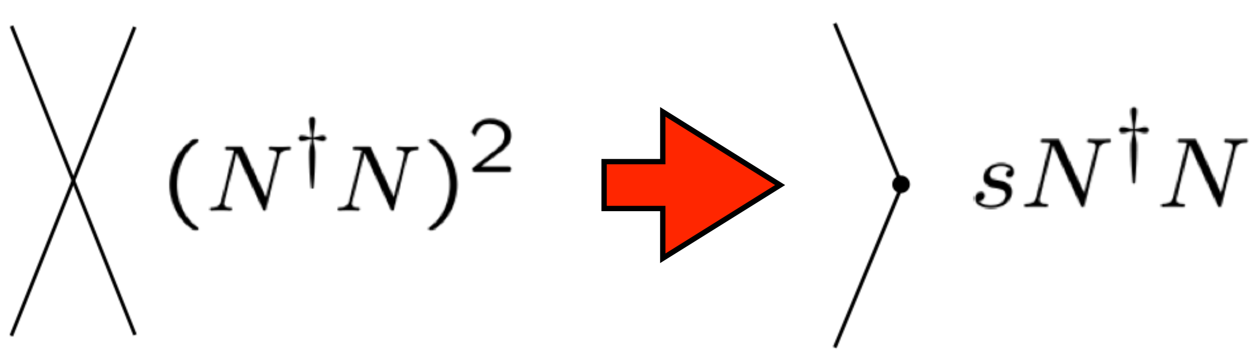
Decoupling of nucleon-nucleon interactions

Hubbard-Stratonovich transformation ...

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

Replace interactions between nucleons with interactions of each nucleus with a background field





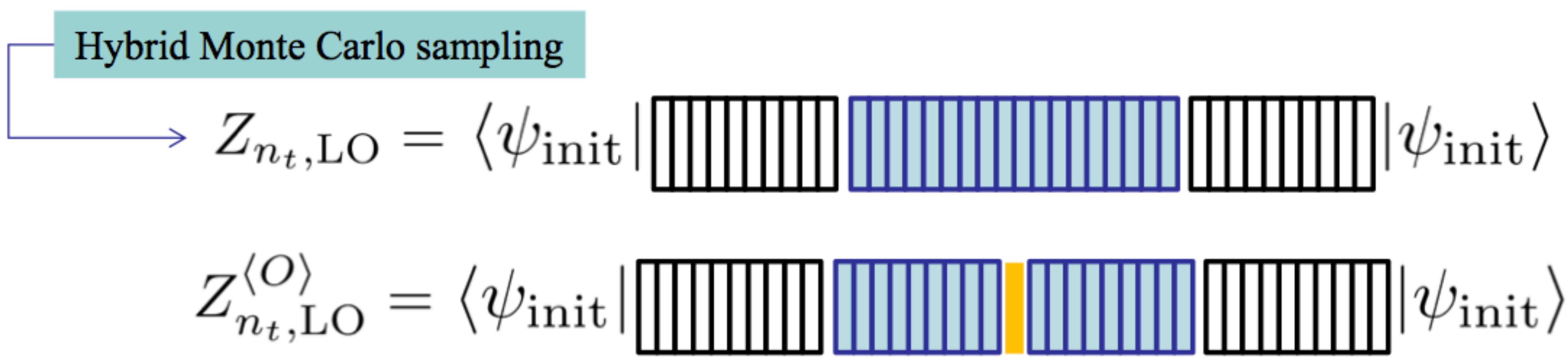
Auxiliary Field Quantum Monte Carlo (AFQMC)

Discretized Euclidean time evolution …

[blue box] $= M_{\rm LO}$ — sign problem (not too severe)

[white box] $= M_{\rm approx}$ — positive definite, strength can be varied

[yellow box] $= O_{\rm observable}$



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

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

For a thorough review, see:
Lee, Prog. Part. Nucl. Phys. 63 (2009) 179

AFQMC + Hybrid Monte Carlo

Substantial investment of supercomputing time …

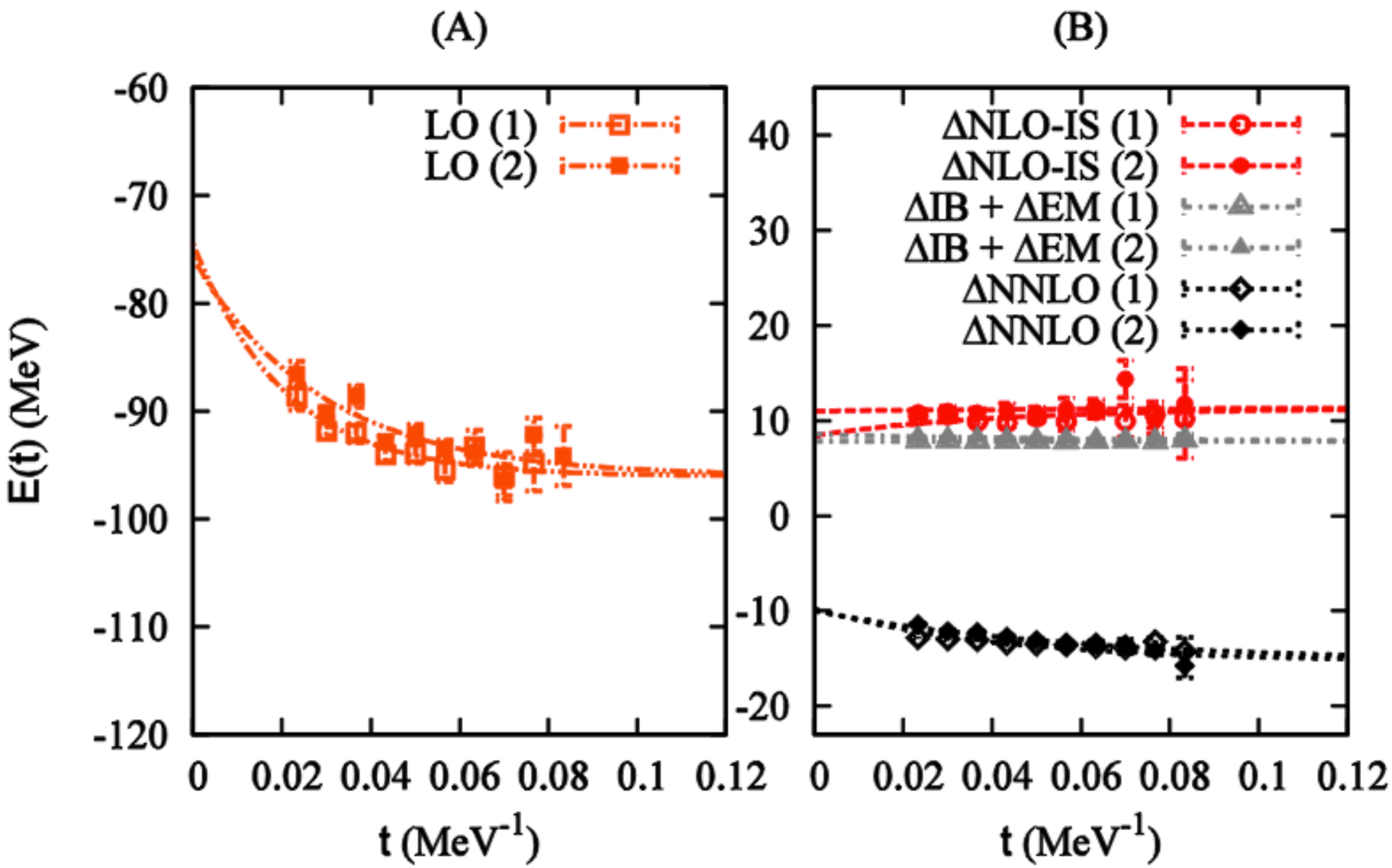
CPU time allocations:

- JUQUEEN (FZ Jülich), 30 Mcore-h (project) + > 100 Mcore-h (institutional)
- RWTH cluster (Aachen), 1.3 Mcore-h (project) + "free CPU time" (long queue)

Figure courtesy of Jülich Supercomputer Centre (JSC)

AFQMC results for ^{12}C (ground state)

Improved NNLO interaction ... a = 1.97 fm



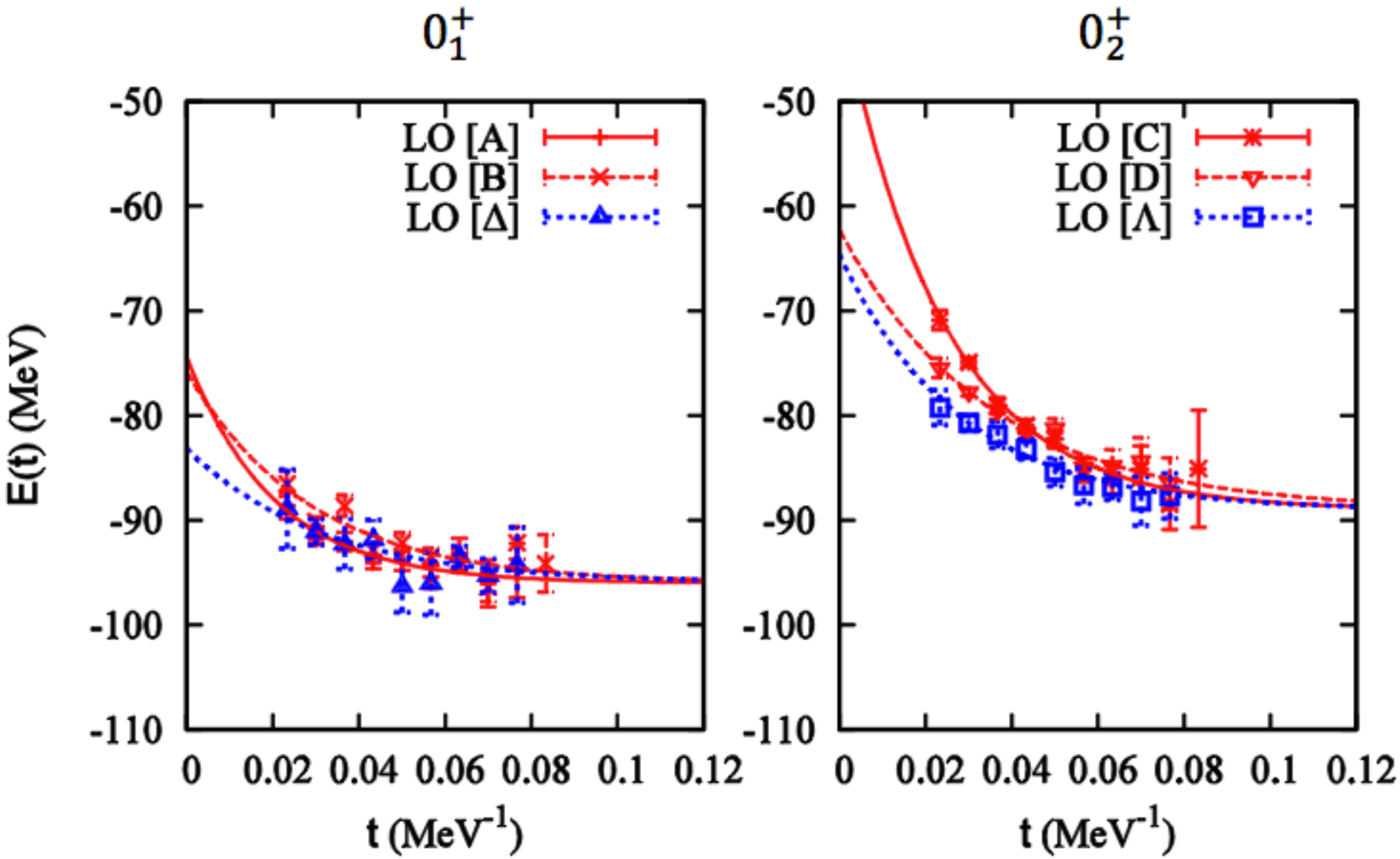
Epelbaum, Krebs, D.L, Meißner, PRL 106 (2011) 192501

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

AFQMC – ground and Hoyle states of ^{12}C

Multiple trial wavefunctions ...

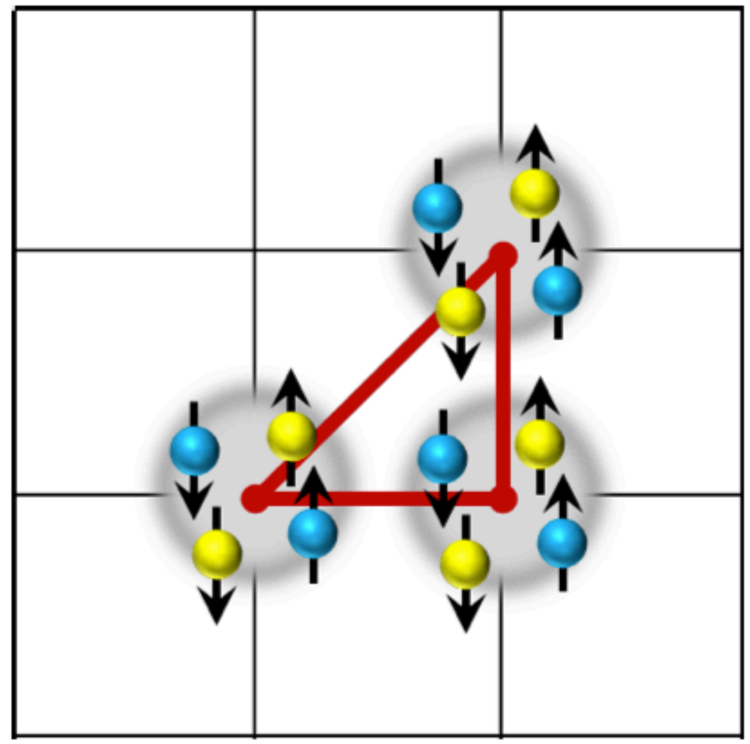
a = 1.97 fm



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

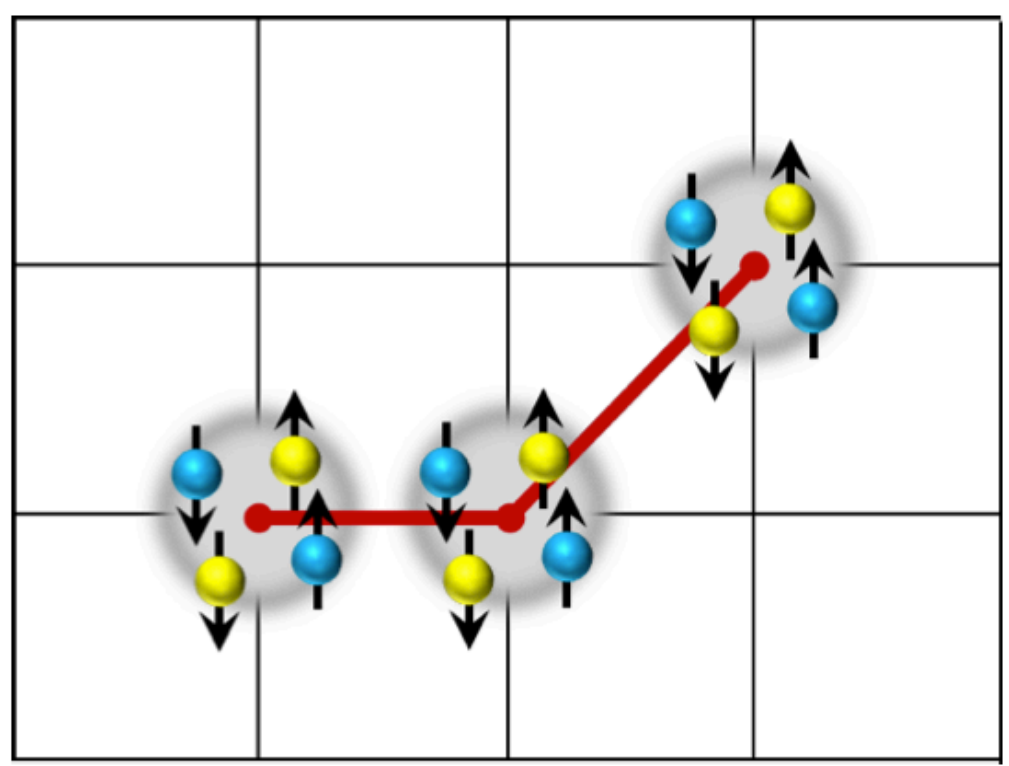
Alpha cluster structure of ^{12}C ...

Ground state



12 rotational orientations

Hoyle state



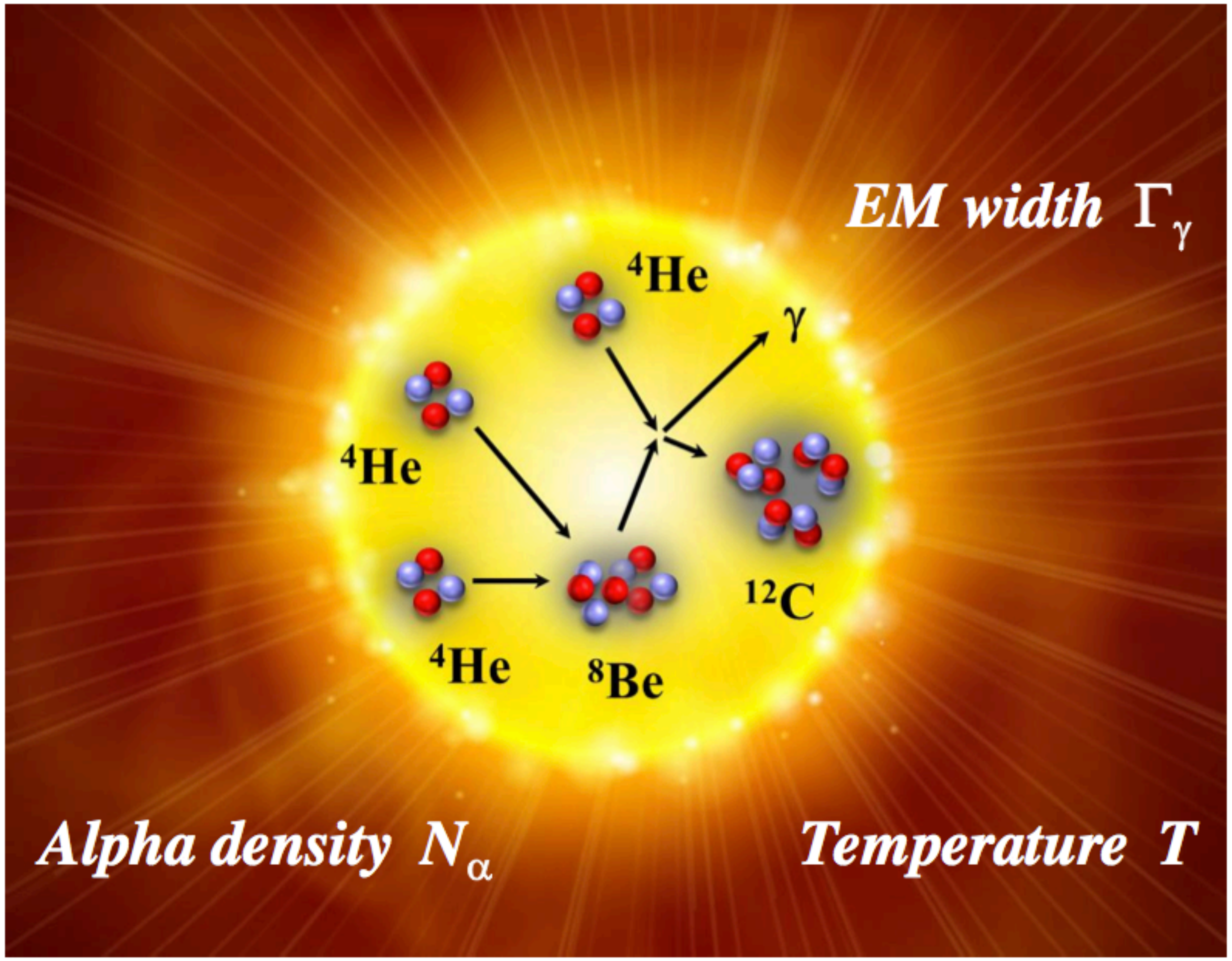
24 rotational orientations

Production of ^{12}C in red giant stars

Resonant production via ^{8}Be and Hoyle state ...

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

Is the Universe fine-tuned?



Energy of Hoyle state in ^{12}C relative to triple alpha

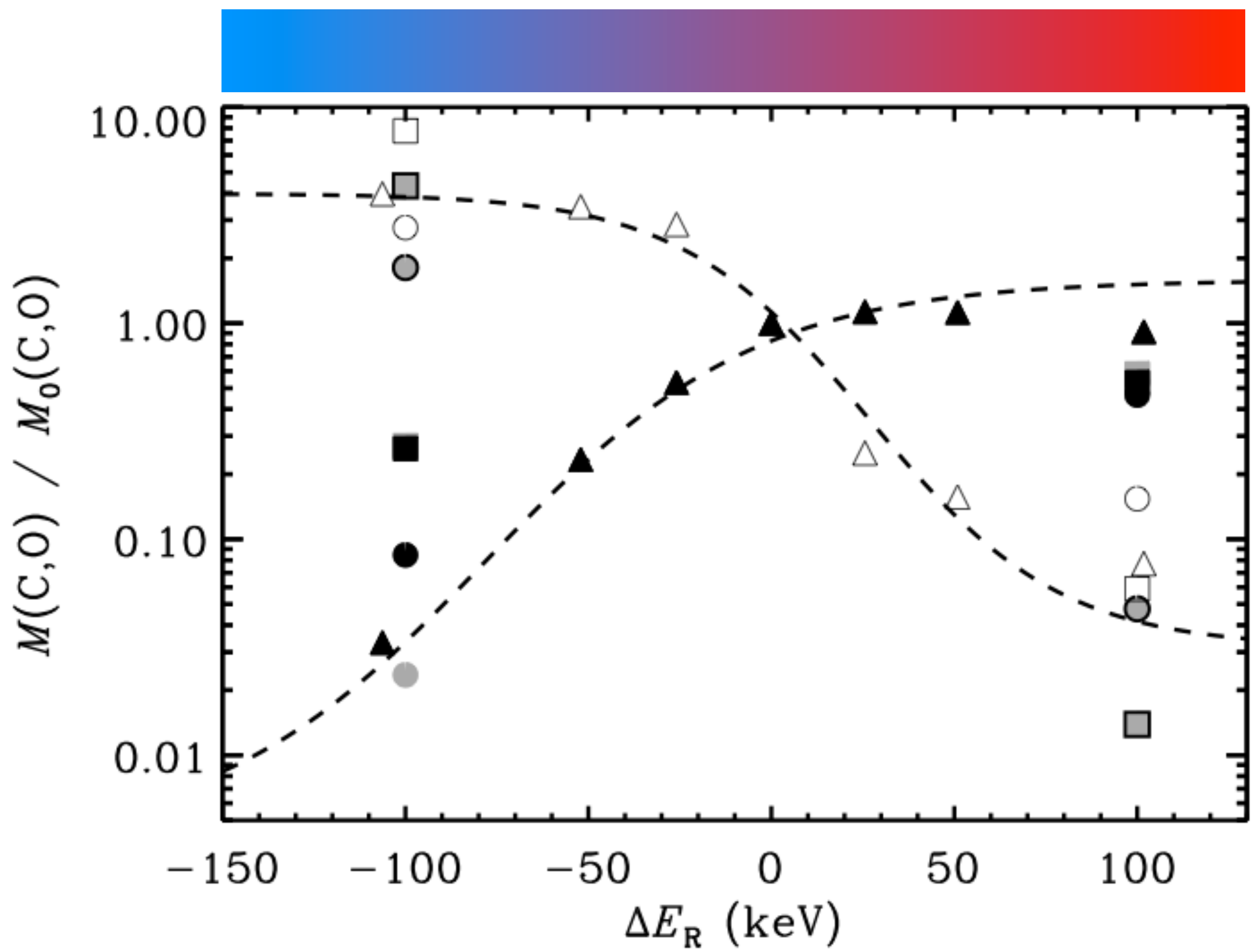
$$\Delta E_b + \Delta E_h = E_{12}^\star - 3E_4$$

Experiment: 379.47 ± 0.18 keV

What if the Hoyle state is moved?

Calculations of stellar nucleosynthesis …

Very little ^{16}O produced: $^{12}C + {}^{4}He \rightarrow {}^{16}O$ too inefficient



All ^{12}C converted to ^{16}O: $^{12}C + {}^{4}He \rightarrow {}^{16}O$ too efficient

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

$$|\delta(\Delta E_{h+b})| < 100 \text{ keV}$$

Anthropic bound on (ad hoc) variation of the Hoyle state

More fundamental description - Chiral EFT

Sources of quark mass dependence ...

ChPT:

$$m_{\pi^\pm}^2 \sim (m_u + m_d)$$

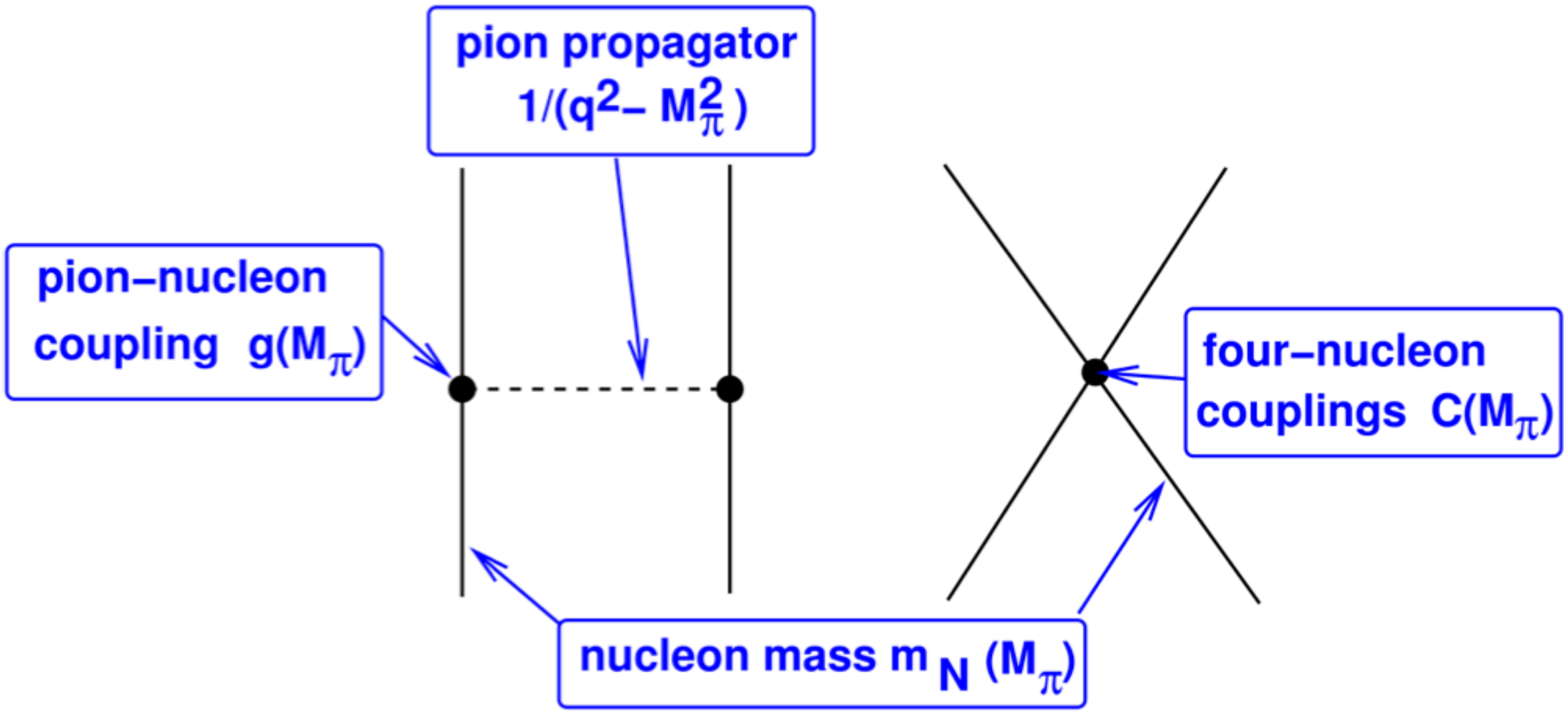


Figure courtesy of U.-G. Meißner

AFQMC calculation for ^{4}He, ^{8}Be and ^{12}C ...

$$E_i = E_i(\tilde{M}_\pi, m_N(M_\pi), \tilde{g}_{\pi N}(M_\pi), C_0(M_\pi), C_I(M_\pi))$$

$$\frac{\partial E_i}{\partial M_\pi}\bigg|_{M_\pi^{\rm ph}} = \frac{\partial E_i}{\partial \tilde{M}_\pi}\bigg|_{M_\pi^{\rm ph}} + x_1 \frac{\partial E_i}{\partial m_N}\bigg|_{m_N^{\rm ph}} + x_2 \frac{\partial E_i}{\partial \tilde{g}_{\pi N}}\bigg|_{\tilde{g}_{\pi N}^{\rm ph}}$$

$$+ x_3 \frac{\partial E_i}{\partial C_0}\bigg|_{C_0^{\rm ph}} + x_4 \frac{\partial E_i}{\partial C_I}\bigg|_{C_I^{\rm ph}}$$

Small shifts around the physical point

$$x_1 := \frac{\partial m_N}{\partial M_\pi}\bigg|_{M_\pi^{\rm ph}}$$

$$x_2 := \frac{\partial \tilde{g}_{\pi N}}{\partial M_\pi}\bigg|_{M_\pi^{\rm ph}} = \frac{1}{2F_\pi}\frac{\partial g_A}{\partial M_\pi}\bigg|_{M_\pi^{\rm ph}} - \frac{g_A}{2F_\pi^2}\frac{\partial F_\pi}{\partial M_\pi}\bigg|_{M_\pi^{\rm ph}}$$

$$x_3 := \frac{\partial C_0}{\partial M_\pi}\bigg|_{M_\pi^{\rm ph}}, \quad x_4 := \frac{\partial C_I}{\partial M_\pi}\bigg|_{M_\pi^{\rm ph}}$$

AFQMC
A = 4 - 12

ChPT,
Lattice QCD

Two-nucleon
scattering

Parameterization of the short-range terms

Lüscher formula ...

$$p\cot\delta = \frac{1}{\pi L}S(\eta) \approx -\frac{1}{a}, \qquad \eta := m_N E\left(\frac{L}{2\pi}\right)^2$$

$$\zeta_i := \frac{m_N L}{4\pi^3}S'(\eta_i)$$

$$q_i := \left.\frac{\partial E_i}{\partial C_0}\right|_{C_0^{\mathrm{ph}}}$$

$$\bar{A} = \frac{\partial a^{-1}}{\partial M_\pi} = -\frac{1}{\pi L}S'(\eta)\frac{\partial \eta}{\partial M_\pi}$$

$$-\zeta_s^{-1}\,\bar{A}_s = \left.\frac{\partial E_s}{\partial \tilde{M}_\pi}\right|_{M_\pi^{\mathrm{ph}}} + x_1\frac{E_s}{m_N} + x_1\left.\frac{\partial E_s}{\partial m_N}\right|_{m_N^{\mathrm{ph}}} + x_2\left.\frac{\partial E_s}{\partial \tilde{g}_{\pi N}}\right|_{\tilde{g}_{\pi N}^{\mathrm{ph}}} + x_3 q_s + x_4 q_s\,,$$

$$-\zeta_t^{-1}\,\bar{A}_t = \left.\frac{\partial E_t}{\partial \tilde{M}_\pi}\right|_{M_\pi^{\mathrm{ph}}} + x_1\frac{E_t}{m_N} + x_1\left.\frac{\partial E_t}{\partial m_N}\right|_{m_N^{\mathrm{ph}}} + x_2\left.\frac{\partial E_t}{\partial \tilde{g}_{\pi N}}\right|_{\tilde{g}_{\pi N}^{\mathrm{ph}}} + x_3 q_t - 3x_4 q_t\,,$$

Two-nucleon problem (no AFQMC)

Theory (ChPT) + Lattice QCD

^{4}He

$$\left.\frac{\partial E_4}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} = -0.339(5) \left.\frac{\partial a_s^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} - 0.697(4) \left.\frac{\partial a_t^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} + 0.0380(14)^{+0.008}_{-0.006}$$

^{8}Be

$$\left.\frac{\partial E_8}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} = -0.794(32) \left.\frac{\partial a_s^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} - 1.584(23) \left.\frac{\partial a_t^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} + 0.089(9)^{+0.017}_{-0.011}$$

^{12}C (ground)

$$\left.\frac{\partial E_{12}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} = -1.52(3) \left.\frac{\partial a_s^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} - 2.88(2) \left.\frac{\partial a_t^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} + 0.159(7)^{+0.023}_{-0.018}$$

^{12}C (Hoyle)

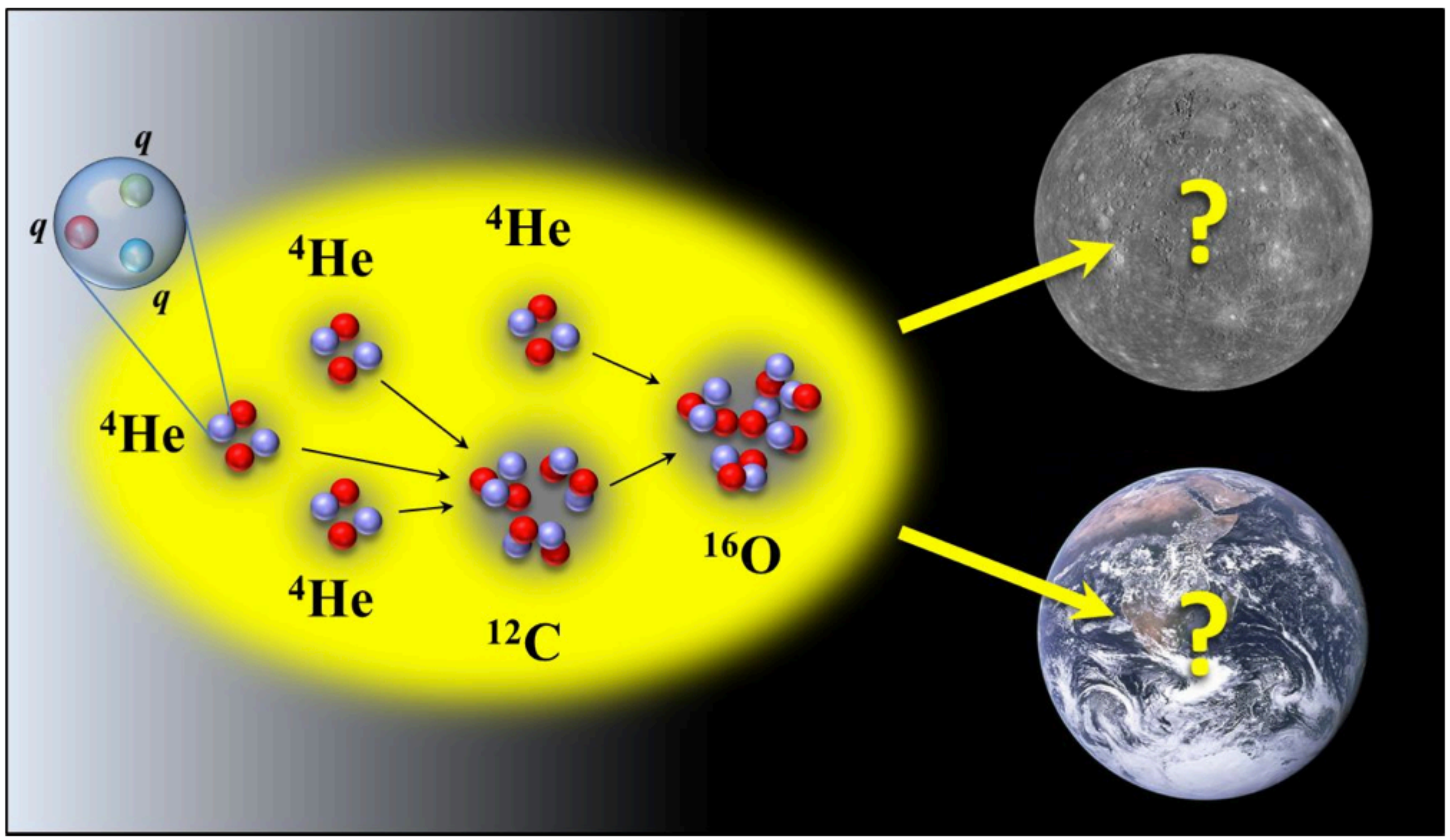
$$\left.\frac{\partial E_{12}^\star}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} = -1.588(11) \left.\frac{\partial a_s^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} - 3.025(8) \left.\frac{\partial a_t^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} + 0.178(4)^{+0.026}_{-0.021}$$

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

$$\left.\frac{\partial \Delta E_{h+b}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} = -0.572(19) \left.\frac{\partial a_s^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} - 0.933(15) \left.\frac{\partial a_t^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} + 0.064(6)^{+0.010}_{-0.009}$$

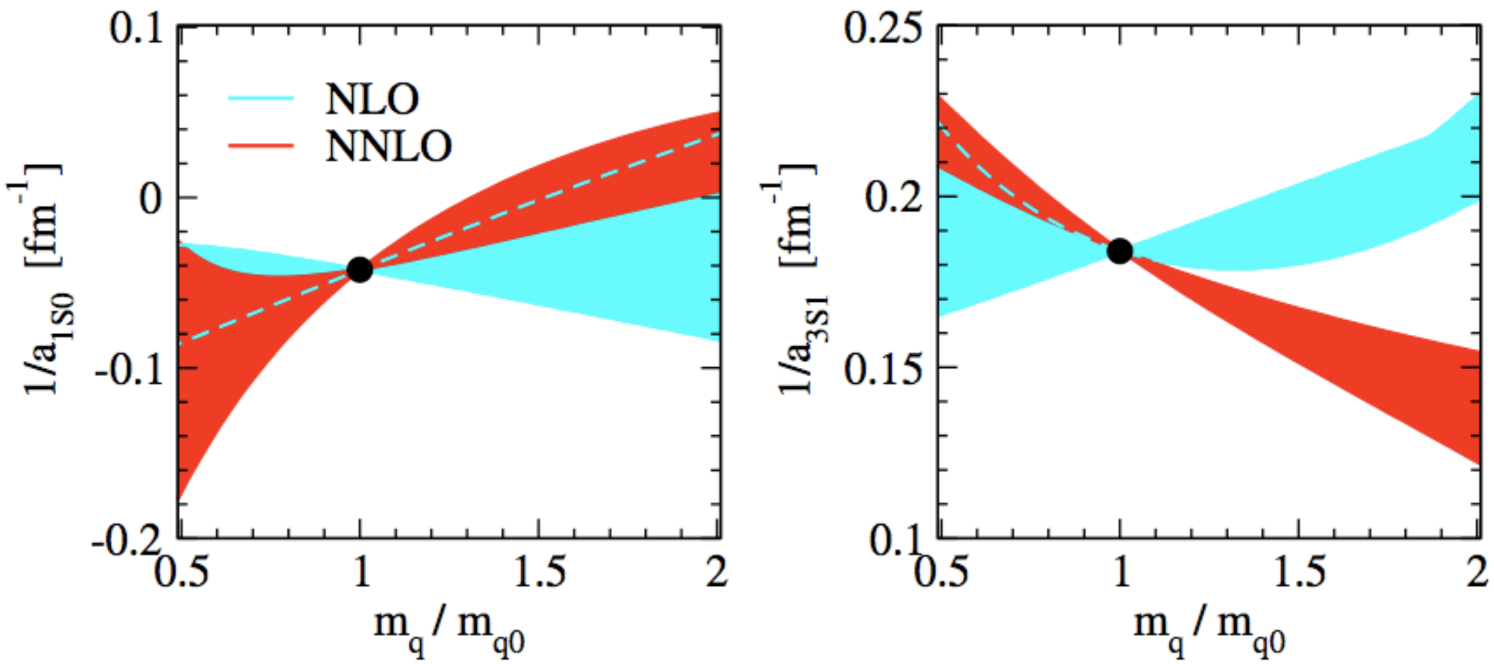
--> Viability of carbon-oxygen based life: $|\delta(\Delta E_{h+b})| < 100 \text{ keV}$

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



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

Current theoretical knowledge of the quark mass dependence of the S-wave scattering lengths ...



$$-\frac{\partial a_s^{-1}}{\partial m_\pi} \equiv \frac{A_s}{a_s m_\pi}, \quad A_s \equiv \frac{K^q_{a_s}}{K^q_\pi},$$

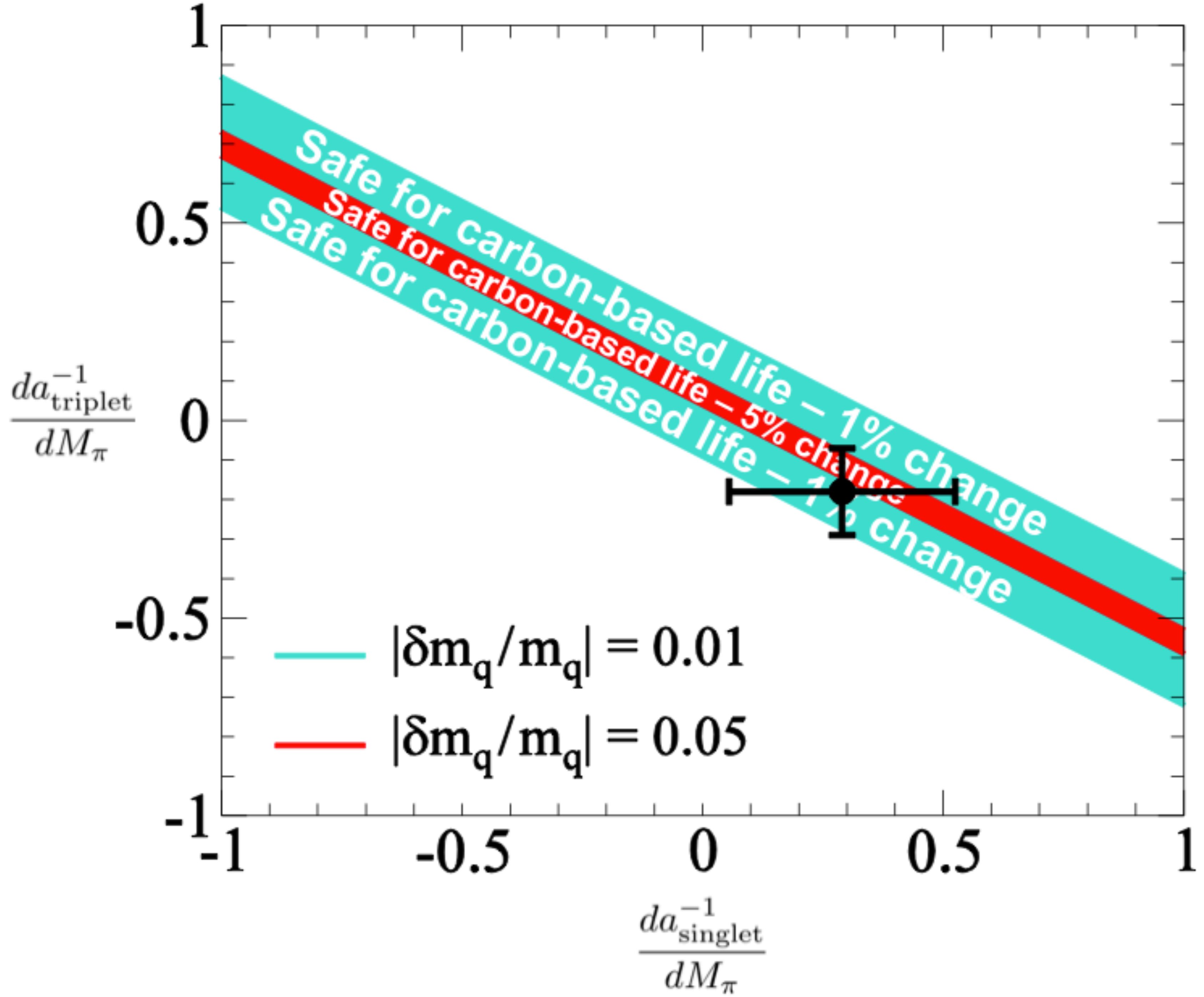
$$\boxed{K^q_{a_s} = 2.3^{+1.9}_{-1.8}, \qquad K^q_{a_t} = 0.32^{+0.17}_{-0.18}}$$

$$\bar{A}_t \equiv \left.\frac{\partial a_t^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} = \frac{-197.33 \text{ MeV fm}}{5.4 \text{ fm} \times 134.98 \text{ MeV}} \times \frac{0.32^{+0.17}_{-0.18}}{0.494^{+0.009}_{-0.013}} \simeq -0.18^{+0.10}_{-0.10}$$

$$\bar{A}_s \equiv \left.\frac{\partial a_s^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}} = \frac{-197.33 \text{ MeV fm}}{-23.8 \text{ fm} \times 134.98 \text{ MeV}} \times \frac{2.3^{+1.9}_{-1.8}}{0.494^{+0.009}_{-0.013}} \simeq 0.29^{+0.25}_{-0.23}$$

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

The "end of the world" plot :)



Epelbaum, Krebs, Lähde, Lee, Meißner,
Phys. Rev. Lett. 110 (2013) 112502; arXiv:1303.4856

Upcoming results

Spectra of Oxygen-16 and Neon-20

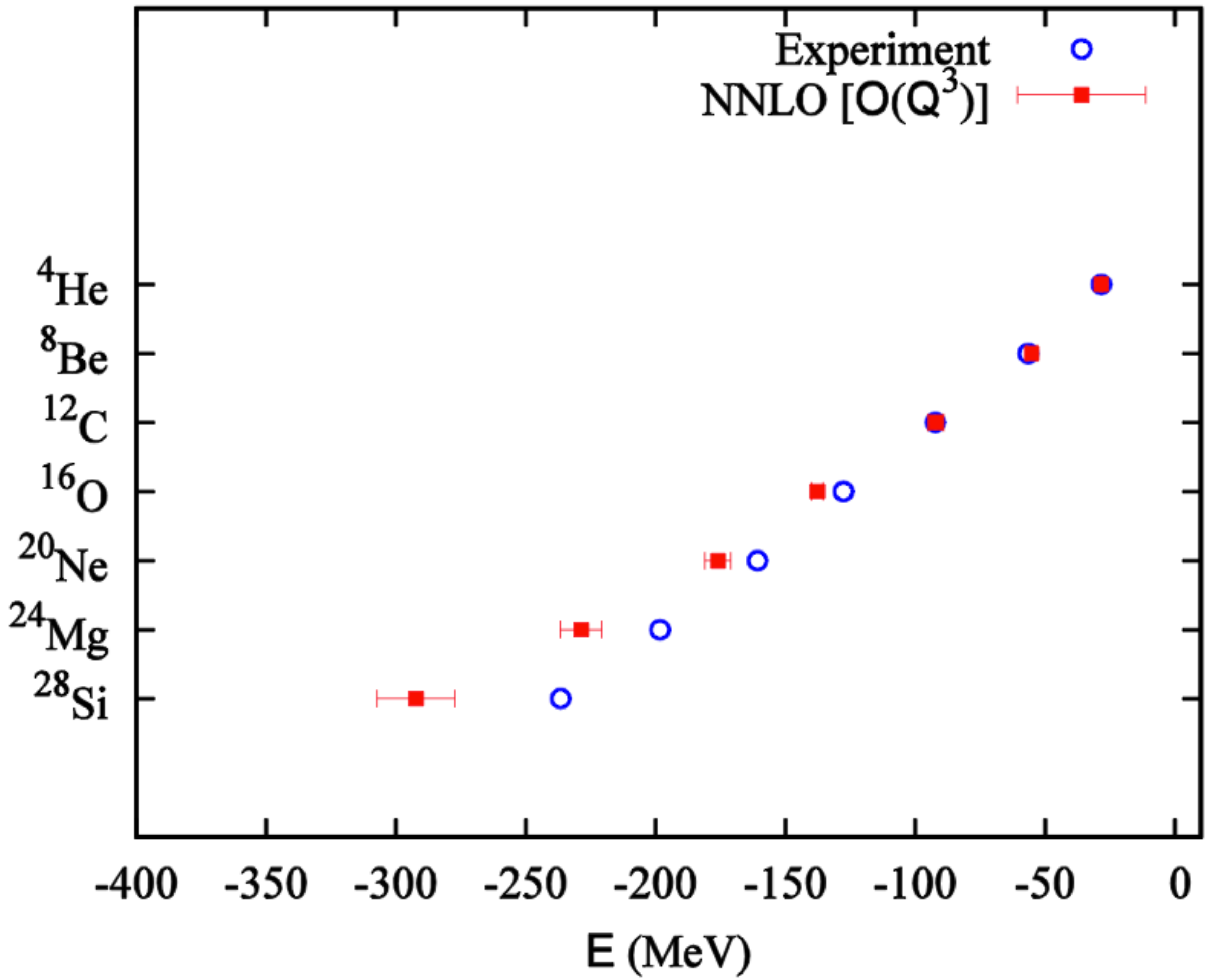
Extension of nuclear lattice EFT up to A = 28

First AFQMC results for non-alpha-cluster nuclei

Extension of chiral NN interaction to N3LO

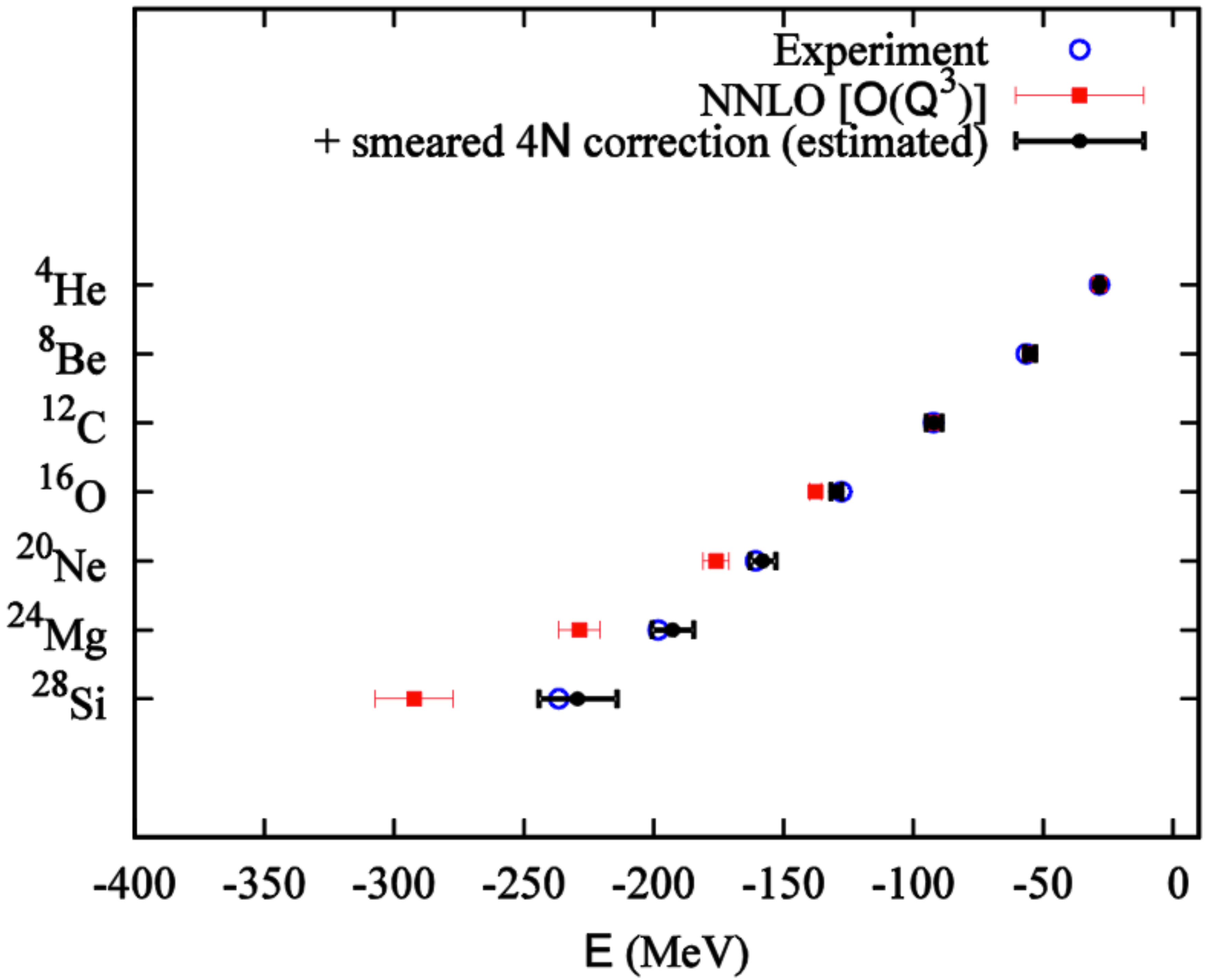
Effects of lattice spacing and finite volume

Preliminary results for binding energies up to A = 28 ...



Improved NNLO interaction
(includes contact 4N correction)

Preliminary results for binding energies up to A = 28 ...



Improved NNLO interaction
+ smeared 4N correction