Lattice Nuclear Physics

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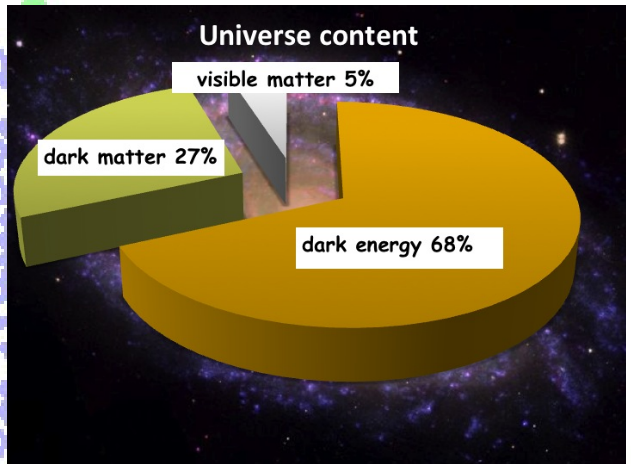
CONTENTS

- Introduction: The BIG picture
- Basics of nuclear lattice simulations
- Results from nuclear lattice simulations
- Ab initio alpha-alpha scattering
- New insights into nuclear clustering
- Summary & outlook

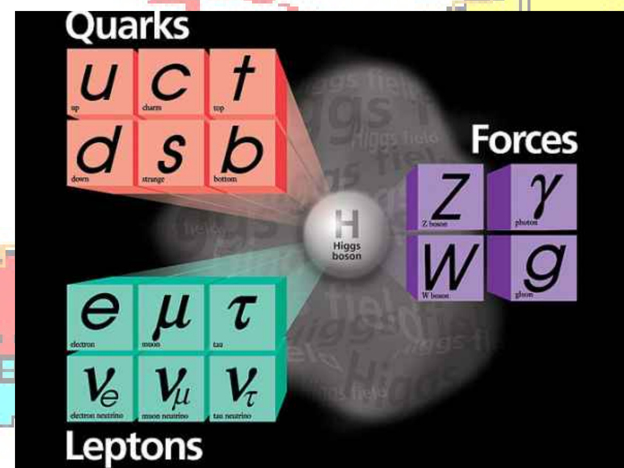
The BIG Picture

WHY NUCLEAR PHYSICS?

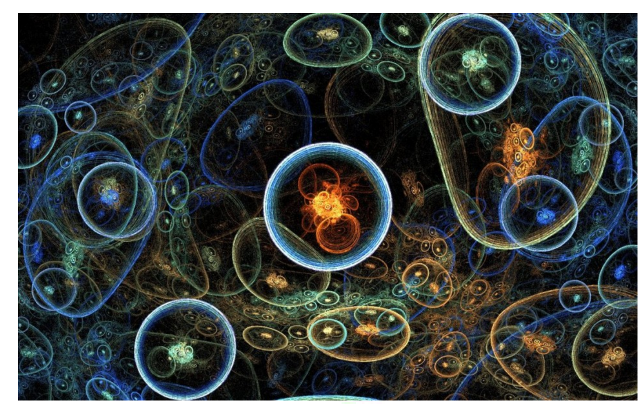
- The matter we are made off



- The last frontier of the SM

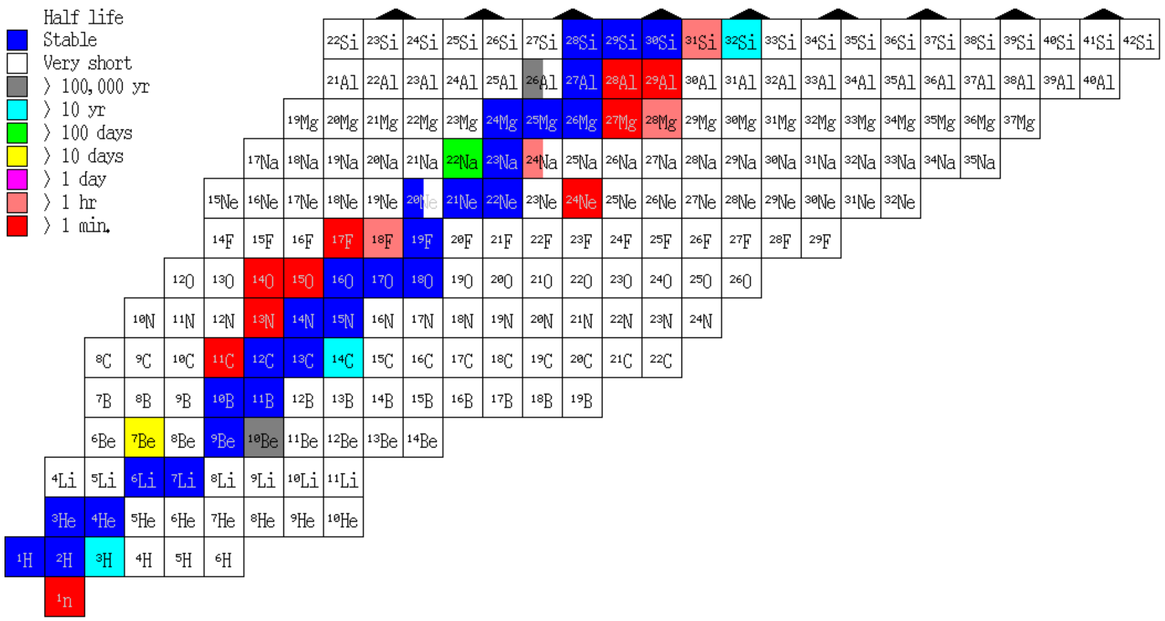


- Access to the Multiverse



AB INITIO NUCLEAR STRUCTURE and SCATTERING

- Nuclear structure:
  - ⋆ 3-nucleon forces
  - ⋆ limits of stability
  - ⋆ alpha-clustering
  - ⋮

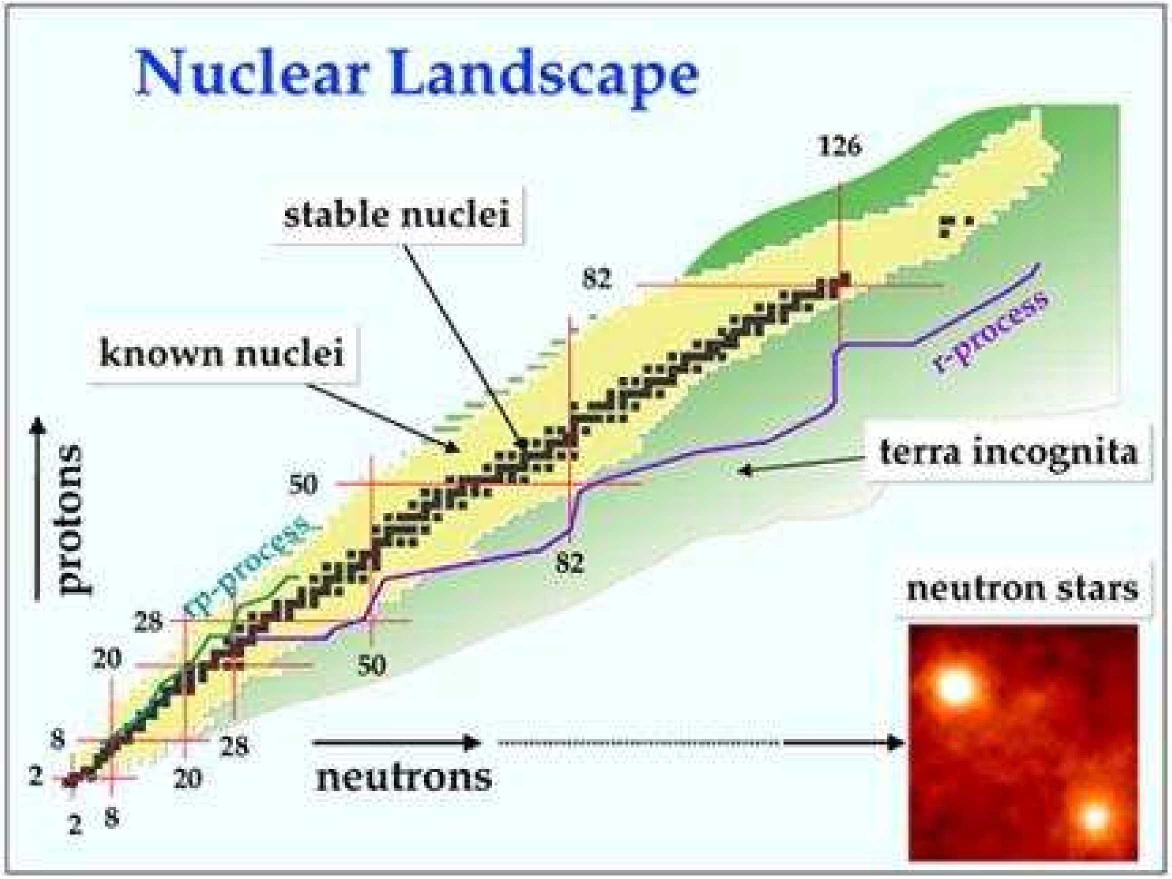


ⓒ National Nuclear Data Center

- Nuclear scattering: processes relevant for nuclear astrophysics
  - ⋆ alpha-particle scattering: $^4\text{He} + {}^4\text{He} \to {}^4\text{He} + {}^4\text{He}$
  - ⋆ triple-alpha reaction: $^4\text{He} + {}^4\text{He} + {}^4\text{He} \to {}^{12}\text{C} + \gamma$
  - ⋆ alpha-capture on carbon: $^4\text{He} + {}^{12}\text{C} \to {}^{16}\text{O} + \gamma$
  - ⋮

THE NUCLEAR LANDSCAPE: AIMS & METHODS

- Theoretical methods:
  - Lattice QCD: A = 0,1,2, . . .
  - NCSM, Faddeev-Yakubowsky, GFMC, ... : A = 3 - 16
  - coupled cluster, . . .: A = 16 -100
  - density functional theory, . . .: $A \geq 100$
- Chiral EFT:
  - provides **accurate 2N, 3N and 4N forces**
  - successfully applied in light nuclei with A = 2, 3, 4
  - combine with simulations to get to larger A



⇒ Chiral Nuclear Lattice Effective Field Theory

Basics of nuclear lattice simulations

for an easy intro, see: UGM, Nucl. Phys. News **24** (2014) 11

for an early review, see: D. Lee, Pr og. Part. Nucl. Phys. **63** (2009) 117

upcoming textbook, see: T. Lähde, UGM, Springer Lecture Notes in Physics

NUCLEAR LATTICE EFFECTIVE FIELD THEORY

Frank, Brockmann (1992), Koonin, Müller, Seki, van Kolck (2000) , Lee, Schäfer (2004), . . .
Borasoy, Krebs, Lee, UGM, Nucl. Phys. **A768** (2006) 179; Borasoy, Epelbaum, Krebs, Lee, UGM, Eur. Phys. J. **A31** (2007) 105

- *new method* to tackle the nuclear many-body problem

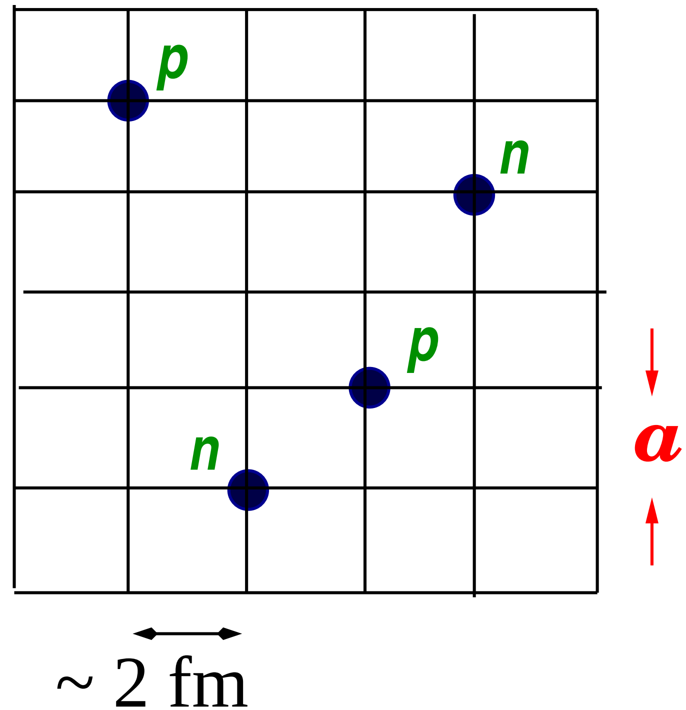
- discretize space-time $V = L_s \times L_s \times L_s \times L_t$:
  nucleons are point-like particles on the sites

- discretized chiral potential w/ pion exchanges
  and contact interactions + Coulomb

→ see Epelbaum, Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773

- typical lattice parameters

$$p_{\rm max} = \frac{\pi}{a} \simeq 314\ \text{MeV [UV cutoff]}$$



- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

E. Wigner, Phys. Rev. **51** (1937) 106; T. Mehen et al., Phys. Rev. Lett. **83** (1999) 931; J. W. Chen et al., Phys. Rev. Lett. **93** (2004) 242302

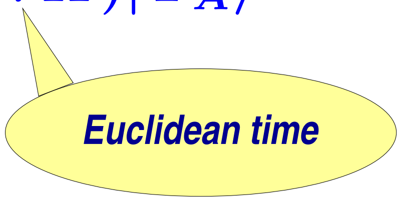
- physics independent of the lattice spacing for $a = 1 \ldots 2$ fm

J. Alarcon et al., EPJA **53** (2017) 83

TRANSFER MATRIX METHOD

- Correlation–function for A nucleons: $Z_A(\tau) = \langle \Psi_A | \exp(-\tau H) | \Psi_A \rangle$

  with Ψ_A a Slater determinant for A free nucleons
  [or a more sophisticated (correlated) initial/final state]



- Transient energy

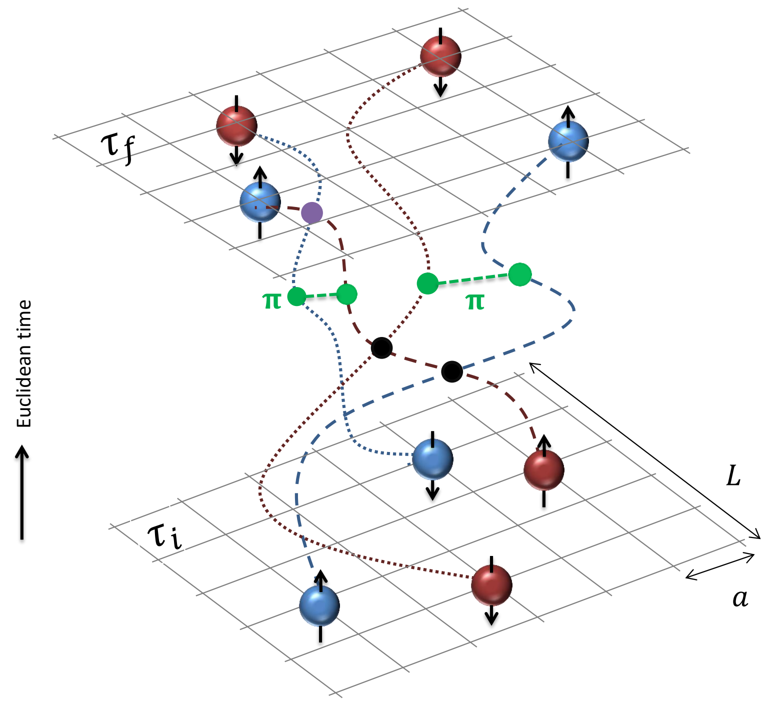
$$E_A(\tau) = -\frac{d}{d\tau} \ln Z_A(\tau)$$

$\rightarrow$ ground state: $E_A^0 = \lim_{\tau\to\infty} E_A(\tau)$

- Exp. value of any normal–ordered operator $\mathcal{O}$

$$Z_A^{\mathcal{O}} = \langle \Psi_A | \exp(-\tau H/2)\, \mathcal{O}\, \exp(-\tau H/2)\, | \Psi_A \rangle$$

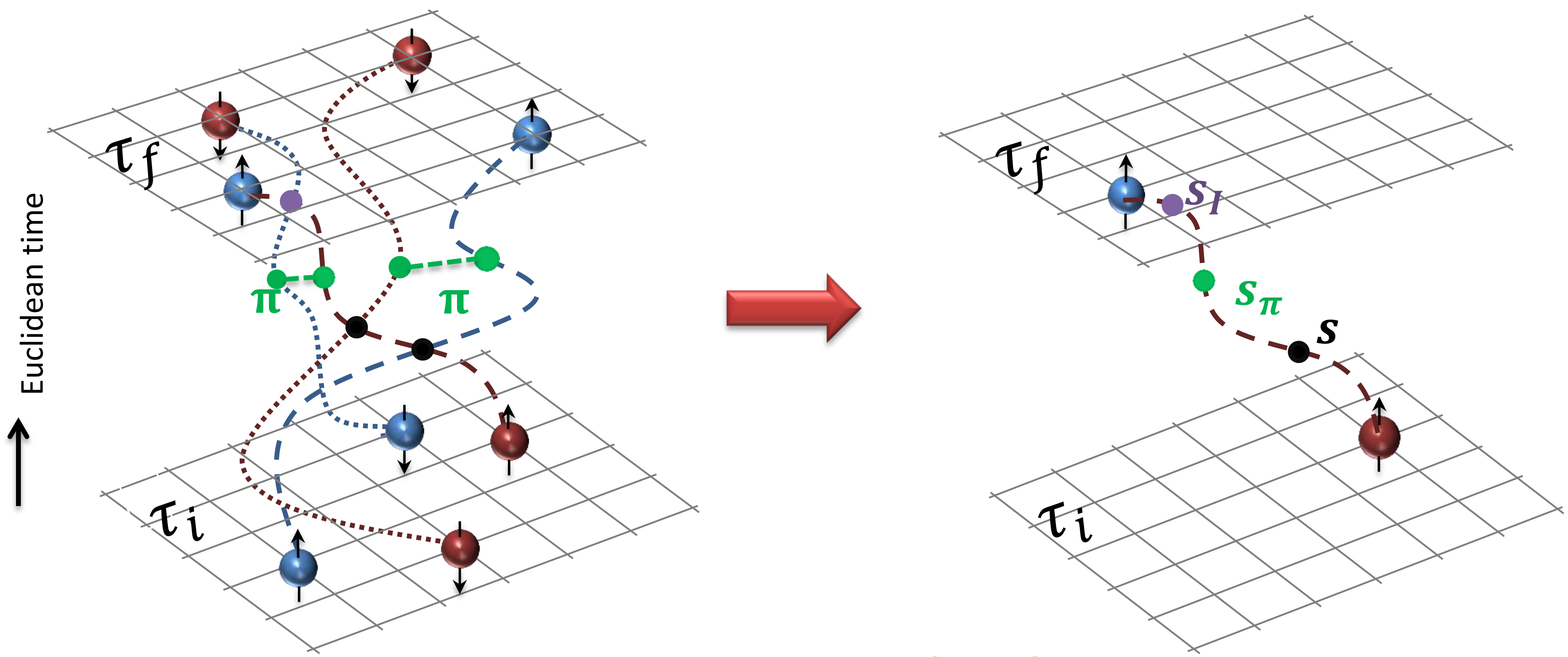
$$\lim_{\tau\to\infty} \frac{Z_A^{\mathcal{O}}(\tau)}{Z_A(\tau)} = \langle \Psi_A | \mathcal{O}\, | \Psi_A \rangle$$



AUXILIARY FIELD METHOD

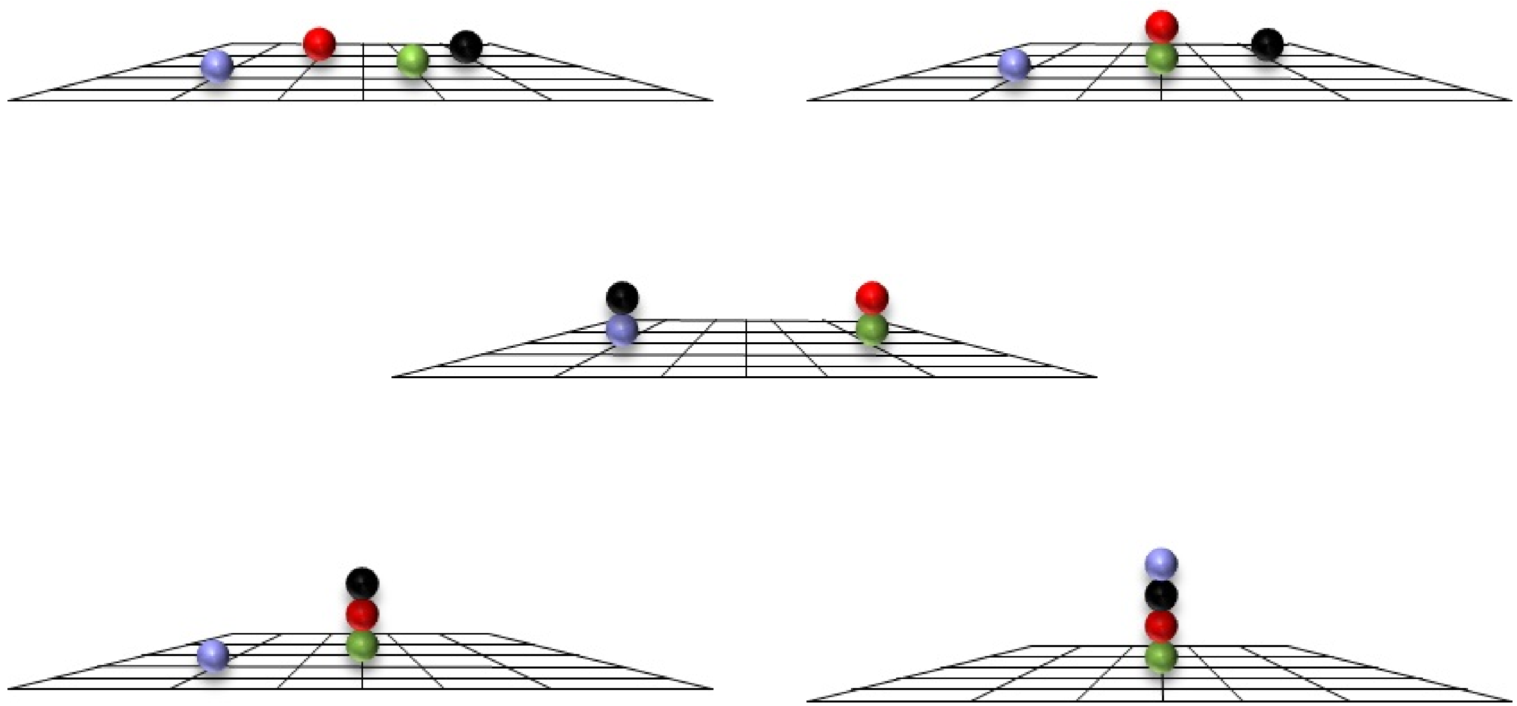
- Represent interactions by auxiliary fields [Gaussian quadrature]:

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



→ PARALLELISATION

CONFIGURATIONS



⇒ all *possible* configurations are sampled

⇒ preparation of *all possible* initial/final states

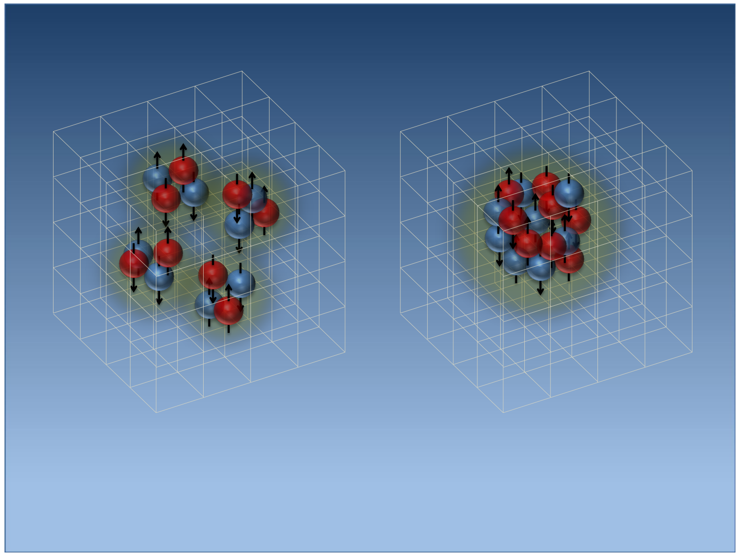
⇒ *clustering* emerges *naturally*

COMPUTATIONAL EQUIPMENT

- Present = JUQUEEN (BlueGene/Q)
- Soon = GPU-coding (QBiG, TITAN, . . .)

6 Pflops

Lattice: some results



NLEFT

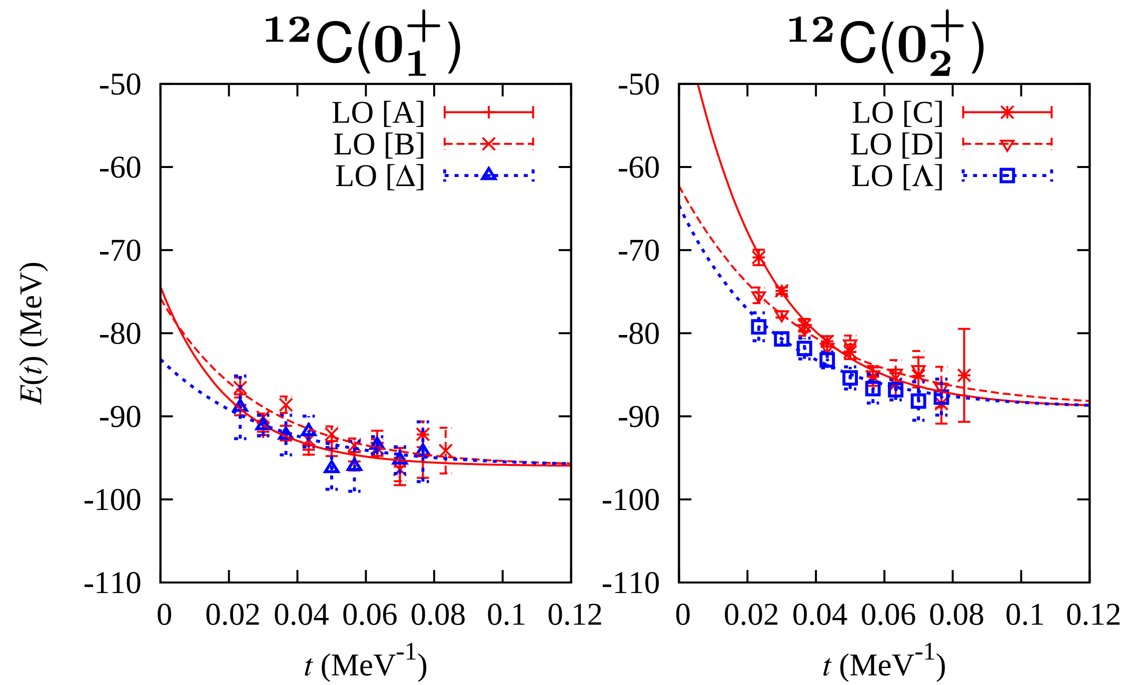
Epelbaum, Krebs, Lähde, Lee, Luu, UGM, Rupak + post-docs + students

FIXING PARAMETERS and FIRST RESULTS

Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. **104** (2010) 142501; Eur. Phys. J. A **45** (2010) 335; . . .

- some groundstate energies and differences [NNLO, 11+2 LECs]

	E [MeV]	NLEFT	Exp.
old algorithm	^{3}He - ^{3}H	0.78(5)	0.76
	^{4}He	−28.3(6)	−28.3
	^{8}Be	−55(2)	−56.5
	^{12}C	−92(3)	−92.2
new algorithm	^{16}O	−131(1)	−127.6
	^{20}Ne	−166(1)	−160.6
	^{24}Mg	−198(2)	−198.3
	^{28}Si	−234(3)	−236.5



- promising results ⇒ uncertainties down to the 1% level
- excited states more difficult ⇒ projection MC method + triangulation

A SHORT HISTORY of the HOYLE STATE

- Heavy element generation in massive stars: triple-α process

Bethe 1938, Öpik 1952, Salpeter 1952, Hoyle 1954, ...

$$^4\text{He} + {}^4\text{He} \rightleftharpoons {}^8\text{Be}$$
$$^8\text{Be} + {}^4\text{He} \rightleftharpoons {}^{12}\text{C}^* \rightarrow {}^{12}\text{C} + \gamma$$
$$^{12}\text{C} + {}^4\text{He} \rightleftharpoons {}^{16}\text{O} + \gamma$$

- Hoyle's contribution: calculation of the relative abundances of ^{4}He, ^{12}C and ^{16}O
  $\Rightarrow$ need a resonance close to the ^{8}Be + ^{4}He threshold at $E_R \simeq 0.37$ MeV
  $\Rightarrow$ this corresponds to a $J^P = 0^+$ excited state 7.7 MeV above the g.s.

- a corresponding state was experimentally confirmed at Caltech at
  $E - E(\text{g.s.}) = 7.653 \pm 0.008$ MeV — Dunbar et al. 1953, Cook et al. 1957

- still on-going experimental activity, e.g. EM transitions at SDALINAC
  M. Chernykh et al., Phys. Rev. Lett. 98 (2007) 032501

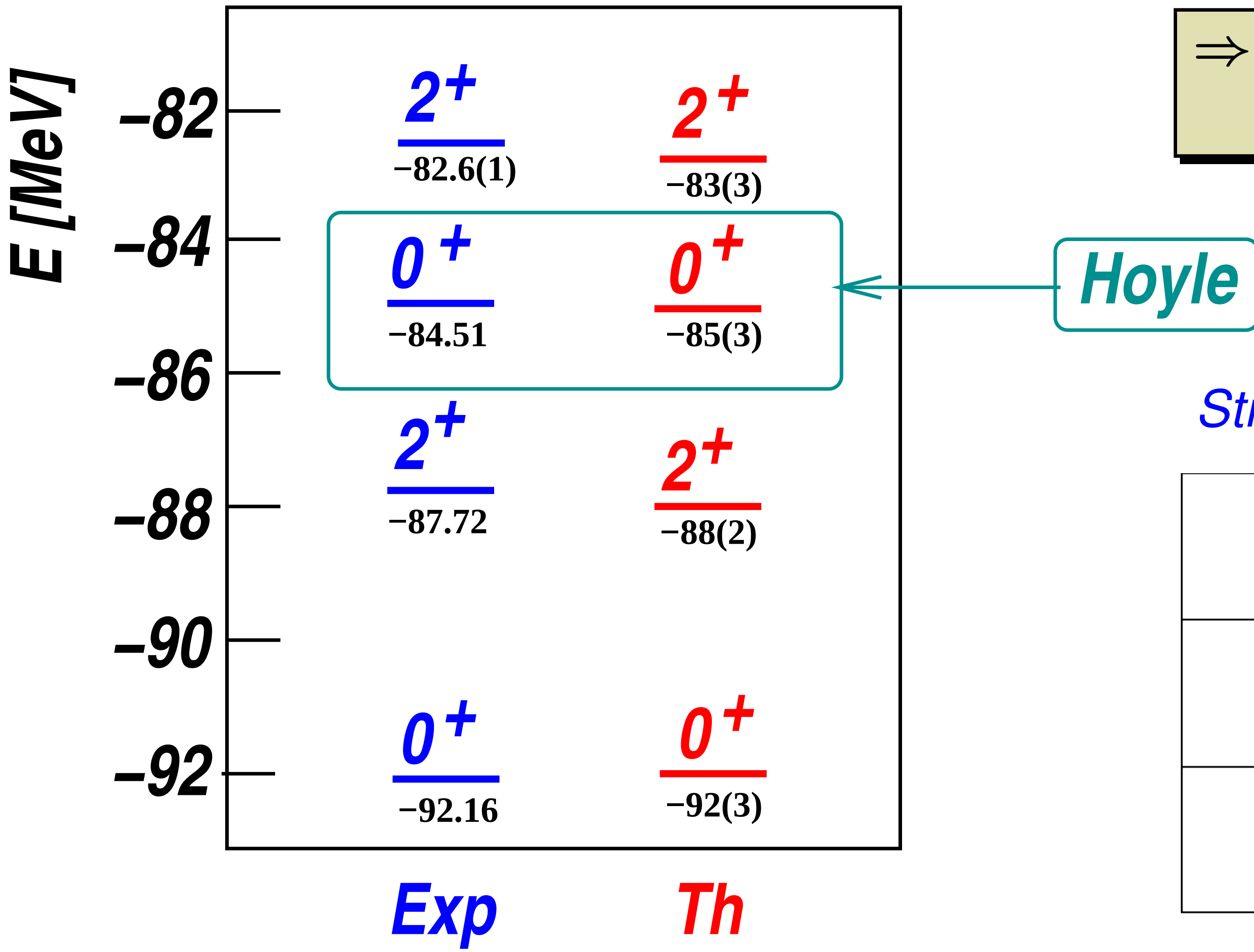
- an **enigma** to *ab initio* nuclear theory until 2011

BREAKTHROUGH: SPECTRUM of CARBON-12

Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. 106 (2011) 192501

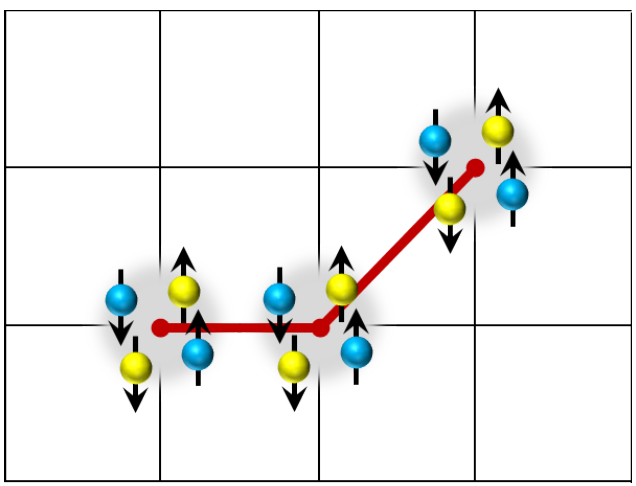
Epelbaum, Krebs, Lähde, Lee, UGM, Phys. Rev. Lett. 109 (2012) 252501

- After $8 \cdot 10^6$ hrs JUGENE/JUQUEEN (and "some" human work)

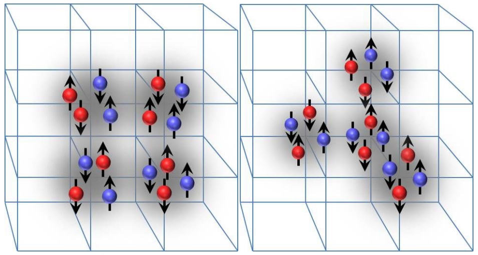


⇒ First ab initio calculation of the Hoyle state ✓

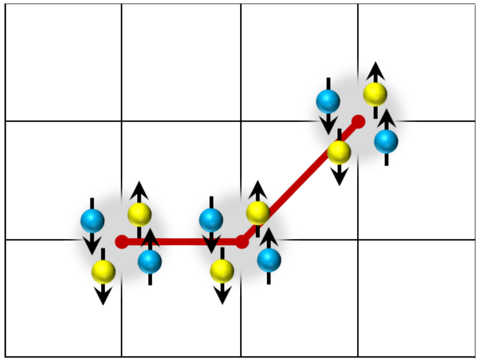
Structure of the Hoyle state:

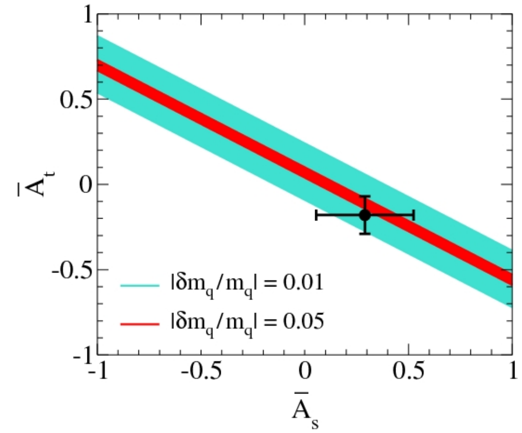


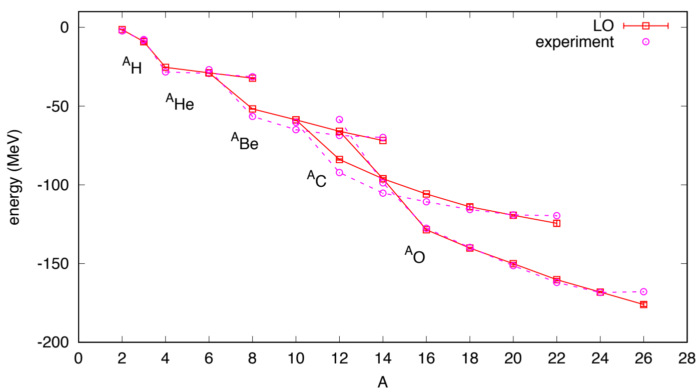
RESULTS from LATTICE NUCLEAR EFT

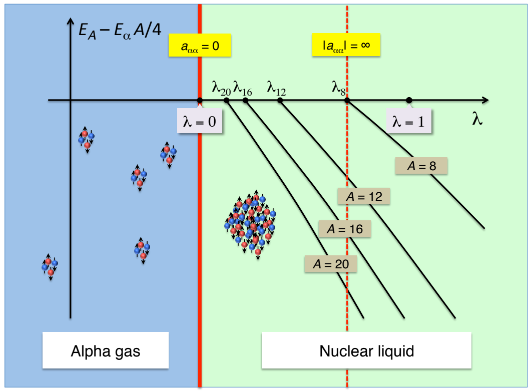


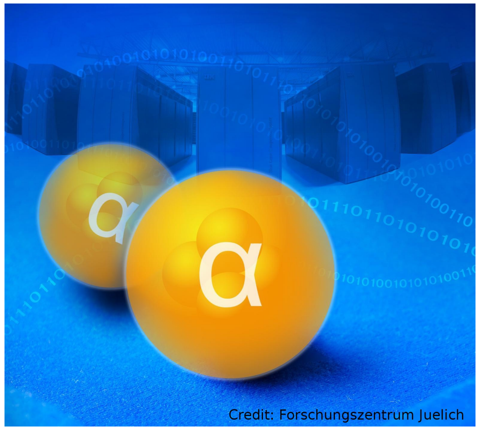
- ☐ Lattice EFT calculations for A=3,4,6,12 nuclei, PRL 104 (2010) 142501
- ☐ *Ab initio* calculation of the Hoyle state, PRL 106 (2011) 192501
- ☐ Structure and rotations of the Hoyle state, PRL 109 (2012) 142501
- ☐ Validity of Carbon-Based Life as a Function of the Light Quark Mass
  PRL 110 (2013) 142501
- ☐ *Ab initio* calculation of the Spectrum and Structure of ^{16}O,
  PRL 112 (2014) 142501
- ☐ *Ab initio* alpha-alpha scattering, Nature 528 (2015) 111
- ☐ Nuclear Binding Near a Quantum Phase Transition, PRL 117 (2016) 132501
- ☐ *Ab initio* calculations of the isotopic dependence of nuclear clustering,
  arXiv:1702.05177, PRL (2017) in print



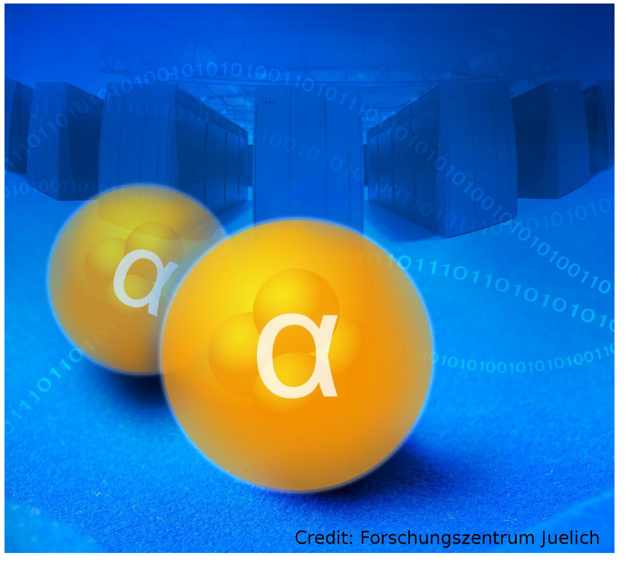








Ab initio calculation of α-α scattering

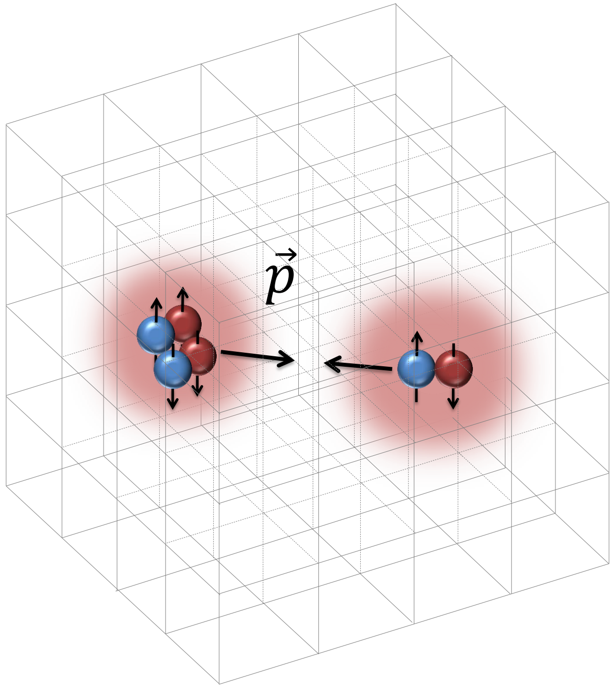


Elhatisari, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, UGM,
Nature **528** (2015) 111 [arXiv:1506.03513]

NUCLEUS–NUCLEUS SCATTERING on the LATTICE

- Processes involving α-particles and α-type nuclei comprise a major part of stellar nucleosynthesis, and control the production of certain elements in stars

- Ab initio calculations of scattering and reactions suffer from computational scaling with the number of nucleons in the clusters



Lattice EFT computational scaling $\Rightarrow$ $(A_1 + A_2)^2$

Rupak, Lee, Phys. Rev. Lett. **111** (2013) 032502
Pine, Lee, Rupak, Eur. Phys. J. A **49** (2013) 151
Elhatisari, Lee, Phys. Rev. C **90** (2014) 064001
Elhatisari et al., Phys.Rev. C **92** (2015) 054612
Elhatisari, Lee, UGM, Rupak, Eur. Phys. J. A **52** (2016) 174

ADIABATIC PROJECTION METHOD

- Basic idea to treat scattering and inelastic reactions:
  split the problem into two parts

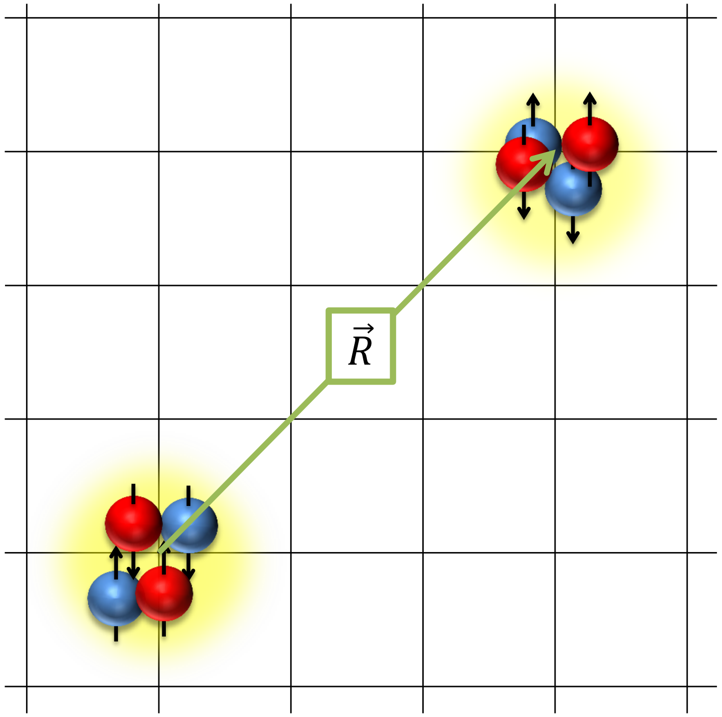
First part:

use Euclidean time projection to construct an *ab initio* low-energy cluster Hamiltonian, called the **adiabatic Hamiltonian**

Second part:

compute the two-cluster scattering phase shifts or reaction amplitudes using the adiabatic Hamiltonian

ADIABATIC PROJECTION METHOD II



- Construct a low-energy effective theory for clusters

- Use initial states parameterized by the relative separation between clusters

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r} + \vec{R}\rangle \otimes \vec{r}$$

- project them in Euclidean time with the chiral EFT Hamiltonian H

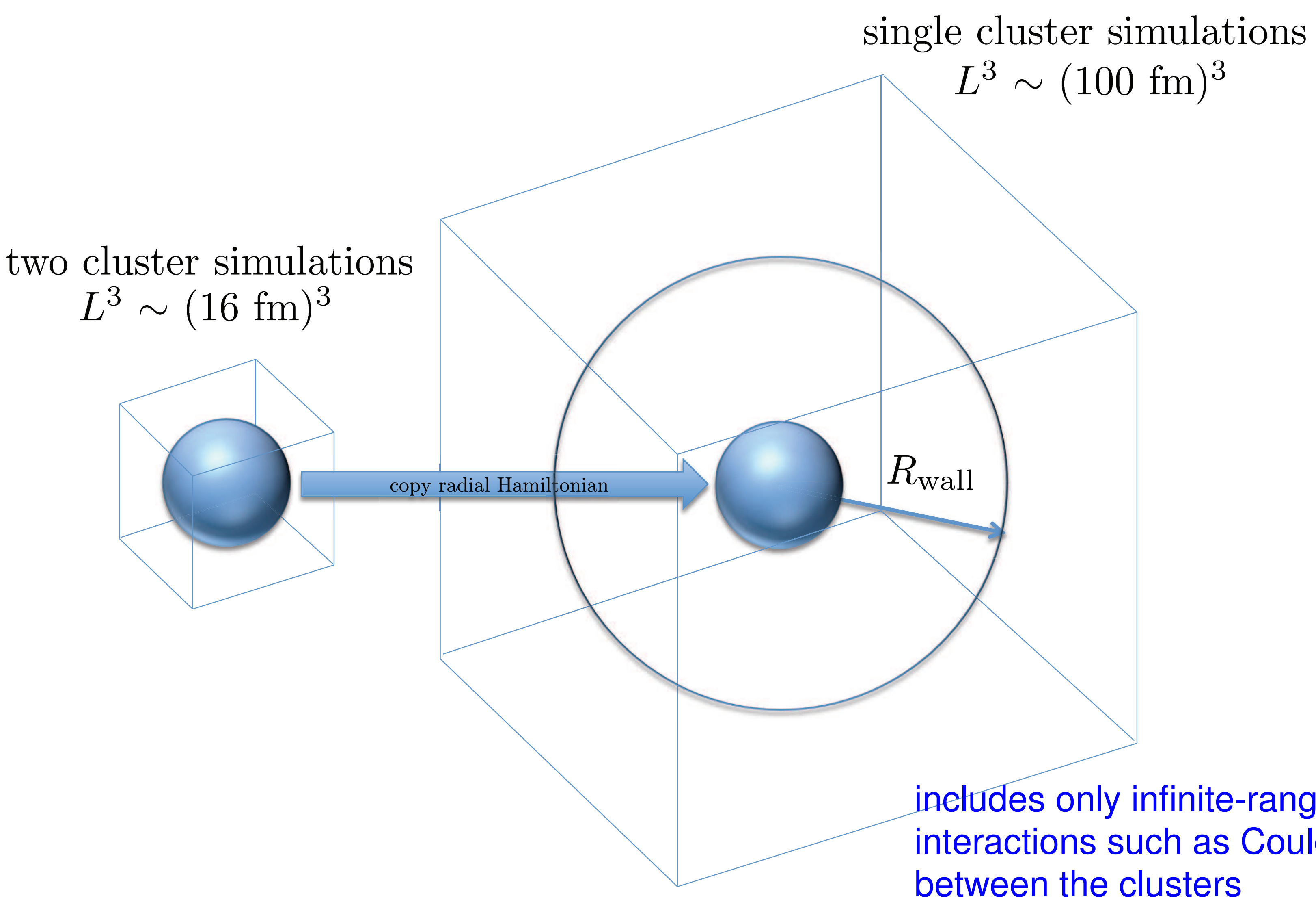
$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$

$\to$ "dressed cluster states" (polarization, deformation, Pauli)

- Adiabatic Hamiltonian (requires norm matrices)

$$[H_\tau]_{\vec{R}\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau$$

ADIABATIC HAMILTONIAN plus COULOMB



includes only infinite-range interactions such as Coulomb between the clusters

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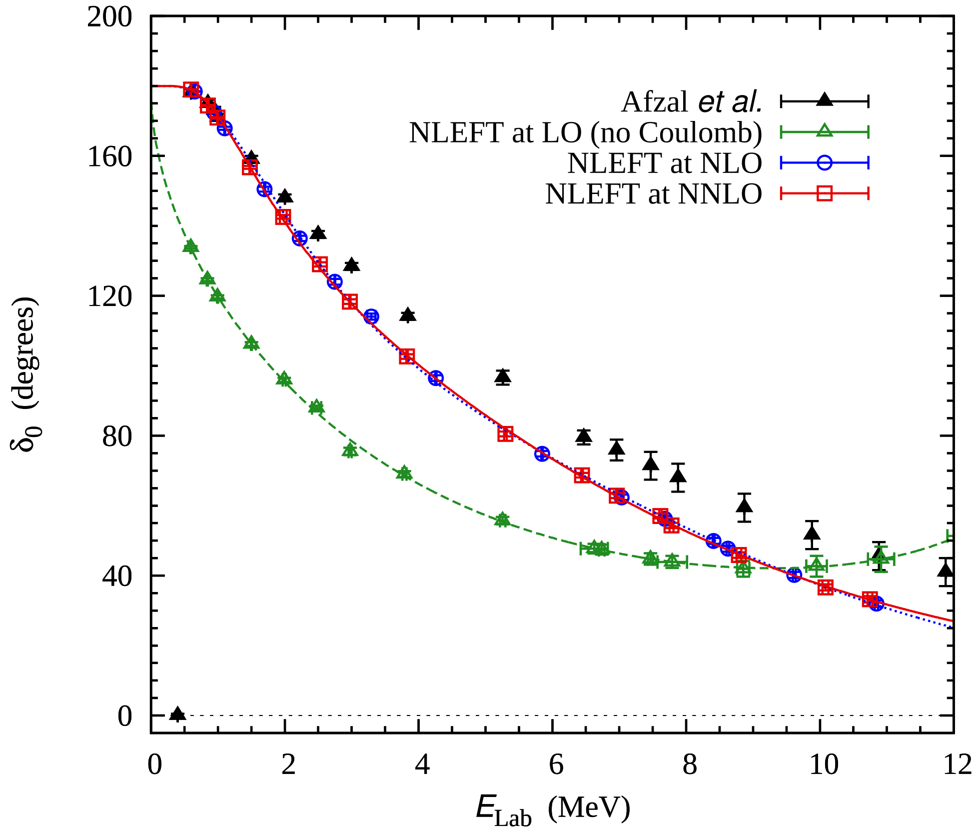
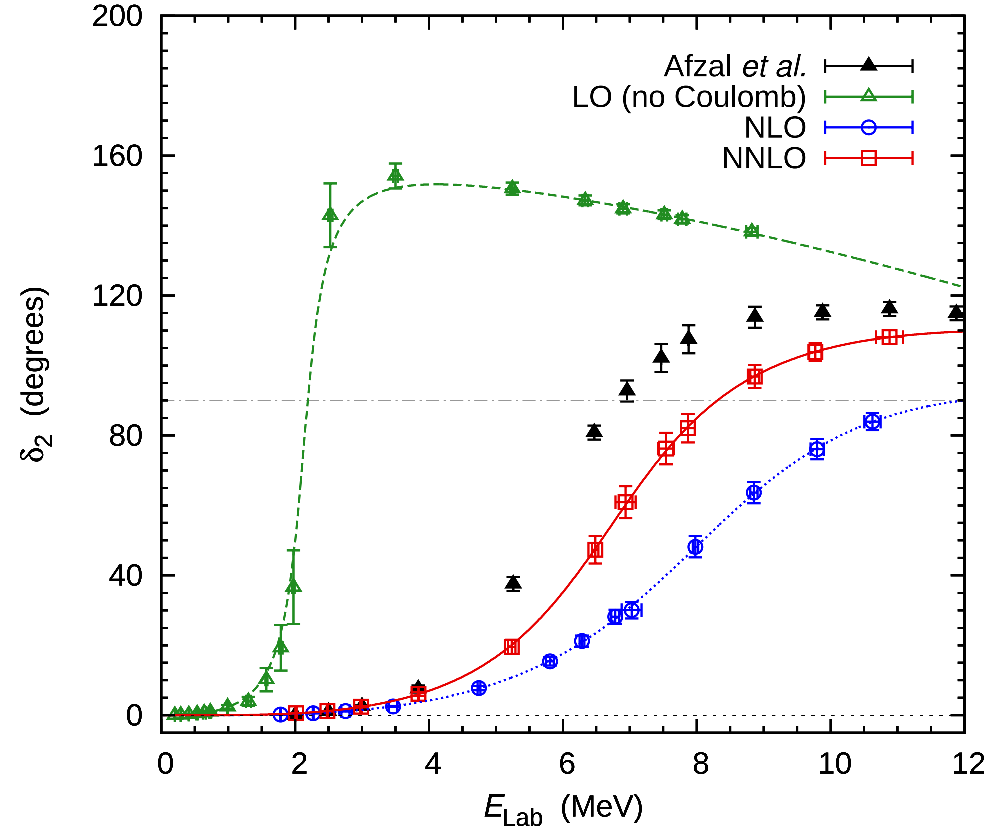
PHASE SHIFTS

- Same NNLO Lagrangian as used for the study of ^{12}C and ^{16}O [only stat. errors]





$$E_R^{\rm NNLO} = -0.11(1)\ \text{MeV} \quad [+0.09\ \text{MeV}]$$

$$E_R^{\rm NNLO} = 3.27(12)\ \text{MeV} \quad [\,2.92(18)\ \text{MeV}]$$

$$\Gamma_R^{\rm NNLO} = 2.09(16)\ \text{MeV} \quad [1.35(50)\ \text{MeV}]$$

Data: Afzal et al., Rev. Mod. Phys. **41** (1969) 247

New insights into nuclear clustering

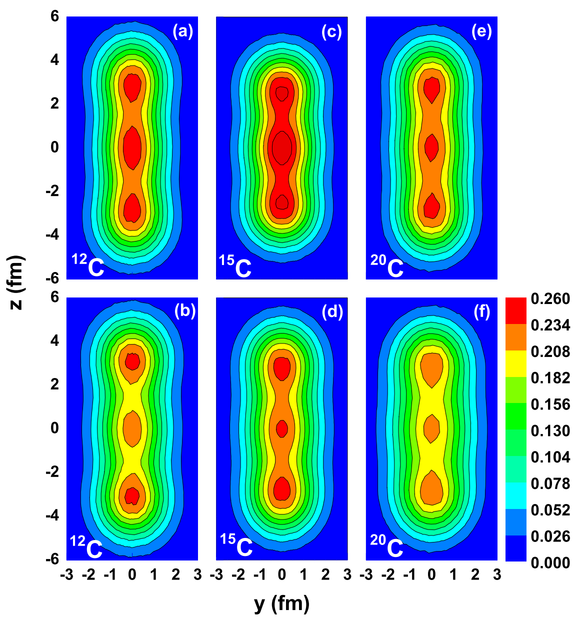
Elhatisari, Epelbaum, Krebs, Lähde, Lee, Li, Lu, UGM, Rupak
[arXiv:1702.05117]

CLUSTERING in NUCLEI

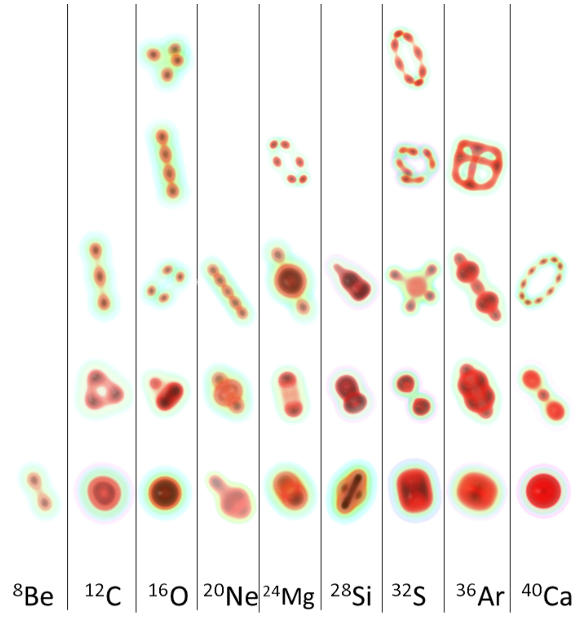
- Introduced theoretically by Wheeler already in 1937:

> John Archibald Wheeler, "Molecular Viewpoints in Nuclear Structure," Physical Review **52** (1937) 1083

- many works since then... Ikeda, Horiuchi, Freer, Schuck, Röpke, Khan, Zhou, Iachello, ...



Zhao, Itagaki, Meng (2015)



Ebran, Khan, Niksic, Vretenar (2014)

α-clusters

$\Rightarrow$ can we understand this phenomenon from *ab initio* calculations?

EARLIER RESULTS on NUCLEAR CLUSTERING

- Already a number of intriguing results on clustering:

  Ab initio calculation of the spectrum and structure of ^{12}C (esp. the Hoyle state)

  Ab initio calculation of the spectrum and structure of ^{16}O

  Ground state energies of α-type nuclei up to ^{28}Si within 1%

  Ab initio calculation of α-α scattering

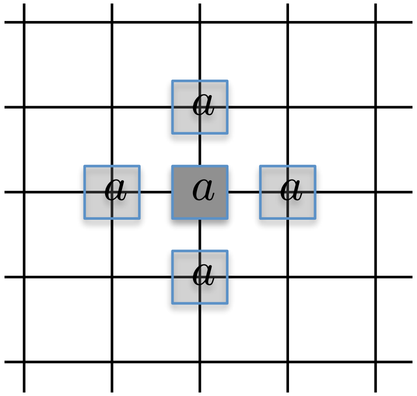
  Quantum phase transition from Bose gas of α's to nuclear liquid for α-type nuclei

- However: when adding extra neutrons/protons, the precision quickly deteriorates due to sign oscillations

- New LO action with smeared SU(4) local+non-local symmetric contact interactions & smeared one-pion exchange

$$a_{\rm NL}(\mathbf{n}) = a(\mathbf{n}) + s_{\rm NL} \sum_{\langle \mathbf{n}' \, \mathbf{n} \rangle} a(\mathbf{n}')$$

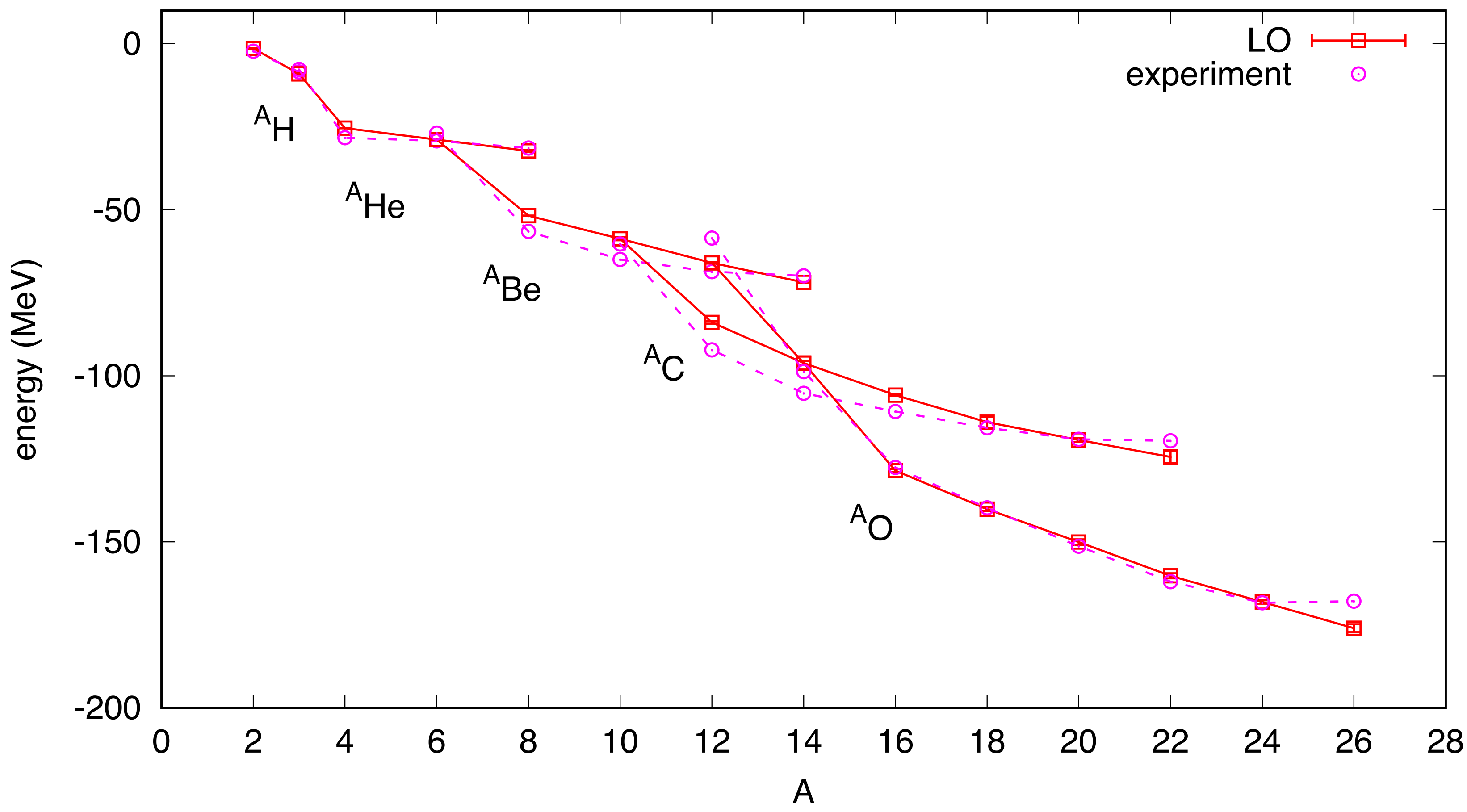
$$a^\dagger_{\rm NL}(\mathbf{n}) = a^\dagger(\mathbf{n}) + s_{\rm NL} \sum_{\langle \mathbf{n}' \, \mathbf{n} \rangle} a^\dagger(\mathbf{n}')$$



GROUND STATE ENERGIES

- Fit 3 parameters to average NN S-wave scattering length and effective range and α-α S-wave scattering length [higher orders in the works]

$\rightarrow$ predict g.s. energies of H, He, Be, C and O isotopes $\rightarrow$ quite accurate (LO)



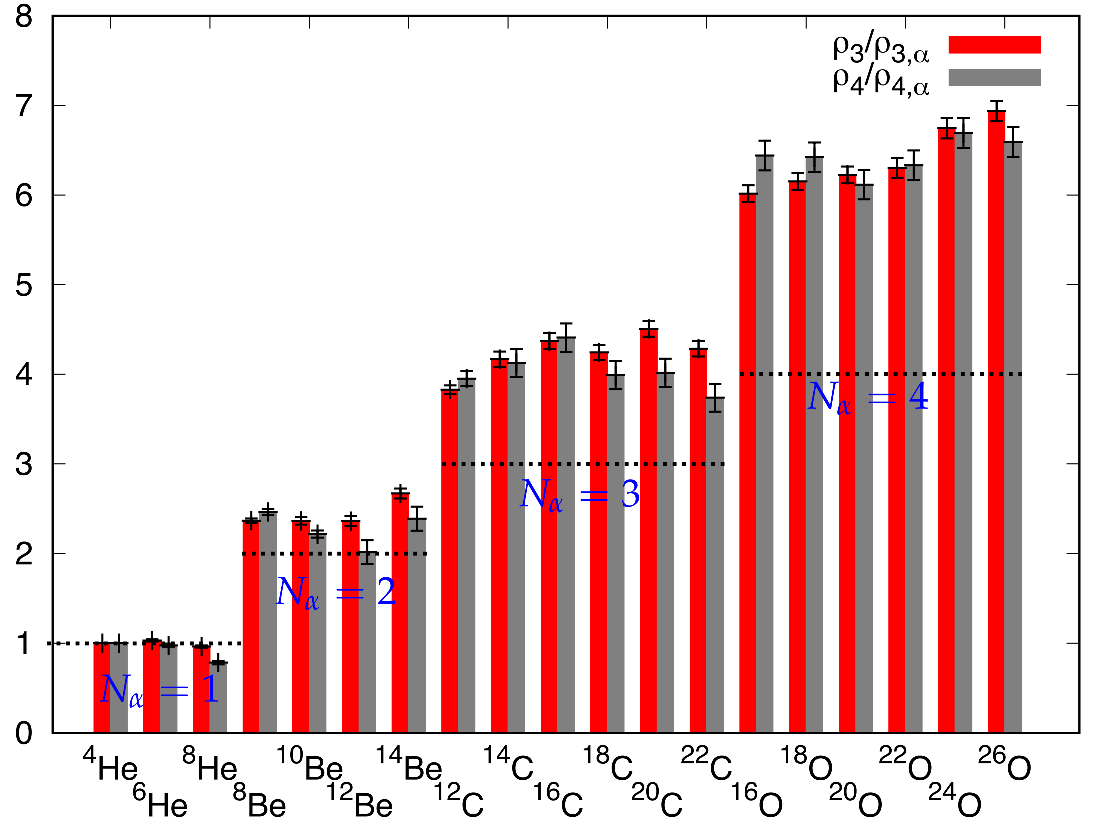
PROBING NUCLEAR CLUSTERING

- Local densities on the lattice: $\rho(\mathbf{n})\ ,\quad \rho_p(\mathbf{n})\ ,\quad \rho_n(\mathbf{n})$
- Probe of alpha clusters: $\rho_4 = \sum_{\mathbf{n}} : \rho^4(\mathbf{n})/4! :$
- Another probe for $Z = N =$ even nuclei: $\rho_3 = \sum_{\mathbf{n}} : \rho^3(\mathbf{n})/3! :$
- ρ_4 couples to the center of the α-cluster while ρ_3 gets contributions from a wider portion of the alpha-particle wave function
- Both ρ_3 and ρ_4 depend on the regulator, a, but not on the nucleus
- The ratios $\rho_3/\rho_{3,\alpha}$ and $\rho_4/\rho_{4,\alpha}$ free of short-distance ambiguities and model-independent
- $\rho_3/\rho_{3,\alpha}$ measures the effective number of alpha-cluster N_α

$\Rightarrow$ Any deviation from $N_\alpha =$ integer measures the entanglement of the α-clusters in a given nucleus

PROBING NUCLEAR CLUSTERING

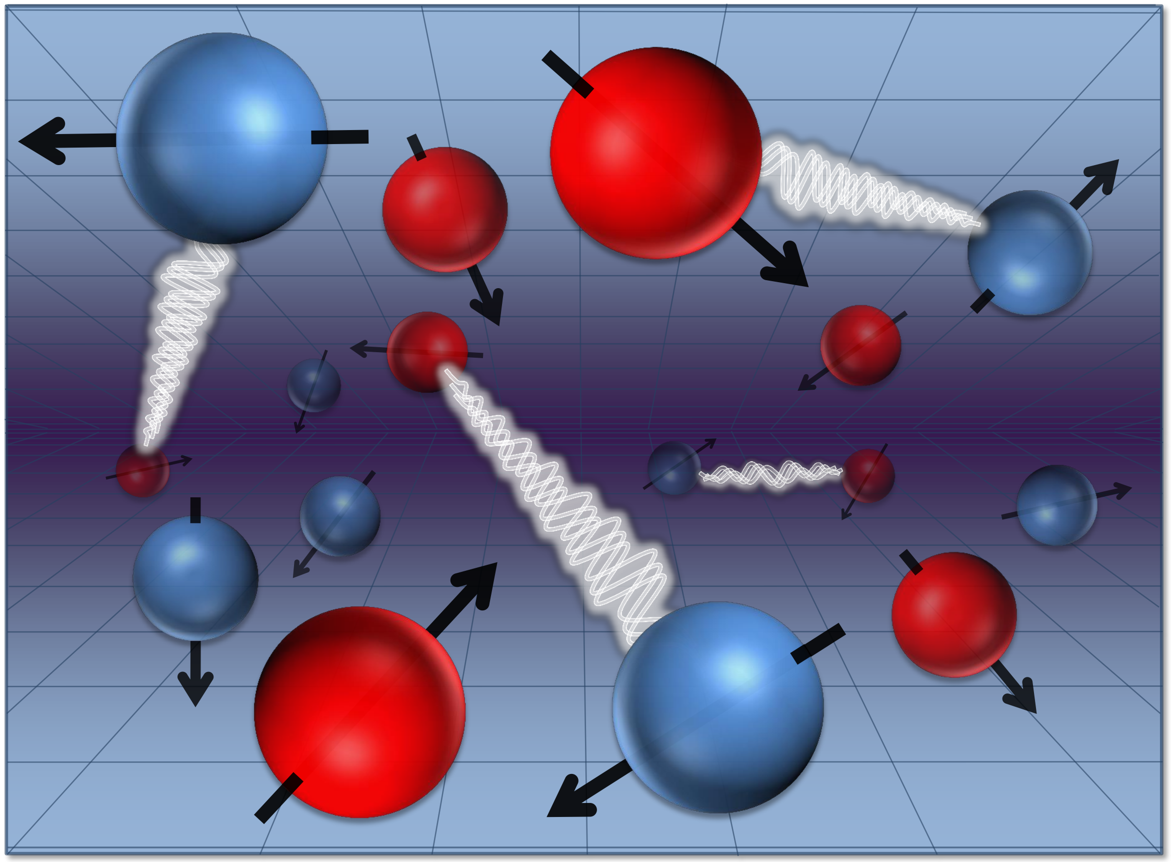
- ρ_3-entanglement of the α-clusters: $$\frac{\Delta_\alpha^{\rho_3}}{N_\alpha} = \frac{\rho_3/\rho_{3,\alpha}}{N_\alpha} - 1$$



Nucleus	^{4,6,8}He	^{8,10,12,14}Be	^{12,14,16,18,20,22}C	^{16,18,20,22,24,26}O
$\Delta_\alpha^{\rho_3}/N_\alpha$	0.00 - 0.03	0.20 - 0.35	0.25 - 0.50	0.50 - 0.75

PROBING NUCLEAR CLUSTERING

- The transition from cluster-like states in light systems to nuclear liquid-like states in heavier systems should not be viewed as a simple suppression of multi-nucleon short-distance correlations, but rather as an increasing *entanglement* of the nucleons involved in the multi-nucleon correlations.



PINHOLE ALGORITHM

- AFQMC calculations involve states that are superpositions of many different center-of-mass positions

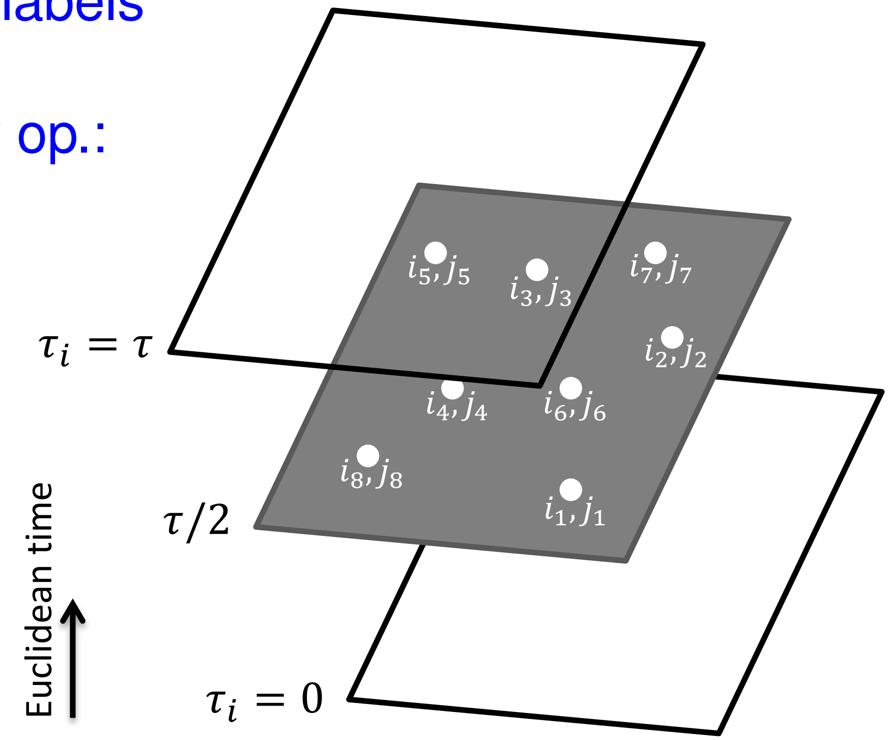
$\longrightarrow$ density distributions of nucleons can not be computed directly

- Insert a screen with pinholes with spin & isospin labels that allows nucleons with corresponding spin & isospin to pass = insertion of the A-body density op.:

$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) \\ = :\rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$

- MC sampling of the amplitude:

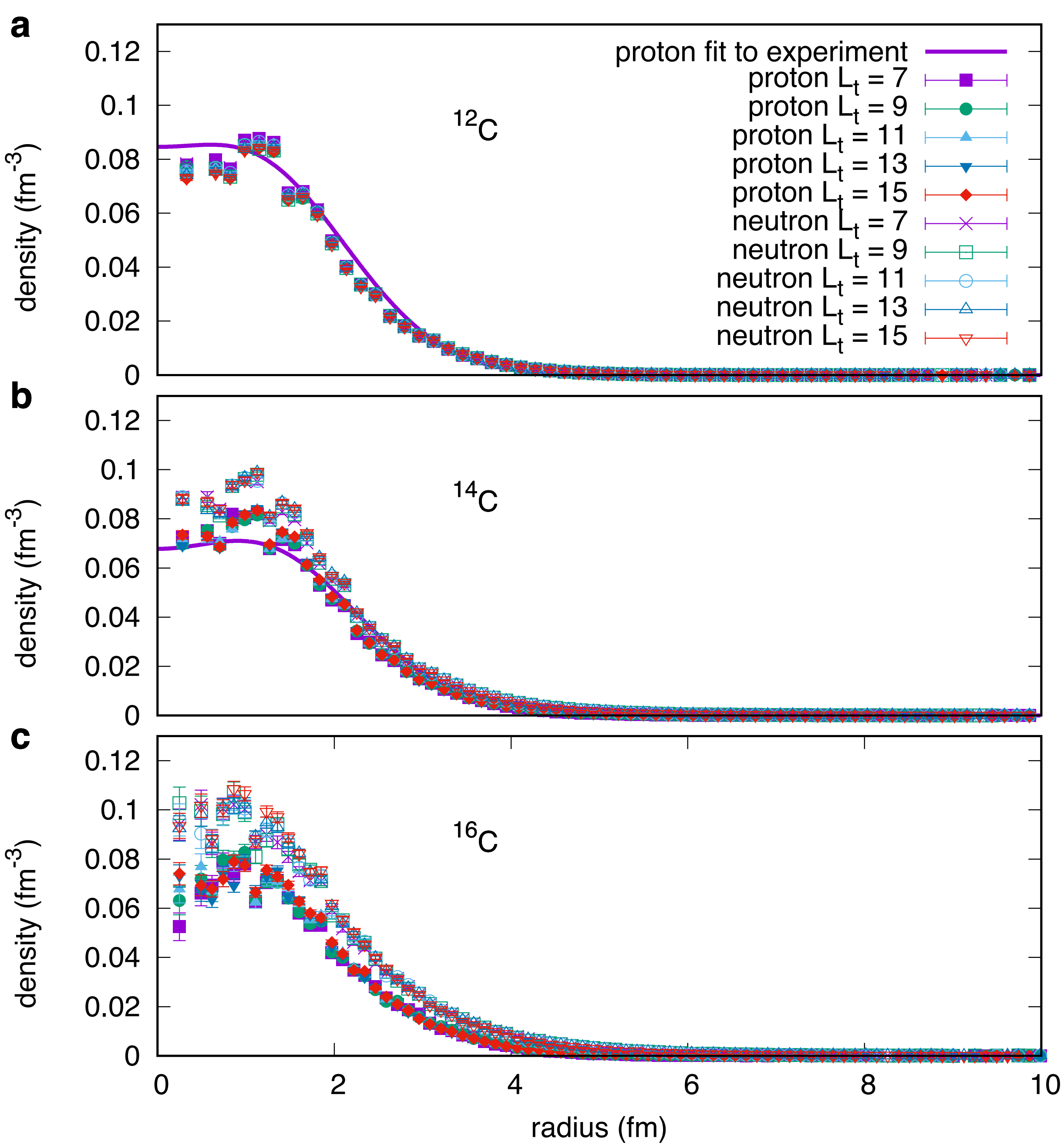
$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A,L_t) \\ = \langle\psi(\tau/2)|\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A)|\psi(\tau/2)\rangle$$



- Allows to measure proton and neutron distributions

- Resolution scale $\sim a/A$ as cm position $\mathbf{r}_{\rm cm}$ is an integer $\mathbf{n}_{\rm cm}$ times a/A

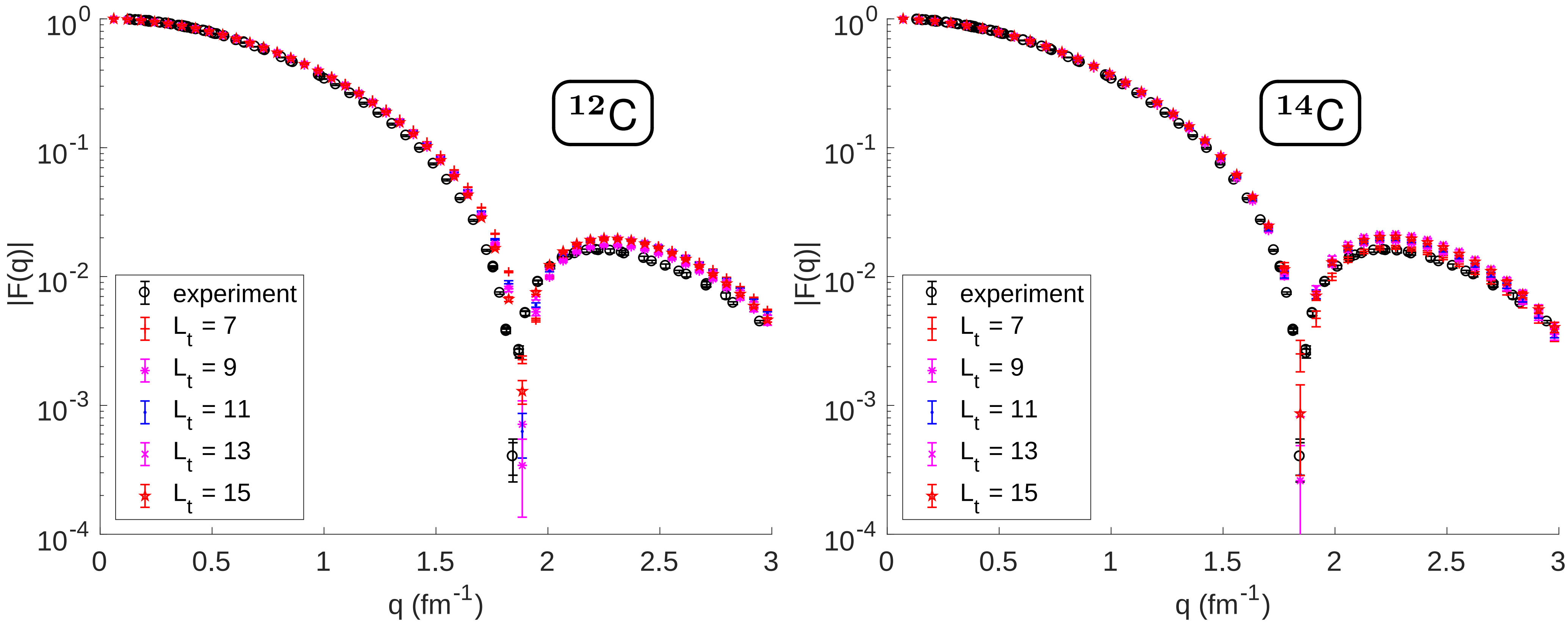
PROTON and NEUTRON DENSITIES in CARBON



- open symbols: neutron
- closed symbols: proton
- proton size accounted for
- asymptotic properties of the distributions from the volume dependence of N-body bound states
  König, Lee, [arXiv:1701.00279]
- consistent with data
- fit to data from
  Kline et al., NPA209 (1973) 381

FORM FACTORS

- Fit charge distributions by a Wood-Saxon shape
  $\hookrightarrow$ get the form factor from the Fourier-transform (FT)
  $\hookrightarrow$ uncertainties from a direct FT of the lattice data



$\Rightarrow$ detailed structure studies become possible

SUMMARY & OUTLOOK

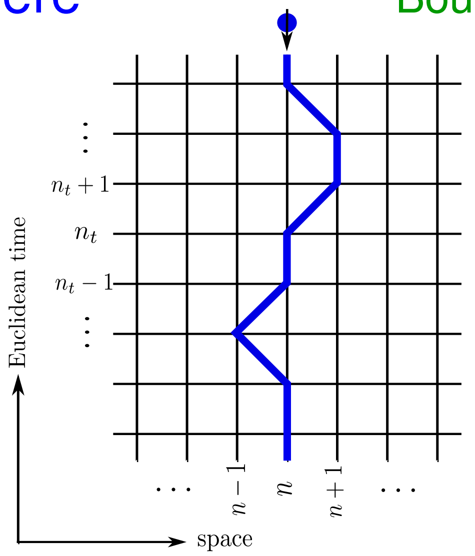
- Nuclear lattice simulations: a new quantum many-body approach
  - $\to$ based on the successful continuum nuclear chiral EFT
  - $\to$ a number of intriguing results already obtained
  - $\to$ clustering emerges naturally, α-cluster nuclei
  - $\to$ fine-tuning in nuclear reactions can be studied
- Various bridges to lattice QCD studies need to be explored
- Many open issues can now be addressed in a truly quantitative manner
  - $\to$ the "holy grail" of nuclear astrophysics ^{4}He+$^{12}\mathrm{C} \to ^{16}\mathrm{O} + \gamma$ Fowler (1983)
  - $\to$ strangeness nuclear physics using the **impurity MC** method

    Bour, Lee, UGM, Phys. Rev. Lett. **115** (2015) 185301 $\to$ slide
  - $\to$ and much more $\hookrightarrow$ stay tuned

OUTLOOK: HYPERNUCLEI

- Naive extension to include hyperons: sign problem to severe

Bour (2009)



- way out: treat the hyperon as an **impurity** in a bath (background) of the nucleons

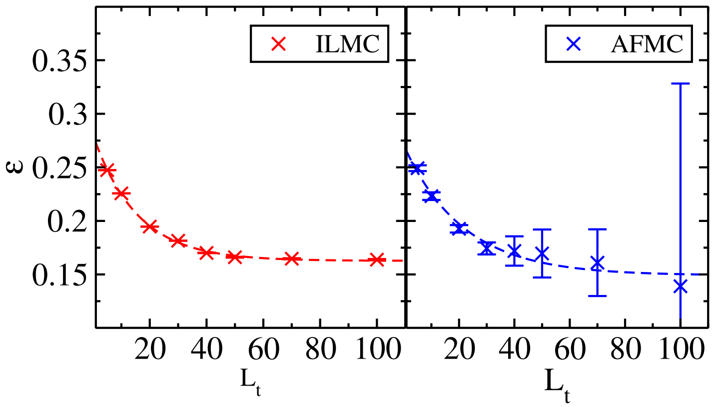
$\hookrightarrow$ using the impurity MC algorithm

Bour, Lee, UGM, PRL **115** (2015) 185301

Elhatisari, Lee, PRC **90** (2014) 064001

- Test cases: simple spin systems and the polaron in 2D & 3D

$9|\uparrow\rangle + 1|\downarrow\rangle, L = 10^3$, zero range int.



polaron in two dimensions