Clustering in Nuclei
from *ab initio* nuclear lattice simulations

Ulf-G. Meißner, Univ. Bonn & FZ Jülich

Supported by DFG, SFB/TR-16
and by DFG, SFB/TR-110
and by EU, I3HP EPOS
and by BMBF 05P12PDFTE
and by HGF VIQCD VH-VI-417
CONTENTS

• Short introduction
• Basics of nuclear lattice simulations
• Results from nuclear lattice simulations
• Summary & outlook
Short introduction
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...

  ⇒ can we understand this phenomenon from *ab initio* calculations?

  Bijker, Iachello (2014)

  Ikeda, Horiuchi, Freer, Schuck, Zhou, Khan, . . .

  Ebran, Khan, Niksic, Vretenar (2014)

  α-clusters
Basics of nuclear lattice simulations

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

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

  \( \rightarrow \) Epelbaum’s talk

• typical lattice parameters

  \( \Lambda = \frac{\pi}{a} \approx 300 \text{ MeV} \) [UV cutoff]

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

  J. W. Chen, D. Lee and T. Schäfer, Phys. Rev. Lett. 93 (2004) 242302, T. Lähde et al., arXiv:1502.06787

• hybrid Monte Carlo & transfer matrix (similar to LQCD)

  – Ulf-G. Meißner, Clustering in nuclei . . . – Chiral Dynamics 2015, July 2015
all possible configurations are sampled
⇒ clustering emerges *naturally*

[NB: smearing necessary → outlook]
NUCLEAR WAVE FUNCTIONS

• General wave function:

\[ \psi_j(\vec{n}) \, , \, j = 1, \ldots, A \]

• States with well-defined momentum (anti-symm.):

\[ \frac{L^{-3/2}}{2} \sum_{\vec{m}} \psi_j(\vec{n} + \vec{m}) \exp(i\vec{P} \cdot \vec{m}) \, , \, j = 1, \ldots, A \]

• Insert clusters of nucleons at initial/final states (spread over some time interval)

\[ \rightarrow \text{allows for all type of wave functions (shell model, clusters, \ldots)} \]
\[ \rightarrow \text{removes directional bias} \]

shell-model type

\[ \psi_j(\vec{n}) = \exp[-c\vec{n}^2] \]
\[ \psi'_j(\vec{n}) = n_x \exp[-c\vec{n}^2] \]
\[ \psi''_j(\vec{n}) = n_y \exp[-c\vec{n}^2] \]
\[ \psi'''_j(\vec{n}) = n_z \exp[-c\vec{n}^2] \]

cluster type

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

• shell-model w.f.s do not have enough 4N correlations \( \sim \langle (N\dagger N)^2 \rangle \)
COMPUTATIONAL EQUIPMENT

- Present = JUQUEEN (BlueGene/Q)

6 Pflops

– Ulf-G. Meißner, Clustering in nuclei ... – Chiral Dynamics 2015, July 2015
Lattice: new results

Epelbaum, Krebs, Lähde, Lee, Luu, UGM, Rupak + post-docs + students
RESULTS from LATTICE NUCLEAR EFT

- Hoyle state in $^{12}$C
  - Structure of the Hoyle state
  - Fate of carbon-based life

- Spectrum of $^{16}$O
  - Going up the $\alpha$-chain
  - Rot. symmetry breaking

\[ E \text{ [MeV]} \]

$^{2+}$
- $^{2+}$
  - $^{2+}$
- $^{0+}$
  - $^{0+}$
- $^{0+}$
  - $^{0+}$

$^{2+}$
- $^{2+}$
  - $^{2+}$
- $^{0+}$
  - $^{0+}$

$^{0+}$
- $^{0+}$
  - $^{0+}$
- $^{0+}$
  - $^{0+}$

$E_{\text{exp}}$
- $E_{\text{exp}}$
  - $E_{\text{exp}}$
- $E_{\text{exp}}$
  - $E_{\text{exp}}$

$E_{\text{Th}}$
- $E_{\text{Th}}$
  - $E_{\text{Th}}$
- $E_{\text{Th}}$
  - $E_{\text{Th}}$

$\delta m_{1}/m_{1}$
- $\delta m_{1}/m_{1}$
  - $\delta m_{1}/m_{1}$
- $\delta m_{1}/m_{1}$
  - $\delta m_{1}/m_{1}$

- Ulf-G. Meißner, Clustering in nuclei ... – Chiral Dynamics 2015, July 2015
GOING up the ALPHA CHAIN

- Consider the $\alpha$ ladder $^{12}\text{C}$, $^{16}\text{O}$, $^{20}\text{Ne}$, $^{24}\text{Mg}$, $^{28}\text{Si}$ as $t_{\text{CPU}} \sim A^2$

- Improved “multi-state” technique to extract ground state energies
  - $\Rightarrow$ higher $A$, better accuracy
  - $\Rightarrow$ overbinding at LO beyond $A = 12$ persists up to NNLO

\[
E = -131.3(5) \quad E = -165.9(9) \quad E = -232(2) \quad E = -308(3)
\]

\[
[-127.62] \quad [-160.64] \quad [-198.26] \quad [-236.54]
\]
REMOVING the OVERBINDING

Lähde, Epelbaum, Krebs, Lee, UGM, Rupak, Phys. Lett. B 732 (2014) 110

- Overbinding is due to four $\alpha$ clusters in close proximity

  $\Rightarrow$ remove this by an effective 4N operator [long term: N3LO]

  \[ V^{(4N_{\text{eff}})} = D^{(4N_{\text{eff}})} \sum_{1 \leq (\vec{n}_i - \vec{n}_j)^2 \leq 2} \rho(\vec{n}_1)\rho(\vec{n}_2)\rho(\vec{n}_3)\rho(\vec{n}_4) \]

- fix the coefficient $D^{(4N_{\text{eff}})}$ from the BE of $^{24}\text{Mg}$

  $\Rightarrow$ excellent description of the ground state energies

| A  | 12       | 16        | 20       | 24       | 28       |
|----|----------|-----------|----------|----------|----------|
| Th | $-90.3(2)$ | $-131.3(5)$ | $-165.9(9)$ | $-198(2)$ | $-233(3)$ |
| Exp| $-92.16$ | $-127.62$ | $-160.64$ | $-198.26$ | $-236.54$ |

$\rightarrow$ ultimately, reduce lattice spacing [interaction more repulsive] & N$^3$LO
GROUND STATE ENERGIES

The graph shows the ground state energies of various isotopes, including 4He, 8Be, 12C, 16O, 20Ne, 24Mg, and 28Si, as a function of energy (E in MeV). The graph includes data from various theoretical models and experimental measurements.

- **Experiment**: Data points for experimental measurements.
- **NNLO**: Data points for the NNLO model.
- **NNLO + 4N\_eff**: Data points for the NNLO + 4N\_eff model.

The graph highlights the comparison between theoretical predictions and experimental results, with a focus on the energy levels of the isotopes mentioned.

- Ulf-G. Mei\ss\,ner, Clustering in nuclei ... – Chiral Dynamics 2015, July 2015
**STRUCTURE of $^{16}$O**

- Mysterious nucleus, despite modern ab initio calcs
  
  Hagen et al. (2010), Roth et al. (2011), Hergert et al. (2013)

- Alpha-cluster models since decades, some exp. evidence
  
  Wheeler (1937), Dennison (1954), Robson (1979), . . ., Freer et al. (2005)

- Spectrum very close to tetrahedral symmetry group
  
  Bijker & Iachello (2014)

- Relevant configurations in lattice simulations:
  
  Tetrahedron (A)  Square (narrow (B) and wide (C))
**DECODING the STRUCTURE of $^{16}$O**

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

- measure the 4N density, where each of the nucleons is placed at adjacent points

  $\Rightarrow 0^+_1$ ground state: mostly tetrahedral config

  $\Rightarrow 0^+_2$ excited state: mostly square configs

  $2^+_1$ excited state: rotational excitation of the $0^+_2$

  overlap w/ tetrahedral config.

  overlap w/ square configs.
RESULTS for $^{16}\text{O}$

- **Spectrum:**

|     | LO     | NNLO(2N) | NNLO(3N) | $4N_{\text{eff}}$ | Exp. |
|-----|--------|----------|----------|------------------|------|
| $0_1^+$ | -147.3(5) | -121.4(5) | -138.8(5) | -131.3(5) | -127.62 |
| $0_2^+$ | -145(2)     | -116(2)   | -136(2)   | -123(2)    | -121.57 |
| $2_1^+$ | -145(2)     | -116(2)   | -136(2)   | -123(2)    | -120.70 |

- **LO charge radius:** $r(0_1^+) = 2.3(1)$ fm  \(\text{Exp.} \ r(0_1^+) = 2.710(15) \text{ fm}\)
  
  $\Rightarrow$ compensate for this by rescaling with appropriate units of $r/r_{\text{LO}}$

- **LO EM properties:**

|                        | LO         | LO(r-scaled) | Exp. |
|------------------------|------------|--------------|------|
| $Q(2_1^+) \ [e \text{ fm}^2]$ | 10(2)      | 15(3)        | —    |
| $B(E2, 2_1^+ \to 0_2^+) \ [e^2 \text{ fm}^4]$ | 22(4)      | 46(8)        | 65(7) |
| $B(E2, 2_1^+ \to 0_1^+) \ [e^2 \text{ fm}^4]$ | 3.0(7)     | 6.2(1.6)     | 7.4(2) |
| $M(E0, 0_2^+ \to 0_2^+) \ [e \text{ fm}^2]$ | 2.1(7)     | 3.0(1.4)     | 3.6(2) |

$\Rightarrow$ gives credit to the interpretation of the $2_1^+$ as rotational excitation

---

- Ulf-G. Meißner, Clustering in nuclei ... – Chiral Dynamics 2015, July 2015
so far: nuclei with $N = Z$, and $A = 4 \times \text{int}$ as these have the least sign problem due to the approximate SU(4) symmetry

$$\langle \text{sign} \rangle = \langle \exp(i\theta) \rangle = \frac{\det M(t_o, t_i, \ldots)}{|\det M(t_o, t_i, \ldots)|}$$

$M(t_o, t_i, \ldots)$ is the transition matrix

- Symmetry-sign extrapolation (SSE) method: control the sign oscillations

$$H_{d_h} = d_h \cdot H_{\text{phys}} + (1 - d_h) \cdot H_{\text{SU}(4)}$$

$$H_{\text{SU}(4)} = \frac{1}{2} C_{\text{SU}(4)} (N^\dagger N)^2$$

$\hookrightarrow$ family of solutions for different SU(4) couplings $C_{\text{SU}(4)}$ that converge on the physical value for $d_h = 1$
RESULTS for $^{12}$C

- generate a few more MC data at large $N_t$ using SSE
  
  | $E_{12}$ (LO) [MeV] | $N_t$ |
  |---------------------|------|
  | -7.0e-5 + SSE       | 0    |
  | -7.0e-5             | 2    |
  | -7.0e-5             | 4    |
  | -7.0e-5             | 6    |
  | -7.0e-5             | 8    |
  | -7.0e-5             | 10   |
  | -7.0e-5             | 12   |
  | -7.0e-5             | 14   |
  | -7.0e-5             | 16   |

  
  | $E_{12}$ (NLO) [MeV] | $N_t$ |
  |---------------------|------|
  | -7.0e-5 + SSE       | 0    |
  | -7.0e-5             | 2    |
  | -7.0e-5             | 4    |
  | -7.0e-5             | 6    |
  | -7.0e-5             | 8    |
  | -7.0e-5             | 10   |
  | -7.0e-5             | 12   |
  | -7.0e-5             | 14   |
  | -7.0e-5             | 16   |

  
  | $E_{12}$ (EMIB) [MeV] | $N_t$ |
  |----------------------|------|
  | -7.0e-5 + SSE        | 0    |
  | -7.0e-5              | 2    |
  | -7.0e-5              | 4    |
  | -7.0e-5              | 6    |
  | -7.0e-5              | 8    |
  | -7.0e-5              | 10   |
  | -7.0e-5              | 12   |
  | -7.0e-5              | 14   |
  | -7.0e-5              | 16   |

  
  | $E_{12}$ (3NF) [MeV] | $N_t$ |
  |---------------------|------|
  | -7.0e-5 + SSE       | 0    |
  | -7.0e-5             | 2    |
  | -7.0e-5             | 4    |
  | -7.0e-5             | 6    |
  | -7.0e-5             | 8    |
  | -7.0e-5             | 10   |
  | -7.0e-5             | 12   |
  | -7.0e-5             | 14   |
  | -7.0e-5             | 16   |

- promising results $\rightarrow$ no more exponential deterioration of the MC data
- results w/ small uncertainties for $d_h \geq 0.8$
RESULTS for $A = 6$

- Simulations for $^{6}\text{He}$ and $^{6}\text{Be}$

⇒ methods works for nuclei with $A \neq Z$

⇒ neutron-rich nuclei can now be systematically explored (larger volumes)
SUMMARY & OUTLOOK

• Nuclear lattice simulations as a new quantum many-body approach
  → clustering emerges naturally, $\alpha$-cluster nuclei
  → symmetry-sign extrapolation method allows to go to the drip lines
  → holy grail of nuclear astrophysics ($\alpha+^{12}\text{C} \rightarrow ^{16}\text{O}+\gamma$) in reach

• Some on-going activities:
  → improving the forces (N3LO, sph. harmonics) ← Alarcon’s talk
  → systematic studies of $\alpha$-independence
    ← Klein, Lee, Liu, UGM, PLB747 (2015) 511
  → finite size effects/averaging procedures
    ← Lu, Lähde, Lee, UGM, arXiv:1504.01685
  → scattering cluster wave functions ← Rokash’s talk
  → $ab\ initio$ alpha-alpha scattering ← Elhatisari’s talk
  → and much more ...
