Clustering in Nuclei
from ab initio nuclear lattice simulations

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

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• Basics of nuclear lattice simulations

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Short introduction
CLUSTERING in NUCLEI

- Introduced theoretically by Wheeler already in 1937:


- many works since then...

⇒ can we understand this phenomenon from \textit{ab initio} calculations?

- Ulf-G. Meißner, Clustering in nuclei ... – Chiral Dynamics 2015, July 2015
Basics of nuclear lattice simulations

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

$\Lambda = \frac{\pi}{a} \simeq 300$ MeV [UV cutoff]

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

hybrid Monte Carlo & transfer matrix (similar to LQCD)
⇒ all possible configurations are sampled
⇒ clustering emerges naturally

[NB: smearing necessary → outlook]
NUCLEAR WAVE FUNCTIONS

- General wave function:
  \[ \psi_j(\vec{n}) , \quad j = 1, \ldots, A \]

- States with well-defined momentum (anti-symm.):
  \[ L^{-3/2} \sum_{\vec{m}} \psi_j(\vec{n} + \vec{m}) \exp(i \vec{P} \cdot \vec{m}) , \quad j = 1, \ldots, A \]

- Insert clusters of nucleons at initial/final states (spread over some time interval)
  \( \rightarrow \) allows for all type of wave functions (shell model, clusters, \ldots)
  \( \rightarrow \) removes directional bias

  shell-model type
  \[
  \begin{align*}
  \psi_j(\vec{n}) &= \exp[-c\vec{n}^2] \\
  \psi'_j(\vec{n}) &= n_x \exp[-c\vec{n}^2] \\
  \psi''_j(\vec{n}) &= n_y \exp[-c\vec{n}^2] \\
  \psi'''_j(\vec{n}) &= n_z \exp[-c\vec{n}^2]
  \end{align*}
  \]

  cluster type
  \[
  \begin{align*}
  \psi_j(\vec{n}) &= \exp[-c(\vec{n} - \vec{m})^2] \\
  \psi'_j(\vec{n}) &= \exp[-c(\vec{n} - \vec{m}')^2] \\
  \psi''_j(\vec{n}) &= \exp[-c(\vec{n} - \vec{m}'')^2] \\
  \psi'''_j(\vec{n}) &= \exp[-c(\vec{n} - \vec{m}''')^2]
  \end{align*}
  \]

- 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 $^{12}\text{C}$**  
PRL 106 (2011)

- **Structure of the Hoyle state**  
PRL 109 (2012)

- **Fate of carbon-based life**  

- **Spectrum of $^{16}\text{O}$**  
PRL 112 (2014)

- **Going up the $\alpha$-chain**  
PLB 732 (2014)

- **Rot. symmetry breaking**  
PRD 90 (2014)

- **Exp**
- **Th**

<table>
<thead>
<tr>
<th>E [MeV]</th>
<th>(2^+)</th>
<th>(0^+)</th>
<th>(2^+)</th>
<th>(0^+)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-92.16</td>
<td>-82.61</td>
<td>-87.72</td>
<td>-84.51</td>
<td>-85.3</td>
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</table>

$\delta m_q/m_q = 0.01$
$\delta m_q/m_q = 0.05$

- Ulf-G. Meißner, Clustering in nuclei ... – Chiral Dynamics 2015, July 2015
• 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
  \[\Rightarrow \text{higher } A, \text{ better accuracy}\]
  \[\Rightarrow \text{overbinding at LO beyond } A = 12 \text{ persists up to NNLO}\]

\[
\begin{align*}
E &= -131.3(5) \\
    &\quad [-127.62] \\
E &= -165.9(9) \\
    &\quad [-160.64] \\
E &= -232(2) \\
    &\quad [-198.26] \\
E &= -308(3) \\
    &\quad [-236.54]
\end{align*}
\]
Overbinding is due to four $\alpha$ clusters in close proximity

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

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

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

$$\Rightarrow \text{excellent description of the ground state energies}$$

<table>
<thead>
<tr>
<th>A</th>
<th>12</th>
<th>16</th>
<th>20</th>
<th>24</th>
<th>28</th>
</tr>
</thead>
<tbody>
<tr>
<td>Th</td>
<td>$-90.3(2)$</td>
<td>$-131.3(5)$</td>
<td>$-165.9(9)$</td>
<td>$-198(2)$</td>
<td>$-233(3)$</td>
</tr>
<tr>
<td>Exp</td>
<td>$-92.16$</td>
<td>$-127.62$</td>
<td>$-160.64$</td>
<td>$-198.26$</td>
<td>$-236.54$</td>
</tr>
</tbody>
</table>

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

- Ulf-G. Meißner, 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


- 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 $^{16}\text{O}$

<table>
<thead>
<tr>
<th></th>
<th>LO</th>
<th>NNLO(2N)</th>
<th>NNLO(3N)</th>
<th>4N$_{\text{eff}}$</th>
<th>Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0^+_1$</td>
<td>-147.3(5)</td>
<td>-121.4(5)</td>
<td>-138.8(5)</td>
<td>-131.3(5)</td>
<td>-127.62</td>
</tr>
<tr>
<td>$0^+_2$</td>
<td>-145(2)</td>
<td>-116(2)</td>
<td>-136(2)</td>
<td>-123(2)</td>
<td>-121.57</td>
</tr>
<tr>
<td>$2^+_1$</td>
<td>-145(2)</td>
<td>-116(2)</td>
<td>-136(2)</td>
<td>-123(2)</td>
<td>-120.70</td>
</tr>
</tbody>
</table>

- **Spectrum:**

- **LO charge radius:** $r(0^+_1) = 2.3(1)\ \text{fm}$ \quad Exp. $r(0^+_1) = 2.710(15)\ \text{fm}$

$\Rightarrow$ compensate for this by rescaling with appropriate units of $r/r_{\text{LO}}$

<table>
<thead>
<tr>
<th></th>
<th>LO</th>
<th>LO(r-scaled)</th>
<th>Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q(2^+_1)$ [e fm$^2$]</td>
<td>10(2)</td>
<td>15(3)</td>
<td>—</td>
</tr>
<tr>
<td>$B(E2, 2^+_1 \rightarrow 0^+_2)$ [e$^2$ fm$^4$]</td>
<td>22(4)</td>
<td>46(8)</td>
<td>65(7)</td>
</tr>
<tr>
<td>$B(E2, 2^+_1 \rightarrow 0^+_1)$ [e$^2$ fm$^4$]</td>
<td>3.0(7)</td>
<td>6.2(1.6)</td>
<td>7.4(2)</td>
</tr>
<tr>
<td>$M(E0, 0^+_2 \rightarrow 0^+_2)$ [e fm$^2$]</td>
<td>2.1(7)</td>
<td>3.0(1.4)</td>
<td>3.6(2)</td>
</tr>
</tbody>
</table>

- **LO EM properties:**

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

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

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

$\leftarrow$ 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

• promising results → 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 $^6\text{Be}$

$\langle e^{i\theta} \rangle$

$N_t$  

$\text{d}_h = 1.00$
$\text{d}_h = 0.85$
$\text{d}_h = 0.75$
$\text{d}_h = 0.65$
$\text{d}_h = 0.55$
$\text{d}_h = 0.35$

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

$\Rightarrow$ 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 $a$-independence
    ← Klein, Lee, Liu, UGM, PLB747 (2015) 511
  → finite size effects/averaging procedures
  → scattering cluster wave functions ← Rokash’s talk
  → ab initio alpha-alpha scattering ← Elhatisari’s talk
  → and much more . . .