Ab initio nuclear structure theory and implications for relativistic heavy-ion collisions

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Physics Colloquium and
STAR Collaboration Meeting
Brookhaven National Laboratory
March 22, 2024
Outline

*Ab initio* methods

Lattice effective field theory

Essential elements for nuclear binding

Emergent geometry and duality of $^{12}$C

Wave function matching

$^{16}$O$^{16}$O collisions at RHIC and LHC energies

$^{16}$O $^{16}$O versus $^{20}$Ne$^{20}$Ne collisions

Outlook
Ab initio methods

adapted from Hergert, Front. Phys. 8, 379 (2020)
Many-Body Perturbation Theory

$$|\Psi\rangle = |\Phi\rangle + \sum_{n=1}^{\infty} \left( \frac{1}{H_0 - E^{(0)}} H_I \right)^n |\Phi\rangle$$

$$E = E^{(0)} + \langle \Phi | \sum_{n=1}^{\infty} H_I \left( \frac{1}{H_0 - E^{(0)}} H_I \right)^n |\Phi\rangle$$

In-Medium Similarity Renormalization Group

Hergert, Front. Phys. 8, 379 (2020)
Coupled Cluster Methods

Self-Consistent Green’s Functions

\[ g_{pq\ldots rs} = \langle \Psi_0^A | T [a_p(t_p)a_q(t_q)\ldots a_s^\dagger(t_s)a_r^\dagger(t_r)] | \Psi_0^A \rangle \]
No-Core Configuration Interaction

\[ |\Psi\rangle = |\Psi\rangle_{\text{core}} \otimes |\Psi\rangle_{\text{valence}} \rightarrow |\Psi\rangle_{\text{all valence}} \]

Symmetry-Adapted No-Core Configuration Interaction
Projected Variational Methods

\[ |\Phi_i(J, M, \pi)\rangle = \sum_{K=-J}^{J} g_K P_{M,K}^{J} P^\pi |\phi_i\rangle \]

\[ |\Psi(J, M, \pi)\rangle = \sum_{i=1}^{N_{\text{basis}}} f_i |\Phi_i(J, M, \pi)\rangle \]

Quantum Monte Carlo
Carlson et al., Rev. Mod. Phys. 87, 1067 (2015); Gandolfi et al, Front. Phys. 8, 117 (2020)

[Foulkes et al., Rev. Mod. Phys. 73, 1 (2001)]
Lattice effective field theory

\[ a \sim 0.5 - 2 \text{ fm} \]

Lähde, Meißner, Nuclear Lattice Effective Field Theory (2019), Springer
Chiral effective field theory

Construct the effective potential order by order

$V_{OPEP}$ Contact interactions

Leading order (LO)

$V_{TPEP}$

Next-to-leading order (NLO)
\[ a = 1.315 \text{ fm} \]
\[ a = 0.987 \text{ fm} \]
Euclidean time projection

\[ \tau = \tau_f \]

\[ \tau = 0 \]

\[ \exp(-H\tau) \]
Auxiliary field method

We can write exponentials of the interaction using a Gaussian integral identity

\[ \exp \left[ -\frac{C}{2} (N^\dagger N)^2 \right] \bigg\rangle (N^\dagger N)^2 \]

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

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.
\[ \tau = \tau_f \]

\[ \psi_I(\vec{r}_3) \rightarrow s_I(\vec{r}_2) \rightarrow s(\vec{r}_1) \]

\[ \text{det } G(s, s_I, \pi_I) \]

\[ G_{ij}(s, s_I, \pi_I) \]

\[ \tau = 0 \]
Essential elements for nuclear binding

What is the minimal nuclear interaction that can reproduce the ground state properties of light nuclei, medium-mass nuclei, and neutron matter simultaneously with no more than a few percent error in the energies and charge radii?

We construct an interaction with only four parameters.

1. Strength of the two-nucleon $S$-wave interaction
2. Range of the two-nucleon $S$-wave interaction
3. Strength of three-nucleon contact interaction
4. Range of the local part of the two-nucleon interaction

fit to $A = 2, 3$ systems

fit to $A > 3$
<table>
<thead>
<tr>
<th></th>
<th>$B$</th>
<th>Exp.</th>
<th>$R_{ch}$</th>
<th>Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^3$H</td>
<td>8.48(2)(0)</td>
<td>8.48</td>
<td>1.90(1)(1)</td>
<td>1.76</td>
</tr>
<tr>
<td>$^3$He</td>
<td>7.75(2)(0)</td>
<td>7.72</td>
<td>1.99(1)(1)</td>
<td>1.97</td>
</tr>
<tr>
<td>$^4$He</td>
<td>28.89(1)(1)</td>
<td>28.3</td>
<td>1.72(1)(3)</td>
<td>1.68</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>121.9(1)(3)</td>
<td>127.6</td>
<td>2.74(1)(1)</td>
<td>2.70</td>
</tr>
<tr>
<td>$^{20}$Ne</td>
<td>161.6(1)(1)</td>
<td>160.6</td>
<td>2.95(1)(1)</td>
<td>3.01</td>
</tr>
<tr>
<td>$^{24}$Mg</td>
<td>193.5(02)(17)</td>
<td>198.3</td>
<td>3.13(1)(2)</td>
<td>3.06</td>
</tr>
<tr>
<td>$^{28}$Si</td>
<td>235.8(04)(17)</td>
<td>236.5</td>
<td>3.26(1)(1)</td>
<td>3.12</td>
</tr>
<tr>
<td>$^{40}$Ca</td>
<td>346.8(6)(5)</td>
<td>342.1</td>
<td>3.42(1)(3)</td>
<td>3.48</td>
</tr>
</tbody>
</table>
Pinhole algorithm
Seeing Structure with Pinholes

Consider the density operator for nucleon with spin $i$ and isospin $j$

$$\rho_{i,j}(n) = a_{i,j}^\dagger(n)a_{i,j}(n)$$

We construct the normal-ordered $A$-body density operator

$$\rho_{i_1,j_1,\ldots,i_A,j_A}(n_1,\ldots,n_A) = :\rho_{i_1,j_1}(n_1)\cdots\rho_{i_A,j_A}(n_A):$$

In the simulations we do Monte Carlo sampling of the amplitude

$$A_{i_1,j_1,\ldots,i_A,j_A}(n_1,\ldots,n_A,t) = \langle \Psi_I | e^{-Ht/2} \rho_{i_1,j_1,\ldots,i_A,j_A}(n_1,\ldots,n_A)e^{-Ht/2} | \Psi_I \rangle$$
$\tau = \tau_f$

$\tau = \tau_f / 2$

$\tau = 0$

Monte Carlo updates of pinholes

Monte Carlo updates of auxiliary/pion fields

Emergent geometry and duality of $^{12}$C

The left panel shows the intrinsic shape of the total nucleon density for $^{10}\text{Be}$. The right panel shows the density distribution of the two neutrons furthest away from the protons in $^{10}\text{Be}$
Wave function matching

Elhatisari et al., Nature, in press
Ground state wave functions

\[ \psi_A \]

\[ \psi_B \]

\[ \psi'_A \]
With wave function matching, we can now compute the eigenenergies starting from the eigenfunctions of $H_B$ and using first-order perturbation theory.

| $E_{A,n} = E'_{A,n}$ (MeV) | $\langle \psi_{B,n} | H_A | \psi_{B,n} \rangle$ (MeV) | $\langle \psi_{B,n} | H'_A | \psi_{B,n} \rangle$ (MeV) |
|--------------------------|----------------------------------|----------------------------------|
| -1.2186                  | 3.0088                           | -1.1597                          |
| 0.2196                   | 0.3289                           | 0.2212                           |
| 0.8523                   | 1.1275                           | 0.8577                           |
| 1.8610                   | 2.2528                           | 1.8719                           |
| 3.2279                   | 3.6991                           | 3.2477                           |
| 4.9454                   | 5.4786                           | 4.9798                           |
| 7.0104                   | 7.5996                           | 7.0680                           |
| 9.4208                   | 10.0674                          | 9.5137                           |
| 12.1721                  | 12.8799                          | 12.3163                          |
| 15.2669                  | 16.0458                          | 15.4840                          |

$R = 2.6$ fm
N3LO chiral effective field theory interaction
Binding energy per nucleon

Elhatisari et al., Nature, in press
Charge radius

Elhatisari et al., Nature, in press
$^{16}\text{O}^{16}\text{O}$ collisions at RHIC and LHC energies

[Summerfield, Lu, Plumberg, D.L., Noronha-Hostler, Timmins PRC 104, L041901 (2021)]

$^{16}\text{O}^{16}\text{O}$ collisions have been proposed at RHIC and LHC to probe dependence on initial states of intermediate size, where alpha clustering is expected to be significant.

We use the TRENTo model to general the initial entropy distribution. Moreland et al., Phys. Rev. C 92, 044903 (2015)

The initial entropy distribution is then passed through a free-streaming phase of duration 0.37 fm/c and used to initialize the hydrodynamics evolution.
We compute the following cumulants of the flow harmonics \( v_n \):

\[
\begin{align*}
  v_n \{2\} &= \left[ \langle v_n^2 \rangle \right]^{\frac{1}{2}} \\
  v_n \{4\} &= \left[ 2 \langle v_n^2 \rangle^2 - \langle v_n^4 \rangle \right]^{\frac{1}{4}}
\end{align*}
\]

We first compute results taking the initial density as a Woods-Saxon potential with density, radius, and diffusive fitted to empirical values. We then consider the same Woods-Saxon potential, taking into account the quark substructure of the nucleons. Lastly, we consider using the nucleon distribution from the lattice effective field theory calculations. This will incorporate correlations such as alpha clustering.

Figure 3. The figure illustrates $v_2\{4\}/v_2\{2\}$ as a function of centrality, defined by charged hadron multiplicity at $|\eta| < 1.5$, in $^{16}$O+$^{16}$O collisions. Additionally, the $\epsilon_2\{4\}/\epsilon_2\{2\}$ ratio from NLEFT, VMC, and two types of 3pF distributions are presented for comparison. Note that an issue is identified in the publicly available PHOBOS Glauber, which affected the implementation of the NLEFT and VMC configuration. This has been corrected in the updated figure.
figure from Giuliano Giacalone
Figure 2. (Color online) Point proton densities in $^{16}$O. The green line refers to the "experimental" result, see text for details.

Lonardoni, Lovato, Pieper, Wiringa, Phys. Rev. C 96, 024326
https://discovery.phys.virginia.edu/research/groups/ncd/plot.html

Nuclear Charge Density Archive - Plots

Select a nuclei from the drop-down box on the right. Then, select a normalization type using the radio buttons that appear (a radio button must be selected). Then click 'PLOT' to add the nuclei to the plot. To remove a plot, simply click the 'REMOVE' button next to the nuclei you would like to remove from the table on the left. To update the axes, use the sliders on the right side, then click 'PLOT' to update. To save an image of the graph, grab a screenshot of the page.

Note that 'non-normalized' $(\rho(r))$ graphs do not have their plots scaled, whereas 'normalized' $((A/Z)\rho(r))$ graphs are scaled by a factor of $(A/Z)$.

Information about specific plot models can be found on the About page.
$^{16}\text{O}^{16}\text{O}$ versus $^{20}\text{Ne}^{20}\text{Ne}$ collisions

Giacalone et al., arXiv:2402.05995
Giacalone et al., arXiv:2402.05995
The elliptic flow of $^{20}\text{Ne}^{20}\text{Ne}$ collisions is enhanced by as much as $1.170(8)\text{stat.}(30)\text{syst.}$ for NLEFT and $1.139(6)\text{stat.}(39)\text{syst.}$ for PGCM relative to $^{16}\text{O}^{16}\text{O}$ collisions for the 1% most central events.
Outlook

This talk started with an overview of different *ab initio* nuclear theory methods, including lattice EFT. It then described how lattice EFT is being used to predict nuclear structure. It also described how pinhole configurations provide *ab initio* data for initial states in relativistic heavy-ion collisions.

In a few years, it will be possible to do *ab initio* calculations of nuclear states across the nuclear chart using lattice EFT. We look forward to collaborating with our relativistic heavy-ion colleagues to explore this new field bringing together two different nuclear science communities.