New Results in Lattice Scattering Using the Adiabatic Projection Method

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Nuclear Lattice EFT Collaboration

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Science objectives

*Ab initio* calculations of scattering and reactions relevant to alpha processes in stellar evolution and Type Ia supernovae

\[ ^4\text{He} + ^4\text{He} \rightarrow ^4\text{He} + ^4\text{He} \]
\[ ^{12}\text{C} + ^4\text{He} \rightarrow ^{16}\text{O} + \gamma \]
\[ ^{20}\text{Ne} + ^4\text{He} \rightarrow ^{24}\text{Mg} + \gamma \]
\[ ^{12}\text{C} + ^{12}\text{C} \rightarrow ^{20}\text{Ne} + ^4\text{He} \]
\[ ^4\text{He} + ^4\text{He} + ^4\text{He} \rightarrow ^{12}\text{C} + \gamma \]
\[ ^{16}\text{O} + ^4\text{He} \rightarrow ^{20}\text{Ne} + \gamma \]
\[ ^{24}\text{Mg} + ^4\text{He} \rightarrow ^{28}\text{Si} + \gamma \]
\[ ^{16}\text{O} + ^{16}\text{O} \rightarrow ^{28}\text{Si} + ^4\text{He} \]

Challenges

How to reduce computational scaling with number of nucleons in participating nuclei? Can we provide useful *ab initio* input for halo/cluster EFT calculations?
Outline

Lattice effective field theory
Cluster structures in $^{12}$C and $^{16}$O
Adiabatic projection method
Lüscher’s finite-volume method
Asymptotic cluster wave functions

$^4$He + $^4$He $\rightarrow$ $^4$He + $^4$He

Summary and outlook
Lattice chiral effective field theory

\[ a \sim 1 - 2 \text{ fm} \]

Construct the effective potential order by order

\[ V_{\text{OPEP}} \quad \text{Contact interactions} \]

\[ V_{\text{TPEP}} \]

Leading order (LO)

Next-to-leading order (NLO)
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

\[
\exp \left[ -\frac{C}{2} (N^\dagger N)^2 \right] \quad \left\langle \begin{array}{c} \quad (N^\dagger N)^2 \\
\end{array} \right. \\
= \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} ds \exp \left[ -\frac{1}{2} s^2 + \sqrt{-C} \, s(N^\dagger N) \right] \\
\left\langle \begin{array}{c} \quad \quad sN^\dagger N \
\end{array} \right.
\]

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.
Sign oscillations in determinant suppressed by approximate Wigner SU(4) symmetry
Carbon-12

$0^+_1$, $2^+_1$  

$0^+_2$, $2^+_2$

Compact triangular  

Bent-arm structure

$a = 1.97 \text{ fm}$

PRL 106, 192501, 2011; PRL 109, 252501, 2012
Oxygen-16

$0^+_1$

Tetrahedral structure

$0^+_2$, $2^+_1$

Square-like structure

$a = 1.97$ fm

PRL 112, 102501, 2014
Adiabatic projection method

Development inspired by progress using no-core shell model with resonating group method to describe \textit{ab initio} scattering and reactions in light nuclei.

Navratil, Roth, Quaglioni, PRC 82 034609 (2010); Navratil, Quaglioni, PRC 83 044609 (2011); etc.

Strategy is to divide the problem into two parts. In the first part, we use Euclidean time projection and lattice Monte Carlo to derive an \textit{ab initio} low-energy cluster Hamiltonian, called the adiabatic Hamiltonian (adiabatic transfer matrix for nonzero temporal lattice spacing).

In the second part, we use the adiabatic Hamiltonian to compute scattering phase shifts or reaction amplitudes.
Start with localized cluster states for all possible separation vectors $\vec{R}$

$$|\vec{R}\rangle = \sum_{\vec{r'}} |\vec{r'} + \vec{R}\rangle_1 \otimes |\vec{r'}\rangle_2$$
Cluster evolution with Euclidean time

\[ |\vec{R}\rangle_{\tau} = \exp(-H\tau)|\vec{R}\rangle \]
Use projection Monte Carlo to propagate cluster wavefunctions in Euclidean time to form dressed cluster states

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

Evaluate matrix elements of the full microscopic Hamiltonian with respect to the dressed cluster states,

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

Since the dressed cluster states are in general not orthogonal, we construct a norm matrix given by the inner product

\[ [N_\tau]_{\vec{R},\vec{R}'} = \tau \langle \vec{R}|\vec{R}'\rangle_\tau \]
The adiabatic Hamiltonian is defined by the matrix product

\[
[H^a_\tau]_{\vec{R}, \vec{R'}} = \left[ N^{-1/2}_\tau H_\tau N^{-1/2}_\tau \right]_{\vec{R}, \vec{R'}}
\]

One can see the similarity to no-core shell model with resonating group method. But in the adiabatic projection method we don’t need to include excitations of the participating nuclei unless the energy is above the corresponding inelastic threshold.

Distortion and polarization of the nuclear wave functions are automatically produced by the Euclidean time projection.

As we increase the projection time, the adiabatic Hamiltonian exactly reproduces the low-energy spectrum of the full microscopic Hamiltonian.
Quartet neutron-deuteron scattering (pionless EFT)

Convergence $L=7$, $b=1/100$ MeV

$E$(MeV) vs $t$(MeV$^{-1}$)

Lüscher’s finite-volume formula


Two-particle energy levels near threshold in a periodic cube are related to the elastic phase shifts

\[ p \cot \delta_0(p) = \frac{1}{\pi L} S(\eta), \quad \eta = \left(\frac{Lp}{2\pi}\right)^2 \]

\[ S(\eta) = \lim_{\Lambda \to \infty} \left[ \sum_{\vec{n}} \frac{\theta(\Lambda^2 - \vec{n}^2)}{\vec{n}^2 - \eta} - 4\pi\Lambda \right] \]
Signal-to-noise problems for finite-volume energy extraction

Nuclear binding

energy shift

free scattering energy
Asymptotic cluster scattering wave functions

In the far asymptotic region where our dressed clusters are widely separated, they interact only through infinite-range forces such as the Coulomb interaction. Therefore we can describe everything with an effective cluster Hamiltonian $H^{\text{eff}}$ that is nothing more than a free lattice Hamiltonian for two point particles plus any infinite-range interactions inherited from the full microscopic Hamiltonian. So in the asymptotic region we have

\[
[N_\tau]_{\vec{R},\vec{R}'} = c \cdot \left[ e^{-2H^{\text{eff}} \tau} \right]_{\vec{R},\vec{R}'} ,
\]

\[
[H_\tau]_{\vec{R},\vec{R}'} = c \cdot \left[ e^{-H^{\text{eff}} \tau} H^{\text{eff}} e^{-H^{\text{eff}} \tau} \right]_{\vec{R},\vec{R}'} ,
\]

Since

\[ \left( N_\tau^{-1/2} \right)_{\vec{R},\vec{R}'} = c^{-1/2} \cdot \left[ e^{H_{\text{eff}}^\tau} \right]_{\vec{R},\vec{R}'} \]

we conclude that the adiabatic Hamiltonian coincides with the effective cluster Hamiltonian in the asymptotic region

\[ [H_{\tau}^a]_{\vec{R},\vec{R}'} = [H_{\text{eff}}]_{\vec{R},\vec{R}'} \]

In the asymptotic region, we are inverting the diffusion process when computing the adiabatic Hamiltonian and are left with an effective cluster Hamiltonian in position space basis.
We use projections onto spherical harmonics defined on sets of lattice points with the same distance from the origin.

\[ |\vec{R}\rangle^{L,L_z} = \sum_{\vec{R}'} Y_{L,L_z}(\hat{\vec{R}}') \delta_{R,|\vec{R}'|} |\vec{R}'\rangle \]

Lu, Lähde, Lee, Meißner, arXiv:1506.05652

New algorithm developed for auxiliary field updates and initial/final state updates

\[ [Z_{n_t,LO}]_{R,R'}^{L,L_z} = \langle R | L,L_z | \vec{R}' \rangle^{L,L_z} |\vec{R}'\rangle \]

Hybrid Monte Carlo updates

Metropolis updates
two cluster simulations

\[ L^3 \sim (16 \text{ fm})^3 \]

single cluster simulations

\[ L^3 \sim (120 \text{ fm})^3 \]
\[ ^4\text{He} + ^4\text{He} \rightarrow ^4\text{He} + ^4\text{He} \]

We now present *ab initio* results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.


We did calculations for the S-wave and for the $L = 2$, $L_z = 0$ D-wave projections.
The graph shows the wave function $\psi(r)$ as a function of the radial coordinate $r$ (in femtometers, fm). Two states are compared: the $2S$ state (dashed line with crosses) and the $3S$ state (dotted line with stars). The $R_{\text{wall}}$ mark on the right axis indicates a specific radial distance, which is not explicitly defined in the image but typically refers to a boundary or a limit in the context of quantum mechanics. The graph illustrates how the wave function changes with increasing radial distance.
$S$-wave

Afzal et al., RMP 41 247 (1969)

Afzal, Ahmad, Ali, RMP 41 247 (1969)
$S$-wave at NNLO

$\delta_0$ (degrees)

$E_{\text{Lab}}$ (MeV)

$L_t = 4$
$L_t = 5$
$L_t = 6$
$L_t = 7$
$L_t = 8$
$L_t = 9$
$L_t = 10$

Higa et al. (halo EFT)
Afzal et al.

\[ \delta_2 \text{ (degrees)} \]

\[ E_{\text{Lab}} \text{ (MeV)} \]

- NLO
- NNLO

Afzal et al.
$D$-wave at NNLO

\begin{align*}
\delta_2 (\text{degrees}) & \\
E_{\text{Lab}} (\text{MeV}) & \\
\end{align*}

$L_t = 4$
$L_t = 5$
$L_t = 6$
$L_t = 7$
$L_t = 8$
$L_t = 9$
$L_t = 10$

Afzal et al.

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Summary and outlook

More work needs to be done. But alpha processes now appear to be in reach of \textit{ab initio} methods. Since the sign oscillations are mild for alpha nuclei, the scaling is very favorable.

For an $A_1$-body + $A_2$-body scattering or reaction process the computational scaling is typically $\sim (A_1 + A_2)^2$.

For mass and charge transfer processes, we do the same steps but consider coupled channel scattering. For capture reactions, we include one-photon matrix elements and compute overlaps between bound states and scattering states.

Could be useful and interesting to explore connections with halo/cluster EFT calculations. In cases where the separation of scales is good, halo/cluster EFT calculations should agree with adiabatic projection method. In cases where the separation of scales is not large, the halo/cluster EFT calculations can use the adiabatic projection method as guidance.

Would be interesting to see if some of these methods can be used for calculations in relativistic field theories, in particular lattice QCD.