Ab initio alpha-alpha scattering using adiabatic projection method

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[Scattering and reactions]
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Advances in Diagrammatic Monte Carlo Methods for QFT Calculations in Nuclear-, Particle-, and Condensed Matter Physics

5 October, Trento, Italy
- Introduction
- Lattice effective field theory
- Adiabatic projection method
- Scattering cluster wave function
- Alpha-alpha scattering
- Summary
Thermonuclear reaction rates of alpha capture on light nuclei during the stellar nucleosynthesis are critical for the formation of the building blocks of life and the evolution of the universe (the production of Carbon-12, Oxygen-16, ...).

The rates also determine the size of the iron cores formed in Type-II supernovae, which results in the ultimate fate of the collapsed remnant into either neutron star or black hole.

... low energy nuclear scattering and reaction processes relevant for stellar astrophysics

- Scattering of alpha particles. \( ^4\text{He} + ^4\text{He} \rightarrow ^4\text{He} + ^4\text{He} \)

- Triple- alpha reaction. \( ^4\text{He} + ^4\text{He} + ^4\text{He} \rightarrow ^{12}\text{C} + \gamma \)

- Alpha capture. \( ^{12}\text{C} + ^4\text{He} \rightarrow ^{16}\text{O} + \gamma \)

\[ \vdots \]
QMC calculations of neutron-α scattering.  

Ab Initio Many-Body Calculations of n-H₃, n-He⁴, p-He³⁴, and n-Be₁⁰ Scattering.  

Ab initio many-body calculations of the ³H(d, n)⁴He and ³He(d, p)⁴He fusion.  

Elastic proton scattering of medium mass nuclei from coupled-cluster theory.  
Hagen & Michel PRC 86, 021602 (2012).

Coupling the Lorentz Integral Transform (LIT) and the Coupled Cluster (CC) Methods  

***Deuteron is the heaviest projectile in ab initio calculations of scattering on a heavier target that have been achieved.
Ab initio calculations of scattering and reactions suffer from the computational scaling with the number of nucleons in clusters.

It remains a challenge to address important processes relevant for stellar astrophysics

- Scattering of alpha particles. \( ^4\text{He} + ^4\text{He} \rightarrow ^4\text{He} + ^4\text{He} \)

- Triple- alpha reaction. \( ^4\text{He} + ^4\text{He} + ^4\text{He} \rightarrow ^{12}\text{C} + \gamma \)

- Alpha capture. \( ^{12}\text{C} + ^4\text{He} \rightarrow ^{16}\text{O} + \gamma \)

Ab initio alpha-alpha scattering

S.E., Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, & Meißner.

arXiv:1506.03513
Lattice effective field theory
Lattice effective field theory is a powerful numerical method formulated in the framework of effective field theory.
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Effective field theory organizes the nuclear interactions as an expansion in powers of momenta and other low energy scales such as the pion mass.

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Fig. courtesy E.Epelbaum

Ordonez et al. ‘94; Friar & Coon ‘94; Kaiser et al. ‘97; Epelbaum et al. ‘98,’03,’05; Kaiser ‘99-’01; Higa et al. ‘03; ...
Two-body scattering on the lattice

- Two spin-1/2 particles scattering.

- The LECs by fitting the experimental $NN$ scattering data
Nuclear lattice EFT collaboration

Lattice effective field theory – Euclidean time projection

Nucleons

Euclidean time

$\tau_i$

$\tau_f$

$L$

$a \sim 1-2\,\text{fm}$
\[ e^{-H\tau} \]

\[ \tau = L_t \alpha_t \]

- evolve nucleons forward in Euclidean time.
- allow them to interact
The evolution in Euclidean time automatically incorporates the induced deformation and polarization of the clusters as they come near each other.

The deformation and polarization are due to the interactions of individual nucleons between the two clusters, as well as repulsion due to the Pauli exclusion principle for identical fermions.
Lattice simulations

Transfer matrix operator formalism \( M = : \exp(-H \alpha_t) : \)

Microscopic Hamiltonian \( H = H_{\text{free}} + V \)

The free Hamiltonian with the simplest discretized dispersion relation

\[
H_{\text{free}} = \sum_s \sum_i \sum_{\vec{n}} \frac{1}{2m_s} b^\dagger_s(\vec{n}) \left[ 2 b_s(\vec{n}) - b_s(\vec{n} + \hat{l}) - b_s(\vec{n} - \hat{l}) \right]
\]

\[
Z^{(L_t)} = \int Dc \, Dc^* \exp[-S(c, c^*)] = \text{Tr} [M^{L_t}]
\]


The exact equivalence of several different lattice formulations.


\[
e^{-E_0 a_t} = \lim_{L_t \to \infty} \frac{Z^{(L_t+1)}}{Z^{(L_t)}}
\]
Lattice Monte Carlo calculations

Hybrid Monte Carlo sampling

$H_{SU(4)}$ acts as an approximate and inexpensive low energy filter at few first/last time steps. Significant suppression of sign oscillations.


$$|\psi_{\vec{r}_1,\vec{r}_2}(\tau')\rangle = \exp[-H_{SU(4)}\tau'] |\psi_{\vec{r}_1,\vec{r}_2}\rangle$$

$$\tau' = L_t' \alpha_t$$

For time steps in midsection, the full $H_{LO}$ Hamiltonian is used.

$$|\psi_{\vec{r}_1,\vec{r}_2}(\tau/2)\rangle = \exp[-H_{LO}\tau/2] |\psi_{\vec{r}_1,\vec{r}_2}(\tau')\rangle$$

The amplitude

$$Z^{(L_t)} = \langle \psi_{\vec{r}_3,\vec{r}_4}(\tau/2)|\psi_{\vec{r}_1,\vec{r}_2}(\tau/2)\rangle$$

For the observable $\mathcal{O}$

$$Z^{(L_t)}_{\langle\mathcal{O}\rangle,LO} = \langle \psi_{\vec{r}_3,\vec{r}_4}(\tau/2)|\mathcal{O}|\psi_{\vec{r}_1,\vec{r}_2}(\tau/2)\rangle$$

$$\langle\mathcal{O}\rangle_{0,LO} = \lim_{L_t \to \infty} Z^{(L_t)}_{\langle\mathcal{O}\rangle,LO}/Z^{(L_t)}_{LO}$$
Lattice Monte Carlo calculations

Higher order calculations:

\[ \exp[-H_{\text{NLO}} \alpha_t] : \]
\[ \exp[-H_{\text{NNLO}} \alpha_t] : \]

The amplitude is

\[ Z^{(L_t)}_{\text{NLO}} = \langle \psi_{\vec{r}_3, \vec{r}_4} (\tau/2) | \psi_{\vec{r}_1, \vec{r}_2} (\tau/2) \rangle \]

For the observable \( \mathcal{O} \)

\[ Z^{(L_t)}_{\langle \mathcal{O} \rangle, \text{NLO}} = \langle \psi_{\vec{r}_3, \vec{r}_4} (\tau/2) | \mathcal{O} | \psi_{\vec{r}_1, \vec{r}_2} (\tau/2) \rangle \]

The observable \( \mathcal{O} \) at NLO

\[ \langle \mathcal{O} \rangle_{0, \text{NLO}} = \lim_{L_t \to \infty} \frac{Z^{(L_t)}_{\langle \mathcal{O} \rangle, \text{NLO}}}{Z^{(L_t)}_{\text{NLO}}} \]
Each nucleon evolves as if a single particle in a fluctuating background of pion fields and auxiliary fields.

Using a Gaussian integral identity ($s$ is an auxiliary field coupled to particle density.)

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

Split the problem into two parts.

The first part use Euclidean time projection to construct an ab initio low-energy cluster Hamiltonian, called the adiabatic Hamiltonian.

The second part compute the two-cluster scattering phase shifts or reaction amplitudes using the adiabatic Hamiltonian.

The method constructs a low-energy effective theory for clusters. Use initial states parameterized by the relative spatial separation between clusters, and project them in Euclidean time.

\[ |\vec{R}\rangle = \sum_\vec{r} |\vec{r} + \vec{R}\rangle_1 \otimes |\vec{r}\rangle_2 \]

The adiabatic projection in Euclidean time gives a systematically improvable description of the low-lying scattering cluster states.

\[ |\vec{R}\rangle_\tau = e^{-H_\tau} |\vec{R}\rangle \]

Dressed cluster states

The adiabatic projection in Euclidean time gives a systematically improvable description of the low-lying scattering cluster states.

In the limit of large Euclidean projection time the description becomes exact.

The structure of the adiabatic Hamiltonian, $[H^a_\tau]_{\vec{R} \vec{R'}}$, is similar to the Hamiltonian matrix used in recent calculations of *ab initio* NCSM/RGM for nuclear scattering and reactions.

Microscopic Hamiltonian
\[ L^3(A-1) \times L^3(A-1) \]

Two-cluster (adiabatic) Hamiltonian
\[ L^3 \times L^3 \]

fermion-dimer scattering

Pine, Lee, Rupak, *EPJA 49 (2013) 151*
Scattering phase shifts from finite volumes

\[
\psi_\ell(r) = N \left[ \cos \delta_\ell(p) F_\ell(p r) + \sin \delta_\ell(p) G_\ell(p r) \right]
\]

\[
\psi_\ell(r) = N \left[ \cos \delta_\ell(p) F_\ell(p \, r) + \sin \delta_\ell(p) G_\ell(p \, r) \right]
\]

\[
R'_{\text{wall}} = R_{\text{wall}} + \epsilon \quad -a/2 \leq \epsilon \leq a/2
\]
\[ \psi_\ell(r) = N \left[ \cos \delta_\ell(p) F_\ell(p \, r) + \sin \delta_\ell(p) G_\ell(p \, r) \right] \]

(a)—Use the spectrum of the adiabatic Hamiltonian and the fact that the cluster wave function vanishes for \( r = R'_{\text{wall}} \) to compute the scattering phase shifts directly from

\[ \delta_\ell(p) = \tan^{-1} \frac{F_\ell(p \, R'_{\text{wall}})}{G_\ell(p \, R'_{\text{wall}})} \]


(b)—Use the spherical wall method and extract the scattering phase shifts and momentum by fitting the radial asymptotic wave function to the two-cluster wave function.

neutron-deuteron scattering (pionless EFT)


Gabbiani, Bedaque, Grießhammer, *NPA 675 (2000) 601*
During the Euclidean time interval $\tau_\varepsilon$, each cluster undergoes spatial diffusion

$$d_{\varepsilon,i} = \sqrt{\tau_\varepsilon/M_i}$$

only non-overlapping clusters if

$$|\vec{R}| \gg d_{\varepsilon,i}$$

Define the asymptotic region where the amount of overlap between cluster wave packages is less than $\varepsilon$

$$|\vec{R}| > R_\varepsilon$$

$\varepsilon$ is the relative error.

For $|\vec{R}| > R_\epsilon$, the dressed cluster states are widely separated, and we can describe the system in terms of an effective cluster Hamiltonian, $H^{\text{eff}}$, which is a free lattice Hamiltonian for two clusters plus infinite-range interactions.

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

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

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

Simulations for \((A_1 + A_2)\) system

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

Simulations for cluster \(A_1\) and cluster \(A_2\)

\[ L^3 \sim (120 \text{ fm})^3 \]

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

\[ A_1 + A_2 \rightarrow A_1 + A_2 \]
Define “radial adiabatic Hamiltonian” by coherently adding 3D position states \( |n_x, n_y, n_z\rangle \) weighted by the spherical harmonics

\[
|R\rangle^{\ell,\ell_z} = \sum_{\tilde{R}'} Y_{\ell,\ell_z} (\hat{R}') \delta_{R,|\tilde{R}'|} |\tilde{R}'\rangle
\]


Precise determination of lattice phase shifts and mixing angles

Lu, Lähde, Lee, Meißner, arXiv:1506.05652
Radial adiabatic Hamiltonian

\[ n_x^2 + n_y^2 + n_z^2 = \begin{cases} 0 & \text{for } Y_{0,0} (\hat{R}') \\ 1 & \text{for } Y_{0,1} (\hat{R}') \\ 2 & \text{for } Y_{0,2} (\hat{R}') \end{cases} \]

\[ |R\rangle^{\ell,\ell_z} = \sum_{\tilde{R}'} Y_{\ell,\ell_z} (\hat{R}') \delta_{R,|\tilde{R}'|} |\tilde{R}'\rangle \]
• the same lattice action as in the Hoyle state of $^{12}\text{C}$ and the structure of $^{16}\text{O}$,
  \textit{PRL 106 (2011) 192501.}
  \textit{PRL 109 (2012) 252501.}
  \textit{PRL 112 (2014) 102501.}

• a new algorithm for Monte Carlo updates and alpha clusters,

• the adiabatic projection method to construct a two-alpha (adiabatic) Hamiltonian,

• the spherical wall method to extract the scattering phase shifts.

Alpha-alpha scattering

\[ a = 1.97 \text{ fm} \]
\[ a_t = 1.32 \text{ fm} \]

Afzal, Ahmad, Ali, Rev. Mod. Phys. 41, 247 (1969)
\[ \delta_0(L_t, E) = \delta_0(E) + c_0(E) e^{-\Delta E_0} L_t a_t \]

\[ a = 1.97 \text{ fm} \]
\[ a_t = 1.32 \text{ fm} \]

\( a = 1.97 \text{ fm} \)
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\[ a_t = 1.32 \text{ fm} \]

Afzal, Ahmad, Ali, Rev. Mod. Phys. 41, 247 (1969)
\[ \delta_2(L_t, E) = \delta_2(E) + c_2(E) e^{-\Delta E_2 L_t} a_t \]

\[ a = 1.97 \text{ fm} \]

\[ a_t = 1.32 \text{ fm} \]

$a = 1.97 \text{ fm}$

$a_t = 1.32 \text{ fm}$


• The adiabatic projection method is a general framework for scattering and reactions on the lattice.

• Scattering and reaction processes involving alpha particle are in reach of \textit{ab initio} methods.

• The computational scaling for $A_1$-body and $A_2$-body clusters is $(A_1 + A_2)^2$

• The problem of sign oscillations is greatly suppressed for alpha-like nuclei, and this approach appears to be a viable method to study important alpha processes involving heavier nuclei.

Thank you!
Extras
Two-body energy levels below the inelastic threshold in a periodic lattice are related to the scattering phase shifts in continuum.


\[ p^{2\ell+1} \cot \delta_\ell(p) = -\frac{1}{a_\ell} + \frac{1}{2} r_\ell p^2 + \ldots \]

scattering length

Effective range

\[ p \cot \delta_\ell(p) = \frac{2}{\sqrt{\pi L}} \mathcal{Z}_{0,0}(1; \eta) \quad \text{for } \ell = 0,1 \]

Generalized Zeta function

\[ \mathcal{Z}_{\ell,m}(1; \eta) = \sum_{\hat{n}} \frac{|\hat{n}|^\ell Y_{\ell,m}(\hat{n})}{|\hat{n}|^2 - \eta} \quad \eta = \left(\frac{LP}{2\pi}\right)^2 \]
neutron-deuteron scattering (pionless EFT)

\[
E_0 = \lim_{\tau \to \infty} \frac{\langle \psi_{e,p} | H | \psi_{e,p} \rangle_\tau}{\langle \psi_{e,p} | \psi_{e,p} \rangle_\tau}
\]

Gabbiani, Bedaque, Grießhammer, NPA 675 (2000) 601
neutron-deuteron scattering (pionless EFT)

\[ E_0 = \lim_{\tau \to \infty} \frac{\tau \langle \psi_{o,p} | H | \psi_{o,p} \rangle}{\tau \langle \psi_{o,p} | \psi_{o,p} \rangle} \]

Gabbiani, Bedaque, Grießhammer, \textit{NPA 675 (2000) 601}
$$\psi_\ell(r) = N \left[ \cos \tilde{\delta}_\ell(p) F_\ell(p \ r) + \sin \tilde{\delta}_\ell(p) G_\ell(p \ r) \right]$$

$L_t = 4 \quad a = 1.97 \text{ fm} \quad a_t = 1.32 \text{ fm}$