Scattering phase shifts and mixing angles for an arbitrary number of coupled channels on the lattice

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Outline

Introduction

- Chiral lattice EFT (as described by Dean Lee) allows for simulations of light and medium-mass nuclei, e.g. ^{3}H, ^{4}He, ^{12}C, ^{16}O, ^{28}Si.

  Eur. Phys. J. A 41, 125 (2009); Phys. Rev. Lett. 106, 192501 (2011);
  Phys. Rev. Lett. 109, 252501 (2012); Phys. Rev. Lett. 112, no. 10, 102501 (2014);
  Phys. Lett. B 732, 110 (2014)

- It requires a method to extract the infinite-volume scattering amplitude from the lattice data.

- In lattice QCD (as described by Constantia Alexandrou), Lüscher's method can be used to relate the (n-channel) S-matrix to the finite-volume energy spectrum.

  Phys. Rev. D 89, no. 7, 074507 (2014); JHEP 1610, 011 (2016); Phys. Rev. D 97, no. 5, 054513 (2018);
  JHEP 1807, 043 (2018); arXiv:1904.04136

Introduction

- For heavier nuclei in lattice EFT, the finite-volume scattering energies ($\sim 100\ \mathrm{keV}$) are very small compared to the binding energies ($\sim 100\ \mathrm{MeV}$).

- Therefore, the error of the Monte-Carlo energy levels is larger than the separation between these levels.

  $\Rightarrow$ Lüscher's method is not accurate enough for calculations of nucleus-nucleus scattering phase shifts.

  Phys. Lett. B 760, 309 (2016)

- Instead, one can use the adiabatic projection method to compute an effective nucleus-nucleus Hamiltonian.

  Phys. Rev. C 92, no. 5, 054612 (2015); Nature 528, 111 (2015); Eur. Phys. J. A 52, no. 6, 174 (2016)

Introduction

- Once this so-called adiabatic Hamiltonian is calculated, one can extract phase shifts using spherical wall boundary conditions together with projection onto partial waves.

  Nucl. Phys. A 424, 47 (1984); Eur. Phys. J. A 34, 185 (2007); Phys. Lett. B 760, 309 (2016); Eur. Phys. J. A 53, no. 5, 83 (2017); Phys. Rev. C 98, no. 4, 044002 (2018)

- However, this technique has so far only been applied to uncoupled channels or two coupled channels.

- goal: generalization to three or more coupled partial waves (non-trivial)

Benchmark system

scattering of two spin-1 bosons with approximate deuteron mass $m_1 = m_2 = 2m_{\mathrm{N}}$, $m_{\mathrm{N}} = 938.92\ \mathrm{MeV}$:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(\vec{r}_1 - \vec{r}_2)$$

test potential for spin-$1/2$ fermions ("one-pion exchange"):

$$V(\vec{r}\,) = C\left(1 + \frac{3(\vec{r}\cdot\vec{\sigma}_1)(\vec{r}\cdot\vec{\sigma}_2) - (\vec{\sigma}_1\cdot\vec{\sigma}_2)r^2}{r_0^2}\right)e^{-r^2/(2r_0^2)}$$

$C = -2\ \mathrm{MeV}, \quad r_0 = 3.95\ \mathrm{fm}$

$\vec{\sigma}_i$: Pauli matrices for particle $i = 1, 2$

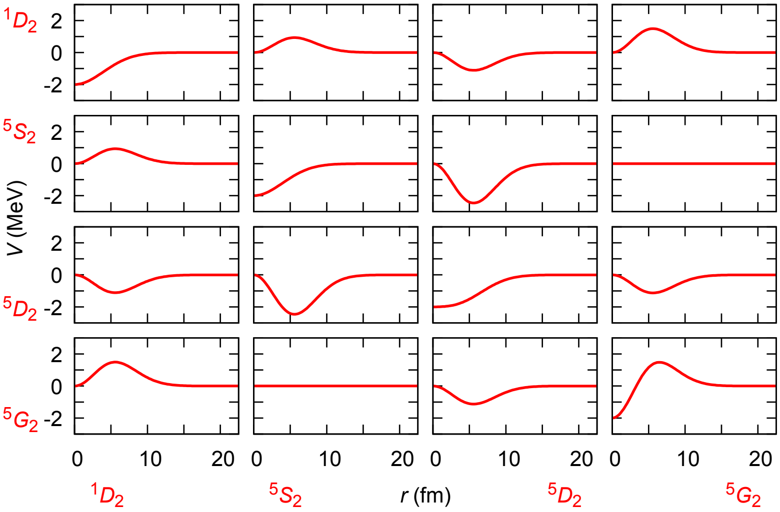
Eur. Phys. J. A 34, 185 (2007); Phys. Lett. B 760, 309 (2016)

replace Pauli matrices $\vec{\sigma}_i$ by spin-1 matrices $\vec{s}_i$:

$$V(\vec{r}\,) = C\left(1 + \frac{3(\vec{r}\cdot\vec{s}_1)(\vec{r}\cdot\vec{s}_2) - (\vec{s}_1\cdot\vec{s}_2)r^2}{r_0^2}\right)e^{-r^2/(2r_0^2)}$$

Benchmark system

projecting $V(\vec{r})$ onto partial waves yields up to four coupled scattering channels:

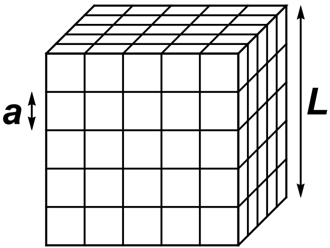


Lattice method: projection onto partial waves

define cubic lattice with spacing $a = 1.97\ \mathrm{fm}$ and length $L = 35a$:

$$\vec{r} = (r_1, r_2, r_3);$$
$$r_i = 0, \ldots, (L-1)a$$
$$= 0, \ldots, (L-1)\ \mathrm{l.u.}$$

(use dimensionless lattice units)



introduce periodic boundary conditions:

$$|\vec{r}\,\rangle = |\vec{r} + L\hat{e}_1\rangle = |\vec{r} + L\hat{e}_2\rangle = |\vec{r} + L\hat{e}_3\rangle$$

consider Hamiltonian in center-of-mass system (CMS):

$$H = \frac{\Delta}{2\mu} + V(\vec{r}\,) \quad \text{with} \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

Lattice method: projection onto partial waves

discretize free term using $O(a^4)$-improved lattice dispersion relation: Eur. Phys. J. A 34, 185 (2007)

$$H\left|\vec{r}\,\right\rangle = \frac{49}{12\mu}\left|\vec{r}\,\right\rangle - \frac{3}{4\mu}\sum_{i=1}^{3}\left(\left|\vec{r}+\hat{e}_i\right\rangle + \left|\vec{r}-\hat{e}_i\right\rangle\right)$$
$$+ \frac{3}{40\mu}\sum_{i=1}^{3}\left(\left|\vec{r}+2\hat{e}_i\right\rangle + \left|\vec{r}-2\hat{e}_i\right\rangle\right)$$
$$- \frac{1}{180\mu}\sum_{i=1}^{3}\left(\left|\vec{r}+3\hat{e}_i\right\rangle + \left|\vec{r}-3\hat{e}_i\right\rangle\right) + V(\vec{r}\,)\left|\vec{r}\right\rangle$$

define radial states for partial wave ${}^{2s+1}l_j$: Phys. Lett. B 760, 309 (2016)

$$\left|R\right\rangle_{s,l,j} = \sum_{\vec{r}}\sum_{l_z,s_z}\sum_{s_{1,z}}\sum_{s_{2,z}} C^{j,l,s}_{0,l_z,s_z} C^{s,1,1}_{s_z,s_{1,z},s_{2,z}} Y_{l,l_z}(\hat{r})\delta_{r,R}\left|\vec{r}\,\right\rangle \otimes \left|s_{1,z}, s_{2,z}\right\rangle$$

Lattice method: projection onto partial waves

consider n coupled channels:

$$|R\rangle_\alpha := |R\rangle_{s_\alpha, l_\alpha, j_\alpha} \text{ for } \alpha = 1, \ldots, n$$

compute norm matrix of radial states:

$$[N(R)]_{\alpha\alpha'} = {}_\alpha\langle R|R\rangle_{\alpha'}$$

project Hamiltonian onto normalized radial states:

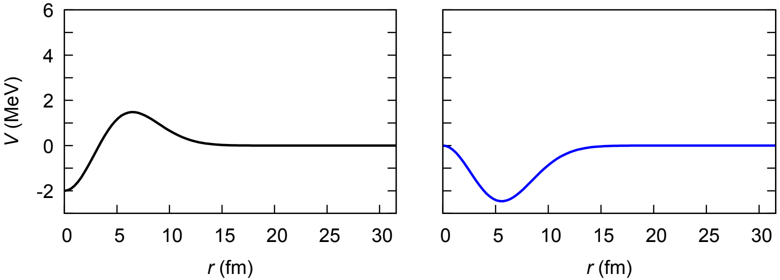
$$[H_R(R_1, R_2)]_{\alpha\beta} = \sum_{\alpha', \beta'=1}^{n} [N^{-1/2}(R_1)]_{\alpha\alpha'} \, {}_{\alpha'}\langle R_1| \, H \, |R_2\rangle_{\beta'} \, [N^{-1/2}(R_2)]_{\beta'\beta}$$

obtain wave functions from eigenvectors $|\psi\rangle$ of H_R:

$$\psi_\alpha(R) = \sum_{\alpha'=1}^{n} [N^{-1/2}(R)]_{\alpha\alpha'} \, {}_{\alpha'}\langle R|\psi\rangle$$

Lattice method: auxiliary potentials

auxiliary potentials on the lattice:



$^{5}G_2$-wave potential (diagonal) $^{5}SD_2$-wave potential (off-diag.)

Eur. Phys. J. A 34, 185 (2007); Phys. Lett. B 760, 309 (2016)

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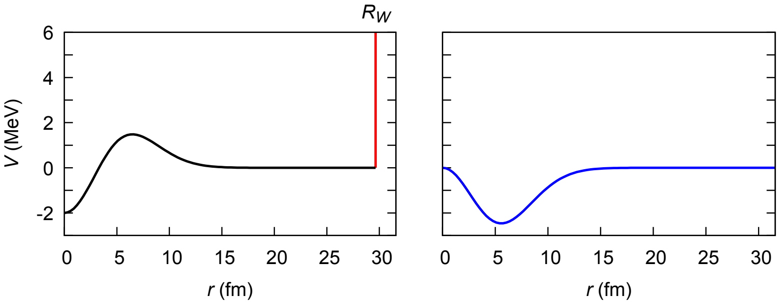

$^5G_2$-wave potential (diagonal) $^5SD_2$-wave potential (off-diag.)

spherical wall

$$V(\vec{r}\,) \to V(\vec{r}\,) + \Lambda\theta(r - R_W), \quad R_W = 15.02a, \quad \Lambda = 10^8\ \mathrm{MeV}$$

(used to avoid artifacts caused by periodic boundary condition)

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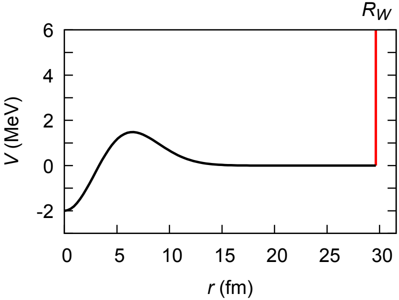

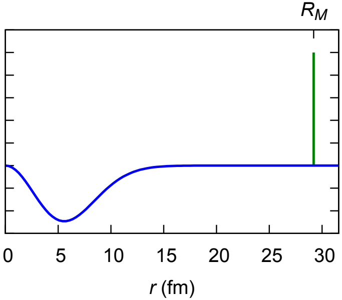

$^5G_2$-wave potential (diagonal) $^5SD_2$-wave potential (off-diag.)

spherical wall mixing potential

$$H_R \to H_R + U_0 \delta_{r,R_M} \left(\ddots \right), \quad R_M \lesssim R_W, \quad U_0 = 5\,\mathrm{MeV}$$

(used to construct full-rank S-matrix)

Eur. Phys. J. A 34, 185 (2007); Phys. Lett. B 760, 309 (2016)

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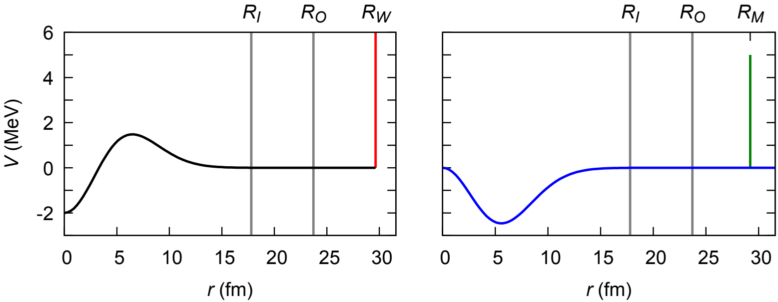

$^5G_2$-wave potential (diagonal)
spherical wall

$^5SD_2$-wave potential (off-diag.)
mixing potential

interval for fitting wave functions: $R_I = 9.02a$, $R_O = 12.02a$

Eur. Phys. J. A 34, 185 (2007); Phys. Lett. B 760, 309 (2016)

Lattice method: determination of S-matrix

extract S-matrix from wave function fit: Phys. Lett. B 760, 309 (2016)

- for one channel: $\psi(r) = Ah_l^-(pr) + Bh_l^+(pr) \Rightarrow S = B/A$

Lattice method: determination of S-matrix

extract S-matrix from wave function fit: Phys. Lett. B 760, 309 (2016)

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- for two channels: $\psi(r) = \begin{pmatrix} A_1 h_{l_1}^-(pr) + B_1 h_{l_1}^+(pr) \\ A_2 h_{l_2}^-(pr) + B_2 h_{l_2}^+(pr) \end{pmatrix}$,

$$\psi^*(r) = \begin{pmatrix} A_1^* h_{l_1}^+(pr) + B_1^* h_{l_1}^-(pr) \\ A_2^* h_{l_2}^+(pr) + B_2^* h_{l_2}^-(pr) \end{pmatrix} \Rightarrow S = (\vec{B}\;\vec{A}^*)(\vec{A}\;\vec{B}^*)^{-1}$$

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problem: $[H, T] = 0 \quad \Rightarrow \quad \psi^* = T\psi = \psi \quad \Rightarrow \quad \vec{A} = \vec{B}^*$

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problem: $[H, T] = 0 \quad \Rightarrow \quad \psi^* = T\psi = \psi \quad \Rightarrow \quad \vec{A} = \vec{B}^*$

$\rightarrow$ time reversal symmetry must be broken to obtain two linearly independent solutions:

$$(H_R + U)\psi(r) = E\psi(r) \quad \text{with} \quad U(r) = U_0 \delta_{r,R_M} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

Lattice method: determination of S-matrix

new: generalization to $n > 2$ coupled channels

$\rightarrow$ need n linearly independent solutions in each channel

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$\rightarrow$ rewrite two-channel wave function:

$$\psi(r) = \begin{pmatrix} \psi_1(r) \\ \psi_2(r) \end{pmatrix} \rightarrow \psi'(r) = \begin{pmatrix} \mathrm{Re}\,\psi_1(r) \\ \mathrm{Im}\,\psi_1(r) \\ \mathrm{Re}\,\psi_2(r) \\ \mathrm{Im}\,\psi_2(r) \end{pmatrix}$$

Lattice method: determination of S-matrix

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$$\Rightarrow H'_R = \left(\begin{array}{cc|cc} [H_R]_{11} & 0 & [H_R]_{12} & 0 \\ 0 & [H_R]_{11} & 0 & [H_R]_{12} \\ \hline [H_R]_{21} & 0 & [H_R]_{22} & 0 \\ 0 & [H_R]_{21} & 0 & [H_R]_{22} \end{array}\right),$$

$$U' = U_0 \delta_{r,R_M} \left(\begin{array}{cc|cc} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{array}\right), \; (H'_R + U')\psi'(r) = E\psi'(r)$$

Lattice method: determination of S-matrix

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Lattice method: determination of S-matrix

possible generalization to $n = 3$ coupled channels:

$$\psi'(r) = \Big(\underbrace{\psi'_1(r), \psi'_2(r), \psi'_3(r)}_{\text{channel 1}}, \underbrace{\psi'_4(r), \psi'_5(r), \psi'_6(r)}_{\text{channel 2}}, \underbrace{\psi'_7(r), \psi'_8(r), \psi'_9(r)}_{\text{channel 3}}\Big)^T$$

Lattice method: determination of S-matrix

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$$H'_R = \left(\begin{array}{ccc|c|ccc}
[H_R]_{11} & 0 & 0 & & [H_R]_{13} & 0 & 0 \\
0 & [H_R]_{11} & 0 & \cdots & 0 & [H_R]_{13} & 0 \\
0 & 0 & [H_R]_{11} & & 0 & 0 & [H_R]_{13} \\
\hline
[H_R]_{21} & 0 & 0 & & [H_R]_{23} & 0 & 0 \\
0 & [H_R]_{21} & 0 & \cdots & 0 & [H_R]_{23} & 0 \\
0 & 0 & [H_R]_{21} & & 0 & 0 & [H_R]_{23} \\
\hline
[H_R]_{31} & 0 & 0 & & [H_R]_{33} & 0 & 0 \\
0 & [H_R]_{31} & 0 & \cdots & 0 & [H_R]_{33} & 0 \\
0 & 0 & [H_R]_{31} & & 0 & 0 & [H_R]_{33}
\end{array}\right)$$

Lattice method: determination of S-matrix

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$$U' = U_0 \delta_{r,R_M} \left(\begin{array}{ccc|ccc|ccc} 0 & 0 & 0 & 0 & -1 & 1 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 \\ \hline 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ -1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & -1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ \hline 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \end{array} \right)$$

Lattice method: determination of S-matrix

construction of S-matrix:

$$\psi'_{\beta+(\alpha-1)n}(r) = A_{\alpha\beta} h^{-}_{l_\alpha}(pr) + B_{\alpha\beta} h^{+}_{l_\alpha}(pr)$$

$$\Rightarrow \quad S = \begin{pmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{n1} & \cdots & B_{nn} \end{pmatrix} \begin{pmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{pmatrix}^{-1}$$

Blatt-Biedenharn parametrization: Phys. Rev. 86, 399 (1952)

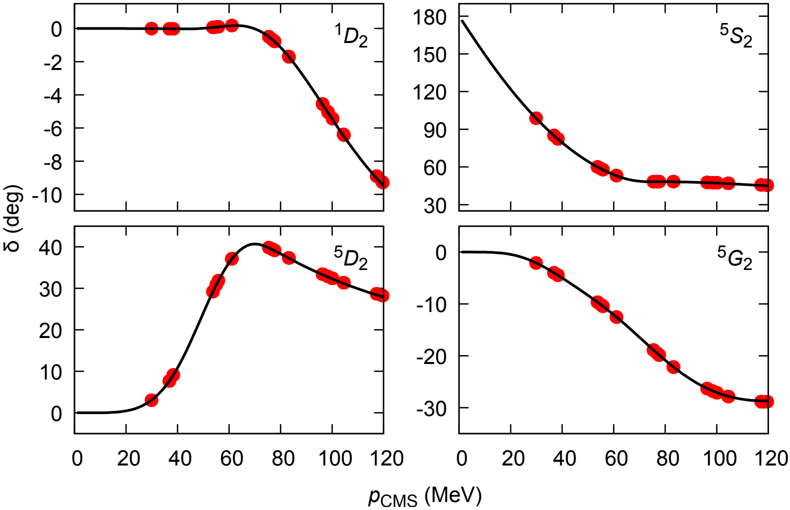
$$S = O^{-1}\,\mathrm{diag}(e^{2i\delta_1}, \ldots, e^{2i\delta_n})\, O$$

with n phase shifts $\delta_1, \ldots, \delta_n$ and $n(n-1)/2$ mixing angles

$$\epsilon_{\alpha\beta} = \tan^{-1} O_{\alpha\beta} \text{ for } \alpha, \beta = 1, \ldots, n \text{ and } \beta > \alpha$$

Computational results

phase shifts for $^1D_2/^5SDG_2$-wave:



continuum lattice

Computational results

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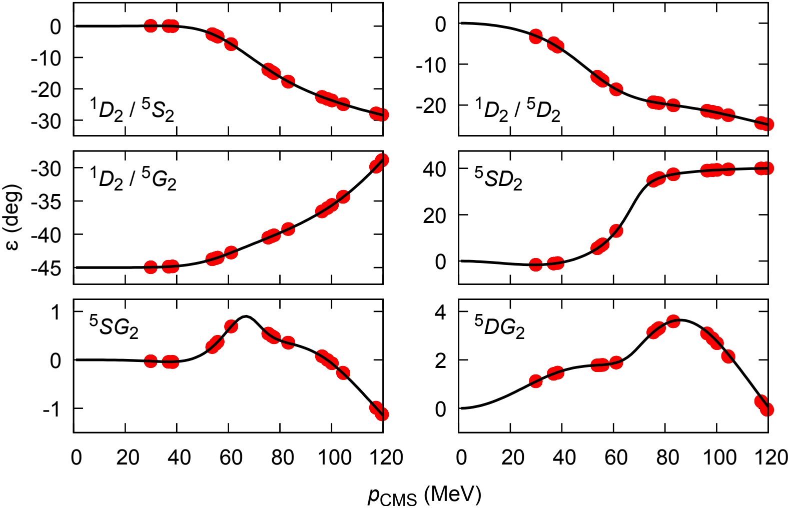

continuum lattice

Summary

- The spherical wall method has been generalized for particles with any spin and an arbitrary number of coupled scattering channels.
- For the benchmark system of two spin-1 bosons, the lattice and continuum results agree for CMS momenta well below the lattice cutoff $\Lambda_{\text{latt}} \sim \pi/a \simeq 314\ \mathrm{MeV}$.
- The presented technique can be combined with the adiabatic projection method, which allows one to consider scattering of particle clusters.
- By using chiral EFT interactions, one can apply the adiabatic projection method to nuclear reactions (e.g. *dd* scattering), where $n > 2$ coupled channels often appear.

Thank you for your attention!