Tutorial: Methods for Few Body Systems

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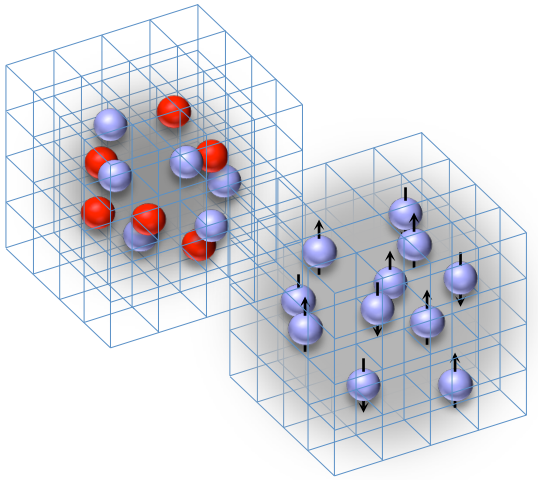
Nuclear Lattice EFT Collaboration



Progress in Diagrammatic Monte Carlo Methods
For Quantum Field Theories in
Particle, Nuclear, and Condensed Matter Physics

Mainz Institute for Theoretical Physics
Johannes Gutenberg University Mainz
September 26, 2017

General reviews:

arXiv:1609.00421
D.L., Lattice Methods and the Nuclear Few- and Many-Body Problem, IN: M. Hjorth-Jensen, M. Lombardo, U. van Kolck (eds.), *An Advanced Course in Computational Nuclear Physics*, Lecture Notes in Physics **936**, 237 (2016).

arXiv:0804.3501
D.L., Lattice simulations for few- and many-body systems, Prog. Part. Nucl. Phys. 63, 117 (2009).

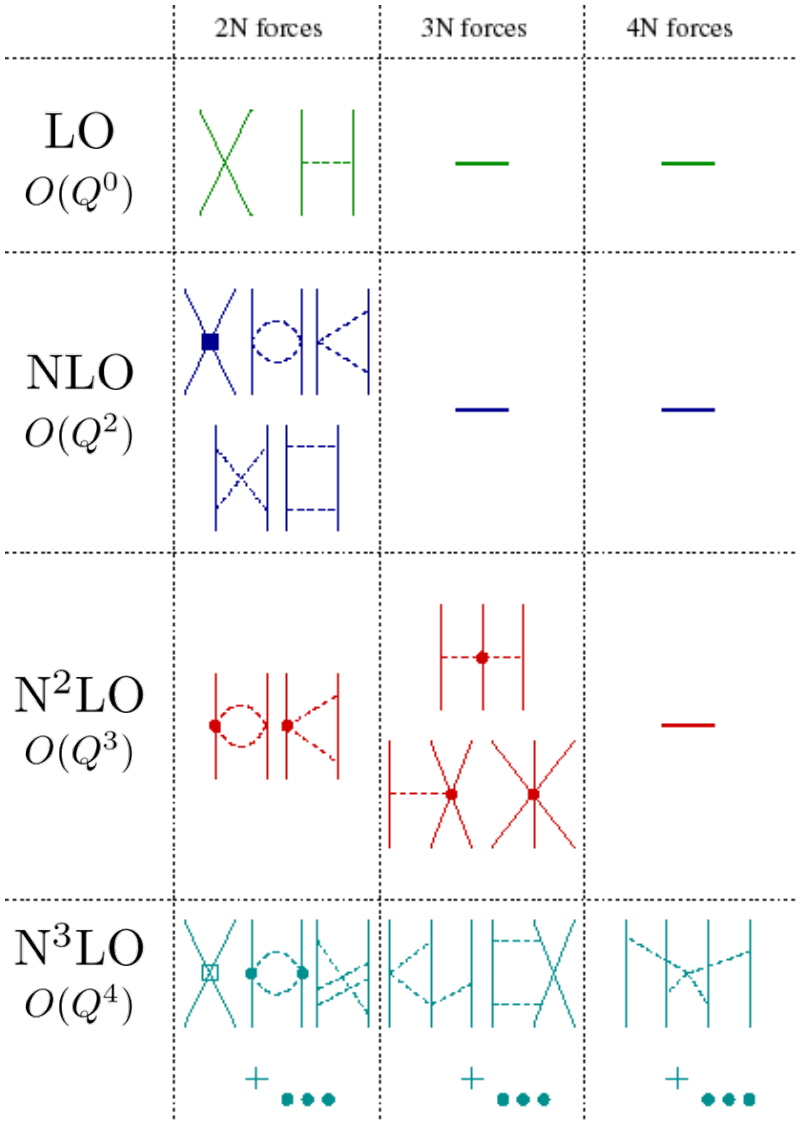
Adiabatic projection method:

arXiv:1603.02333
Elhatisari, D.L., Meißner, Rupak, Nucleon-deuteron scattering using the adiabatic projection method, Eur. Phys. J. A **52**, 174 (2016).

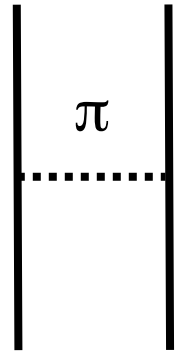
Pinhole method:

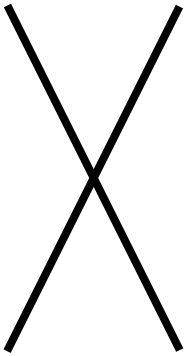
arXiv:1702.05177
Elhatisari *et al.*, Ab initio calculations of the isotopic dependence of nuclear clustering

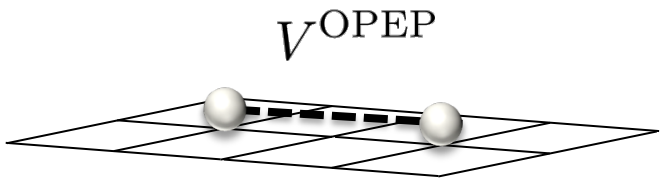
Chiral effective field theory

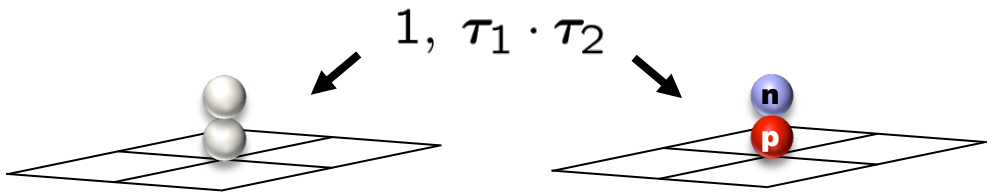


Leading order interactions









Four exactly equivalent lattice formulations at arbitrary spatial and temporal lattice spacings:

Grassmann path integral $\exp[-S(c^*, c)]$	$=$	Transfer matrix M
$\|\|$		$\|\|$
Grassmann path integral with auxiliary fields $\exp[-S(c^*, c, s)]$	$=$	Transfer matrix with auxiliary fields $M(s, n_t)$

Creutz, Found. Phys. 30 (2000) 487

We first consider the leading order chiral EFT interaction on the lattice in the Grassmann path integral formalism

$$\mathcal{Z} = \int DcDc^* \exp\left[-S\left(c^*, c\right)\right]$$

$$S(c^*, c) = S_{\text{free}}(c^*, c) + S_{\text{int}}(c^*, c)$$

$$S_{\text{free}}(c^*, c) = \sum_{\vec{n}, n_t, i} \boxed{c_i^*(\vec{n}, n_t)\left[c_i(\vec{n}, n_t + 1) - c_i(\vec{n}, n_t)\right]} \rightarrow c_i^* \frac{\partial c_i}{\partial t}$$

$$-\frac{\alpha_t}{2m} \sum_{\vec{n}, n_t, i} \sum_{l=1,2,3} \boxed{c_i^*(\vec{n}, n_t)\left[c_i(\vec{n} + \hat{l}, n_t) - 2c_i(\vec{n}, n_t) + c_i(\vec{n} - \hat{l}, n_t)\right]}$$

$$\rightarrow c_i^* \frac{\partial^2 c_i}{\partial x_l^2}$$

It is convenient to view c without indices as a column vector and c^* without indices as a row vector

$$c^* = \left[c_{\uparrow,p}^* c_{\downarrow,p}^* c_{\uparrow,n}^* c_{\downarrow,n}^*\right] \qquad c = \begin{bmatrix} c_{\uparrow,p} \\ c_{\downarrow,p} \\ c_{\uparrow,n} \\ c_{\downarrow,n} \end{bmatrix}$$

The first interaction we consider is the short-range interaction between nucleons which is independent of spin and isospin

$$S^C_{\rm int}(c^*,c) = \alpha_t \frac{C}{2} \sum_{\vec{n},n_t} \left[c^*(\vec{n},n_t)c(\vec{n},n_t)\right]^2$$

Using the auxiliary field s, we can write this interaction as

$$\exp\left[-S^C_{\rm int}(c^*,c)\right] = \int Ds \ \exp\left[-S_{ss}(s) - S_s(c^*,c,s)\right]$$

where

$$S_{ss}(s) = \frac{1}{2} \sum_{\vec{n},n_t} s^2(\vec{n},n_t)$$

$$S_s(c^*,c,s) = \sqrt{-C\alpha_t} \sum_{\vec{n},n_t} s(\vec{n},n_t)c^*(\vec{n},n_t)c(\vec{n},n_t)$$

Next we have the short-range interaction dependent on isospin

$$S_{\rm int}^{C'}(c^*,c) = \alpha_t \frac{C'}{2} \sum_{\vec{n},n_t,I} \left[c^*(\vec{n},n_t)\tau_I c(\vec{n},n_t)\right]^2$$

where we are using the Pauli matrices in isospin space

$$\tau_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_{\rm isospin} \qquad \tau_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}_{\rm isospin} \qquad \tau_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}_{\rm isospin}$$

In terms of three auxiliary fields s_I, we can write the interaction as

$$\exp\left[-S_{\rm int}^{C'}(c^*,c)\right] = \int \prod_I Ds_I \exp\left[-S_{s_I s_I}(s_I) - S_{s_I}(c^*,c,s_I)\right]$$

$$S_{s_I s_I}(s_I) = \tfrac{1}{2} \sum_{\vec{n},n_t,I} s_I^2(\vec{n},n_t)$$

$$S_{s_I}(c^*,c,s_I) = \sqrt{-C'\alpha_t} \sum_{\vec{n},n_t,I} s_I(\vec{n},n_t) c^*(\vec{n},n_t)\tau_I c(\vec{n},n_t)$$

The remaining interaction is the one pion exchange potential (OPEP). We will not include time derivatives in the free pion action, and hence the the pion is not treated as a dynamical field. Instead it resembles an auxiliary field that produces an exchange potential for the nucleons.

$$\exp\left[-S_{\rm int}^{\rm OPEP}(c^*,c)\right] = \int \prod_I D\pi_I \exp\left[-S_{\pi_I\pi_I}(\pi_I) - S_{\pi_I}(c^*,c,\pi_I)\right]$$

$$S_{\pi_I\pi_I}(\pi_I) = \tfrac{1}{2}\alpha_t m_\pi^2 \sum_{\vec{n},n_t,I} \pi_I^2(\vec{n},n_t)$$
$$-\tfrac{1}{2}\alpha_t \sum_{\vec{n},n_t,I,\hat{l}} \pi_I(\vec{n},n_t)\left[\pi_I(\vec{n}+\hat{l},n_t) - 2\pi_I(\vec{n},n_t) + \pi_I(\vec{n}-\hat{l},n_t)\right]$$

The pion coupling to the nucleon is

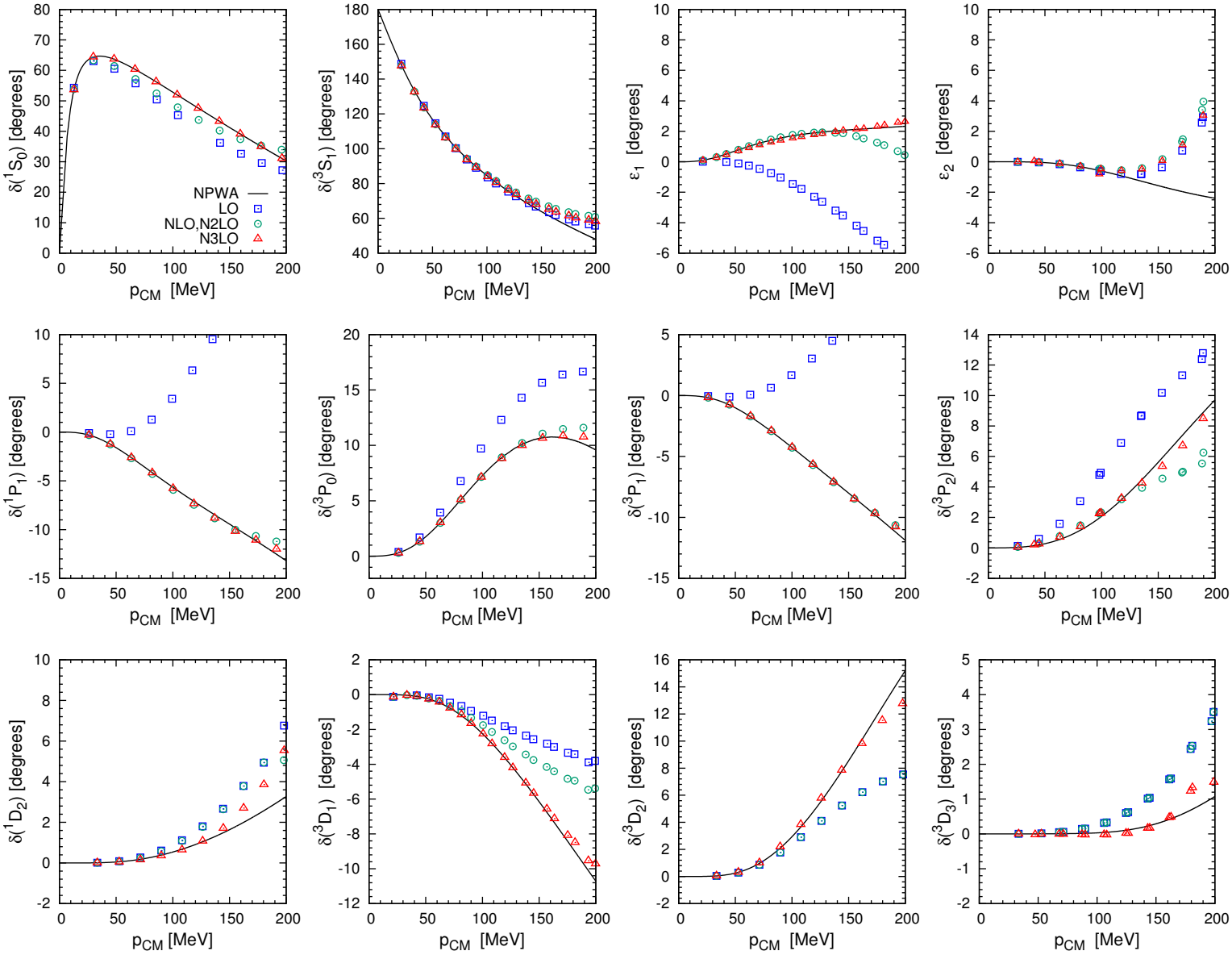
$$S_{\pi_I}(c^*, c, \pi_I) = \frac{g_A \alpha_t}{2 f_\pi} \sum_{\vec{n}, n_t, l, I} \Delta_k \pi_I(\vec{n}, n_t) c^*(\vec{n}, n_t) \sigma_k \tau_I c(\vec{n}, n_t)$$

where g_A is the axial charge, f_π is the pion decay constant, and we have used the Pauli spin matrices

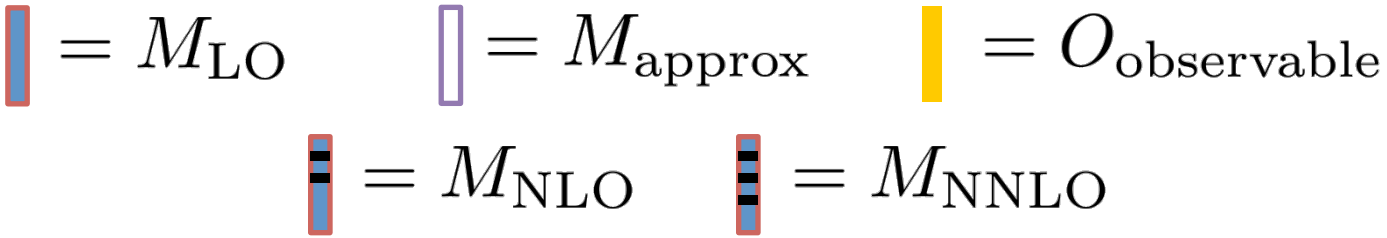
$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_{\text{spin}} \qquad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}_{\text{spin}} \qquad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}_{\text{spin}}$$

And the gradient of the pion field is

$$\Delta_l \pi_I(\vec{n}, n_t) = \frac{1}{2} \left[\pi_I(\vec{n} + \hat{l}, n_t) - \pi_I(\vec{n} - \hat{l}, n_t) \right]$$


δ(1S0) [degrees]
δ(3S1) [degrees]
ε1 [degrees]
ε2 [degrees]
δ(1P1) [degrees]
δ(3P0) [degrees]
δ(3P1) [degrees]
δ(3P2) [degrees]
δ(1D2) [degrees]
δ(3D1) [degrees]
δ(3D2) [degrees]
δ(3D3) [degrees]
pCM [MeV]
NPWA
LO
NLO,N2LO
N3LO

Schematic of lattice Monte Carlo calculations



Hybrid Monte Carlo sampling

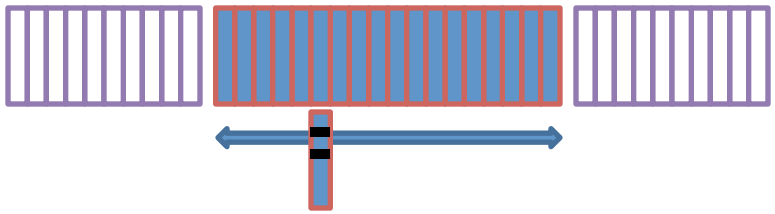
$$Z_{n_t,\mathrm{LO}} = \langle \psi_{\mathrm{init}} | \; \cdots \; | \psi_{\mathrm{init}} \rangle$$

$$Z^{\langle O \rangle}_{n_t,\mathrm{LO}} = \langle \psi_{\mathrm{init}} | \; \cdots \; | \psi_{\mathrm{init}} \rangle$$

$$e^{-E_{0,\mathrm{LO}} a_t} = \lim_{n_t \to \infty} Z_{n_t+1,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

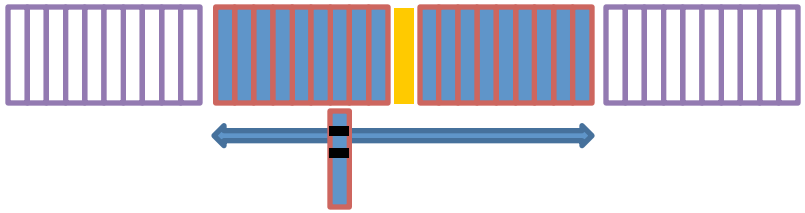
$$\langle O \rangle_{0,\mathrm{LO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

$$Z_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$$



$$| \psi_{\mathrm{init}} \rangle$$

$$Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$$



$$| \psi_{\mathrm{init}} \rangle$$

$$\langle O \rangle_{0,\mathrm{NLO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} / Z_{n_t,\mathrm{NLO}}$$

Science objectives

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

$^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^4\mathrm{He} + {}^4\mathrm{He}$

$^4\mathrm{He} + {}^4\mathrm{He} + {}^4\mathrm{He} \rightarrow {}^{12}\mathrm{C} + \gamma$

$^{12}\mathrm{C} + {}^4\mathrm{He} \rightarrow {}^{16}\mathrm{O} + \gamma$

$^{16}\mathrm{O} + {}^4\mathrm{He} \rightarrow {}^{20}\mathrm{Ne} + \gamma$

$^{20}\mathrm{Ne} + {}^4\mathrm{He} \rightarrow {}^{24}\mathrm{Mg} + \gamma$

$^{24}\mathrm{Mg} + {}^4\mathrm{He} \rightarrow {}^{28}\mathrm{Si} + \gamma$

$^{12}\mathrm{C} + {}^{12}\mathrm{C} \rightarrow {}^{20}\mathrm{Ne} + {}^4\mathrm{He}$

$^{16}\mathrm{O} + {}^{16}\mathrm{O} \rightarrow {}^{28}\mathrm{Si} + {}^4\mathrm{He}$

Challenge

How to reduce computational scaling with number of nucleons in participating nuclei?

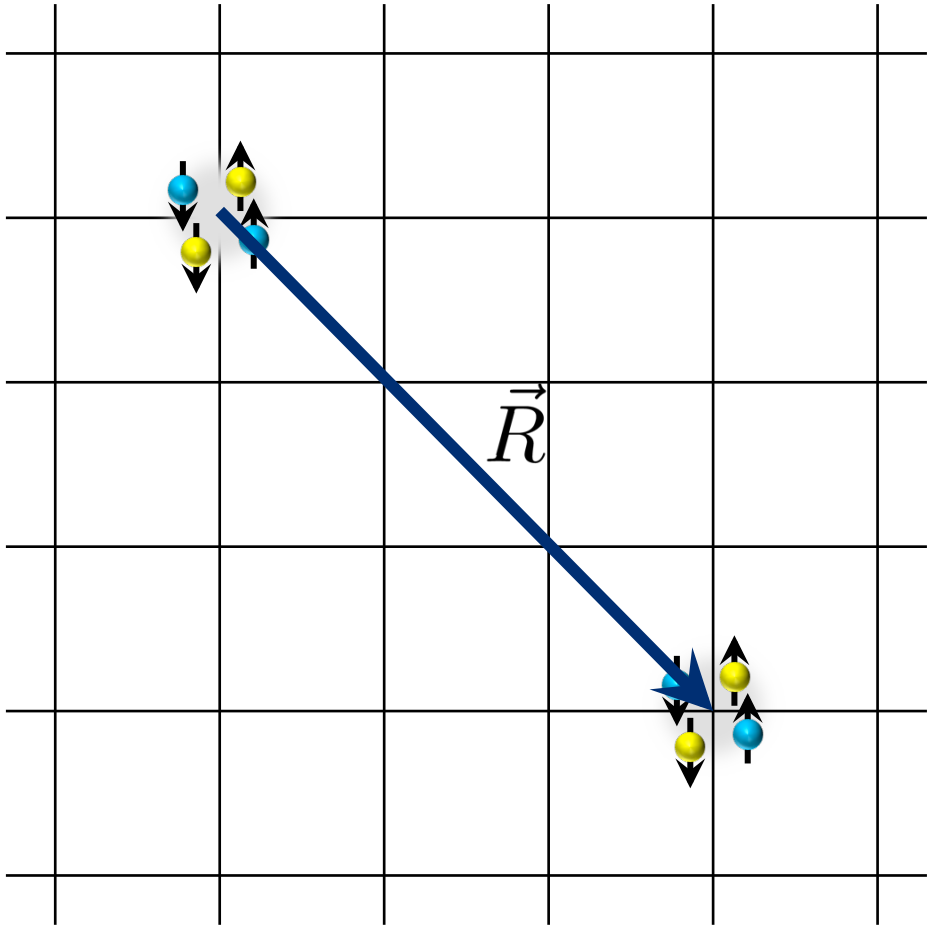
Adiabatic projection method

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 *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 $\vec{R}$

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



For notational simplicity we use the language of continuous time evolution. The actual calculations use normal-ordered transfer matrices.

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,

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

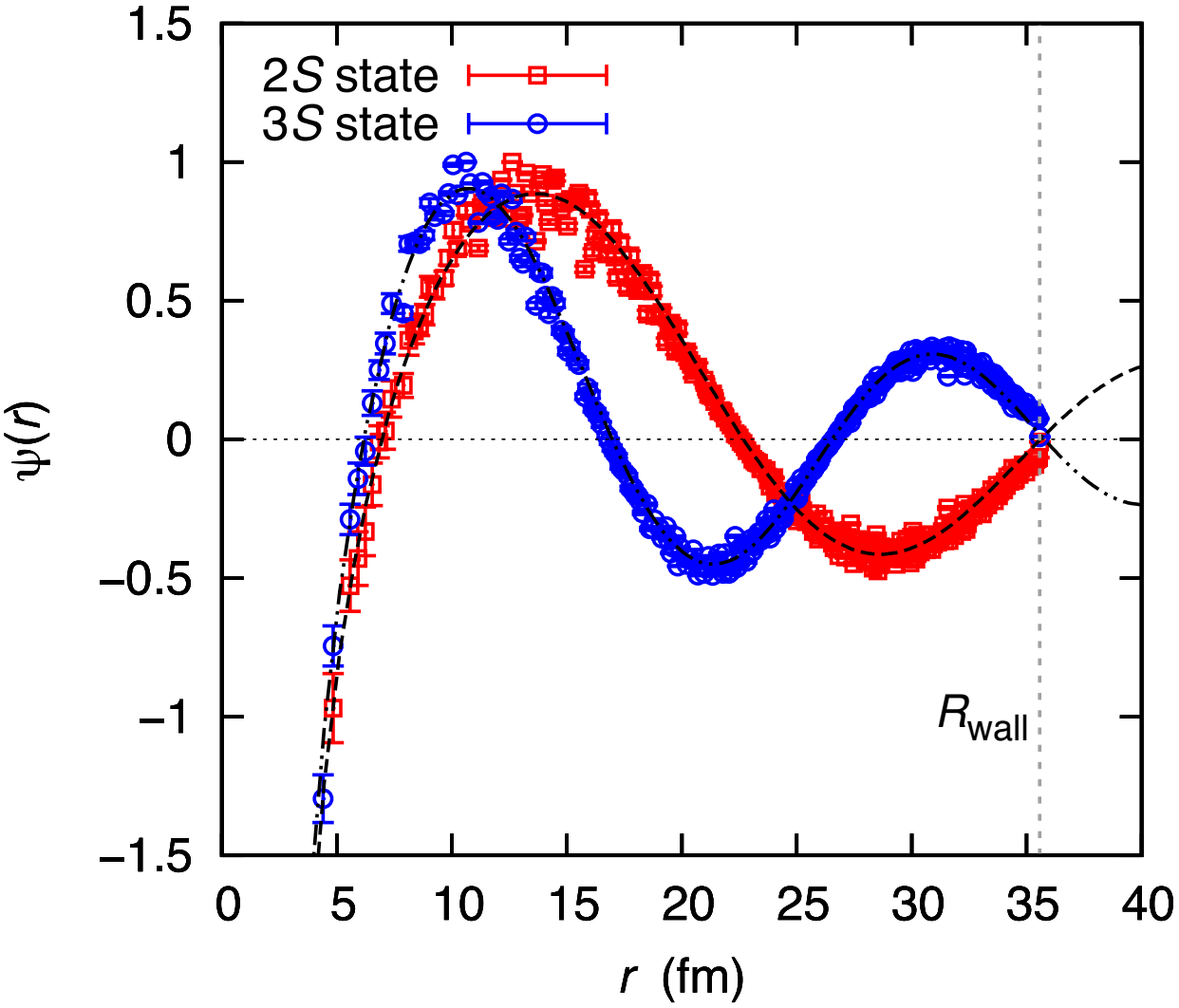
Since the dressed cluster states are in general not orthogonal, we construct a norm matrix given by the inner product

$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle \vec{R}|\vec{R}'\rangle_\tau$$

The adiabatic Hamiltonian is defined by the matrix product

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

We now treat the adiabatic Hamiltonian as an effective two-particle Hamiltonian and determine the phase shifts from the standing wave with spherical boundaries.


2S state
3S state
1.5
1
0.5
0
−0.5
−1
−1.5
ψ(r)
0
5
10
15
20
25
30
35
40
r (fm)
R_wall

Challenge

There was no algorithm available for *ab initio* auxiliary field Monte Carlo simulations to determine the density distribution of particles relative to the center of mass. The problem is that the particle wave functions in the auxiliary field simulation are a superposition of many values for the center of mass.

Pinhole algorithm

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

$$\rho_{i,j}(\mathbf{n}) = a^\dagger_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

We construct the normal-ordered A-body density operator

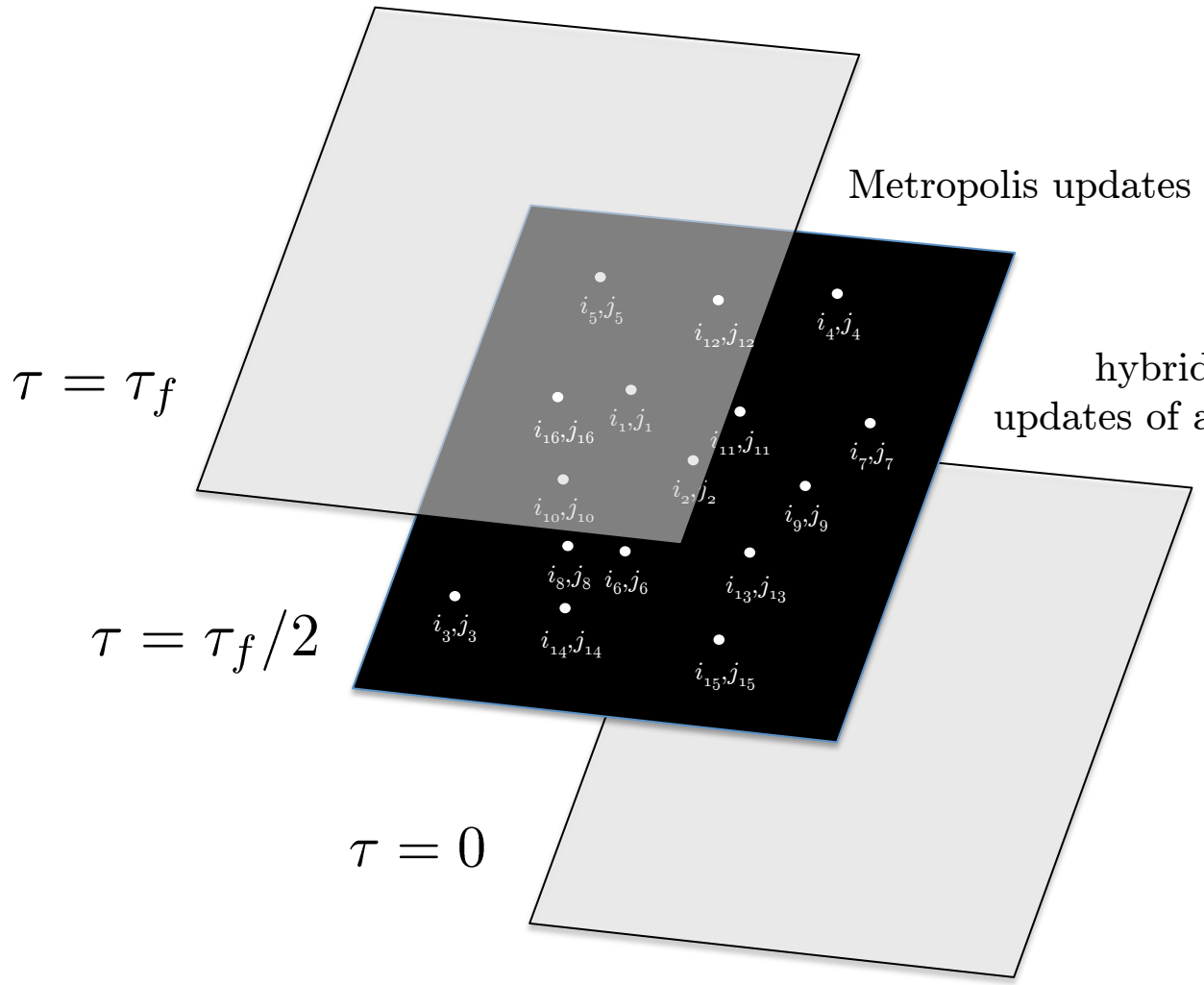
$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) = :\rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$

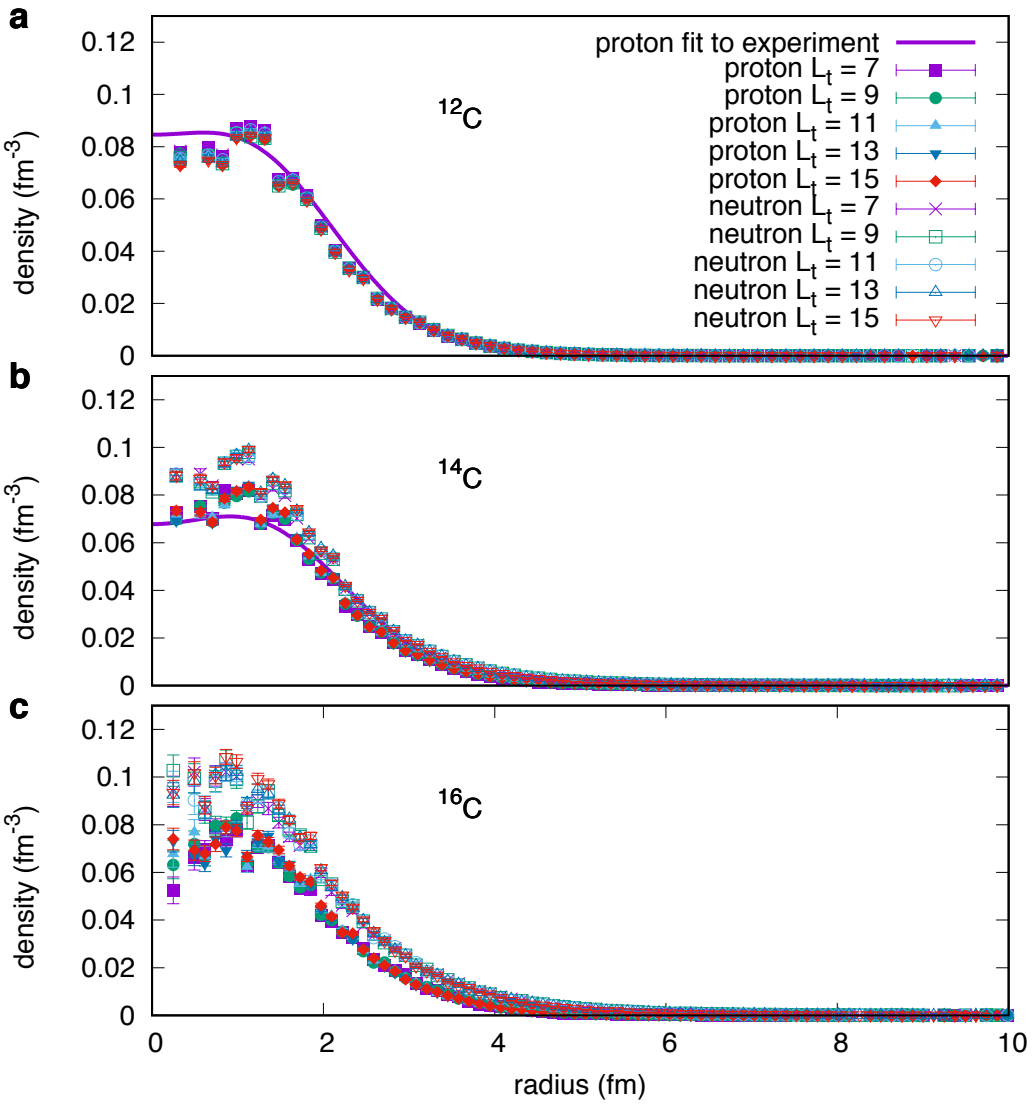
In the A-particle subspace, we have the identity

$$\sum_{i_1,j_1,\cdots i_A,j_A} \sum_{\mathbf{n}_1,\cdots \mathbf{n}_A} \rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) \;= A!$$

In the simulations we do Monte Carlo sampling of the amplitude

$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A, L_t) = \langle \Psi_I | M^{L_t/2} \rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) M^{L_t/2} | \Psi_I \rangle$$


Metropolis updates of pinholes
hybrid Monte Carlo
updates of auxiliary/pion fields
$\tau = \tau_f$
$\tau = \tau_f/2$
$\tau = 0$
i_5,j_5
i_{12},j_{12}
i_4,j_4
i_{16},j_{16}
i_1,j_1
i_{11},j_{11}
i_7,j_7
i_2,j_2
i_{10},j_{10}
i_9,j_9
i_8,j_8
i_6,j_6
i_{13},j_{13}
i_3,j_3
i_{14},j_{14}
i_{15},j_{15}



Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, arXiv:1702.05177

End

Extra Slides

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^{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

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

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

Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, arXiv:1505.02967

Extra Slides

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

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

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.