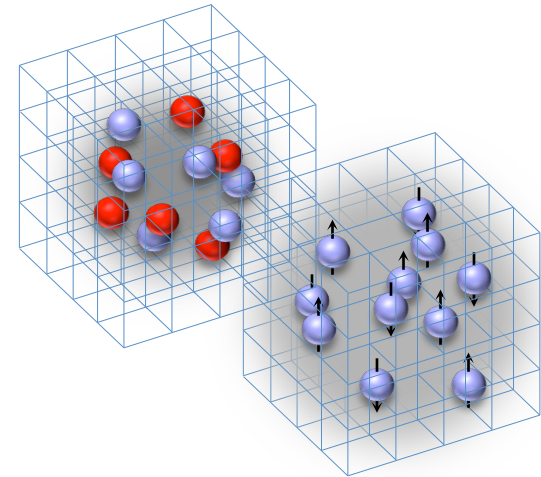


# Nuclear Lattice Simulations

## Lecture 3: Nuclear Structure and Clustering

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## Outline

Projection Monte Carlo with auxiliary fields

Chiral effective field theory at leading order

Spectral convexity and clustering

A tale of two different interactions

Effective forces between bound states

Pinhole algorithm

Model independent probes of clustering

## Projection Monte Carlo with auxiliary fields

Let us consider a system with  $A$  particles. The idea of projection Monte Carlo is to choose a given initial and final state. Very often they are chosen to be the same state. The initial and final state will sandwich a product of a string of transfer matrices. Pictorially the amplitude looks like this:

$$Z(L_t) = \langle \psi_{\text{init}} | \begin{array}{c} \text{MMM} \qquad \qquad \qquad \dots \qquad \qquad \qquad \text{MM} \\ \hline \text{[A row of vertical bars representing a string of transfer matrices]} \end{array} | \psi_{\text{init}} \rangle$$

Using auxiliary fields, we have

$$Z(L_t) = \prod_{\vec{n}, n_t} \left[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(\vec{n}, n_t) e^{-\frac{1}{2}s^2(\vec{n}, n_t)} \right] Z(s, L_t)$$

where the auxiliary field amplitude is

$$Z(s, L_t) = \langle \psi_{\text{init}} | \begin{array}{c} M(s, L_t - 1)M(s, L_t - 2) \quad \cdot \cdot \cdot \quad M(s, 1)M(s, 0) \\ \hline \text{[Diagram of a 1D lattice with } L_t \text{ sites]} \end{array} | \psi_{\text{init}} \rangle$$

For sufficiently large  $L_t$  the amplitude  $Z(L_t)$  will be dominated by the ground state of our quantum system in the sector which is not orthogonal to our initial state. We will see the largest eigenvalue of the transfer matrix  $M$ , which we use to extract the corresponding ground state energy  $E_0$

$$\lim_{L_t \rightarrow +\infty} Z(L_t)/Z(L_t - 1) = \lambda_{\text{max}} = e^{-E_0 \alpha_t}$$

To make the discussion concrete, we continue on with our example of two-component fermions with zero-range interactions.

We can create a general single-particle state on the lattice with a creation operator multiplying a coefficient function  $f$  that depends on the spatial lattice sites and spin component  $i$ .

$$|f\rangle = \sum_{\vec{n},i} a_i^\dagger(\vec{n}) f(\vec{n},i) |0\rangle$$

For our projection Monte Carlo calculation we take our  $A$ -body initial state as an operator product

$$|\psi_{\text{init}}\rangle = |f_1, \dots, f_A\rangle = \left[ \sum_{\vec{n},i} a_i^\dagger(\vec{n}) f_1(\vec{n},i) \right] \cdots \left[ \sum_{\vec{n},i} a_i^\dagger(\vec{n}) f_A(\vec{n},i) \right] |0\rangle$$

For the purposes of coding the projection Monte Carlo calculation, it is convenient to view the identical nucleons as carrying a fictitious label  $[j] = [1], \dots, [A]$  that makes all of the particles distinguishable.

$$a_i(\vec{n}), a_i^\dagger(\vec{n}) \rightarrow a_{i,[j]}(\vec{n}), a_{i,[j]}^\dagger(\vec{n})$$

We will sum over all possible assignments of these operator labels and the anticommuting algebra of the operators will give the proper antisymmetry as required.

With these hidden labels our  $A$ -body initial state is

$$\begin{aligned}
|\psi_{\text{init}}\rangle &= |f_1, \dots, f_A\rangle \\
&\rightarrow \frac{1}{\sqrt{A!}} \sum_P \left[ \sum_{\vec{n}, i} a_{i, [P(1)]}^\dagger(\vec{n}) f_1(\vec{n}, i) \right] \cdots \left[ \sum_{\vec{n}, i} a_{i, [P(A)]}^\dagger(\vec{n}) f_A(\vec{n}, i) \right] |0\rangle \\
&= \frac{1}{\sqrt{A!}} \sum_{P'} \text{sgn}(P') \left[ \sum_{\vec{n}, i} a_{i, [1]}^\dagger(\vec{n}) f_{P'(1)}(\vec{n}, i) \right] \cdots \left[ \sum_{\vec{n}, i} a_{i, [A]}^\dagger(\vec{n}) f_{P'(A)}(\vec{n}, i) \right] |0\rangle
\end{aligned}$$

where the summations are over all permutations, and  $\text{sgn}$  is the sign of the permutation. In the last line we get the usual Slater determinant wave function.

With these hidden indices our normal-ordered auxiliary-field transfer matrix at time step  $n_t$  can be written as

$$\begin{aligned}
M(s, n_t) &\rightarrow \left[ 1 - H_{\text{free}, [1]} \alpha_t + \sum_{\vec{n}} \sqrt{-C} \alpha_t s(\vec{n}, n_t) \rho_{[1]}(\vec{n}) \right] \cdots \\
&\quad \cdots \left[ 1 - H_{\text{free}, [A]} \alpha_t + \sum_{\vec{n}} \sqrt{-C} \alpha_t s(\vec{n}, n_t) \rho_{[A]}(\vec{n}) \right]
\end{aligned}$$

All other terms coming from higher powers coming from the exponential will vanish due to the normal ordering. This is because we have only one particle carrying each fictitious label  $[j] = [1], \dots, [A]$ .

In the projection Monte Carlo calculation we compute the amplitude

$$Z(s, L_t) = \langle f_1, \dots, f_A | M(s, L_t - 1) \cdots M(s, 0) | f_1, \dots, f_A \rangle$$

for each configuration of the auxiliary field  $s$ . We note that this  $A$ -body amplitude is just the determinant of the matrix of single nucleon amplitudes

$$Z(s, L_t) = \det \mathbf{Z}(s, L_t)$$

$$\mathbf{Z}_{i,j}(s, L_t) = \langle f_i | M(s, L_t - 1) \cdots M(s, 0) | f_j \rangle$$

In summary, we want to compute the following ratio for large  $L_t$ :

$$\lim_{L_t \rightarrow +\infty} Z(L_t)/Z(L_t - 1) = \lambda_{\max} = e^{-E_0 \alpha_t}$$

Since we usually write the observable for our Markov chain in the numerator rather than the denominator, we will work with reciprocal of this ratio and calculate using auxiliary fields

$$\frac{Z(L_t - 1)}{Z(L_t)} = \frac{\prod_{\vec{n}, n_t} \left[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(\vec{n}, n_t) e^{-\frac{1}{2} s^2(\vec{n}, n_t)} \right] Z(s, L_t - 1)}{\prod_{\vec{n}, n_t} \left[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(\vec{n}, n_t) e^{-\frac{1}{2} s^2(\vec{n}, n_t)} \right] Z(s, L_t)}$$

where the auxiliary field amplitudes are



$$Z(s, L_t - 1) = \det \mathbf{Z}(s, L_t - 1)$$

$$Z(s, L_t) = \det \mathbf{Z}(s, L_t)$$

$$\mathbf{Z}_{i,j}(s, L_t - 1) = \langle f_i | M(s, L_t - 2) \cdots M(s, 0) | f_j \rangle$$

$$\mathbf{Z}_{i,j}(s, L_t) = \langle f_i | M(s, L_t - 1) \cdots M(s, 0) | f_j \rangle$$

In order to compute this using a Markov chain process, the updating of the auxiliary field is done most efficiently if you store the set of vectors for each single-particle initial state at each time step

$$|v_j(s, n_t)\rangle = M(s, n_t - 1) \cdots M(s, 0) |f_j\rangle$$

as well as the dual vectors at each time step propagating in the reverse temporal direction

$$\langle v_j(s, n_t) | = \langle f_i | M(s, L_t - 1) \cdots M(s, n_t)$$

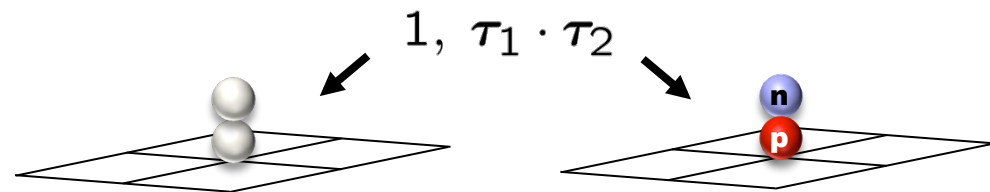
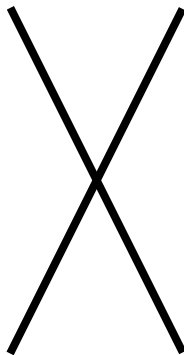
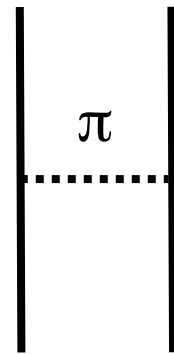
So now if we need to compute the update to an auxiliary field value at time step  $n_t$ , we have an easy way to compute the change in the amplitude

$$\mathbf{Z}_{i,j}(L_t) = \langle v_i(s, n_t + 1) | M(s, n_t) | v_j(s, n_t) \rangle$$



change here  
and re-evaluate

## Lattice chiral EFT at leading order



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

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

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

$$\begin{aligned} S_{\text{free}}(c^*, c) &= \sum_{\vec{n}, n_t, i} \boxed{c_i^*(\vec{n}, n_t) [c_i(\vec{n}, n_t + 1) - c_i(\vec{n}, n_t)]} \rightarrow c_i^* \frac{\partial c_i}{\partial t} \\ &- \frac{\alpha_t}{2m} \sum_{\vec{n}, n_t, i} \sum_{l=1,2,3} \boxed{c_i^*(\vec{n}, n_t) [c_i(\vec{n} + \hat{l}, n_t) - 2c_i(\vec{n}, n_t) + c_i(\vec{n} - \hat{l}, n_t)]} \\ &\rightarrow c_i^* \frac{\partial^2 c_i}{\partial x_l^2} \end{aligned}$$

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

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

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

$$S_{\text{int}}^C(c^*, c) = \alpha_t \frac{C}{2} \sum_{\vec{n}, n_t} [c^*(\vec{n}, n_t) c(\vec{n}, n_t)]^2$$

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

$$\exp [-S_{\text{int}}^C(c^*, c)] = \int Ds \exp [-S_{ss}(s) - S_s(c^*, c, s)]$$

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

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

where we are using the Pauli matrices in isospin space

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

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

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

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

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

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

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

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

The pion coupling to the nucleon is

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

where  $g_A$  is the axial charge,  $f_\pi$  is the pion decay constant, and we have used the Pauli spin matrices

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

And the gradient of the pion field is

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



We can reexpress everything in terms of normal-ordered transfer matrix operators

$$\mathcal{Z} = \int Ds \prod_I (Ds_I D\pi_I) \exp [-S_{ss}(s) - S_{s_I s_I}(s_I) - S_{\pi_I \pi_I}(\pi_I)] \text{Tr} \{ M^{(L_t-1)} \dots M^{(0)} \}$$

where

$$M^{(n_t)} =: \exp [-H^{(n_t)}(a^\dagger, a, s, s_I, \pi_I) \alpha_t]$$

$$H^{(n_t)}(a^\dagger, a, s, s_I, \pi_I) \alpha_t = H_{\text{free}} \alpha_t + S_s^{(n_t)}(a^\dagger, a, s) + S_{s_I}^{(n_t)}(a^\dagger, a, s_I) + S_{\pi_I}^{(n_t)}(a^\dagger, a, \pi_I)$$

with

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

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

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

For the auxiliary-field projection Monte Carlo calculation we compute

$$\begin{aligned} Z(L_t) &= \int Ds \prod_I (Ds_I D\pi_I) \\ &= \exp [-S_{ss}(s) - S_{s_I s_I}(s_I) - S_{\pi_I \pi_I}(\pi_I)] Z(s, s_I, \pi_I, L_t) \end{aligned}$$

where

$$Z(s, s_I, \pi_I, L_t) = \det \mathbf{Z}(s, s_I, \pi_I, L_t)$$

and the matrix of single nucleon amplitudes is

$$\mathbf{Z}_{i,j}(s, s_I, \pi_I, L_t) = \langle f_i | M^{(L_t-1)} \dots M^{(0)} | f_j \rangle$$

We store the set of vectors for each single-particle initial state at each time step

$$|v_j^{(n_t)}\rangle = M^{(n_t-1)} \dots M^{(0)} |f_j\rangle$$

as well as the dual vectors at each time step propagating in the reverse temporal direction

$$\langle v_i^{(n_t)}| = \langle f_i| M^{(L_t-1)} \dots M^{(n_t)}$$

These are useful in computing the update to an auxiliary field value at time step  $n_t$ , using the following relations:

$$Z(s, s_I, \pi_I, L_t) = \det \mathbf{Z}(s, s_I, \pi_I, L_t)$$

$$\mathbf{Z}_{i,j}(s, s_I, \pi_I, L_t) = \langle v_i^{(n_t+1)}| M^{(n_t)}(s, s_I, \pi_I) |v_j^{(n_t)}\rangle$$

It is convenient to redefine the normalization of  $\pi_I$

$$\pi'_I(\vec{n}, n_t) = \pi_I(\vec{n}, n_t) \sqrt{\alpha_t(m_\pi^2 + 6)}$$

So that

$$\begin{aligned} S_{\pi_I \pi_I}(\pi_I) &= \frac{1}{2} \alpha_t m_\pi^2 \sum_{\vec{n}, n_t, I} \pi_I^2(\vec{n}, n_t) \\ &\quad - \frac{1}{2} \alpha_t \sum_{\vec{n}, n_t, I, \hat{l}} \pi_I(\vec{n}, n_t) \left[ \pi_I(\vec{n} + \hat{l}, n_t) - 2\pi_I(\vec{n}, n_t) + \pi_I(\vec{n} - \hat{l}, n_t) \right] \\ &= \frac{1}{2} \sum_{\vec{n}, n_t, I} \pi_I'^2(\vec{n}, n_t) - \frac{\alpha_t}{2q_\pi} \sum_{\vec{n}, n_t, I, \hat{l}} \pi'_I(\vec{n}, n_t) \left[ \pi'_I(\vec{n} + \hat{l}, n_t) + \pi'_I(\vec{n} - \hat{l}, n_t) \right] \end{aligned}$$

and

$$S_{\pi_I}^{(n_t)}(a^\dagger, a, \pi_I) = \frac{g_A \alpha_t}{2f_\pi \sqrt{q_\pi}} \sum_{\vec{n}, k, I} \Delta_k \pi'_I(\vec{n}, n_t) a^\dagger(\vec{n}) \sigma_k \tau_I a(\vec{n})$$

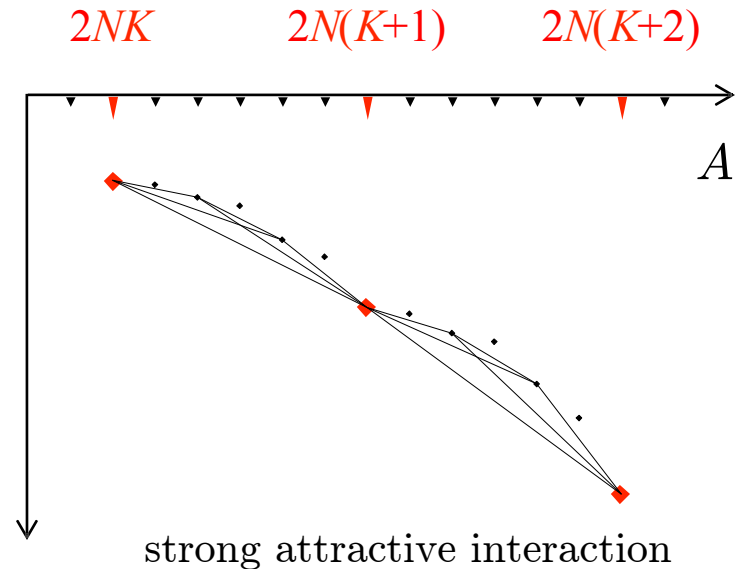
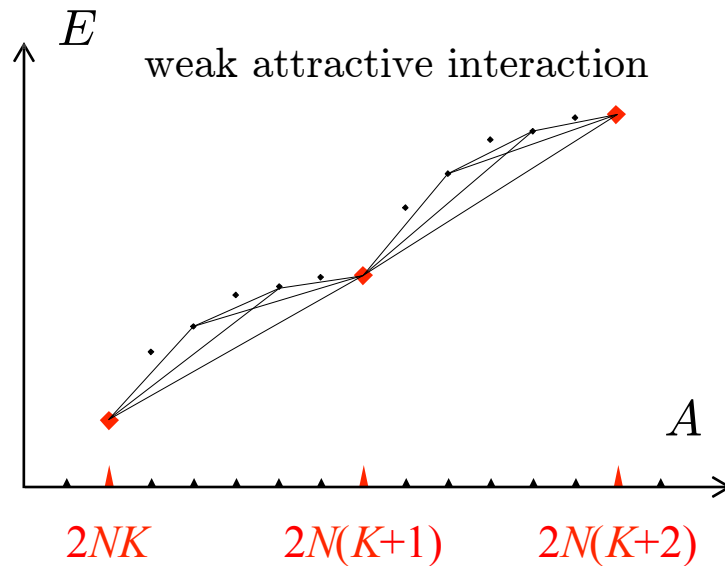
with

$$q_\pi = \alpha_t(m_\pi^2 + 6)$$

Theorem: Any fermionic theory with  $SU(2N)$  symmetry and two-body potential energy that has a negative semi-definite Fourier transform obeys  $SU(2N)$  convexity bounds.

Corollary: The system can be simulated without sign oscillations

Chen, D.L. Schäfer, PRL 93 (2004) 242302;  
D.L., PRL 98 (2007) 182501



There are  $2N$  species of fermions. Let the interaction have the form

$$\frac{1}{2} \sum_{\vec{n}, \vec{m}} \rho(\vec{n}) V(\vec{n} - \vec{m}) \rho(\vec{m})$$

Where  $\rho$  is total density of particles summed over all  $2N$  species. The transfer matrix is

$$M =: \exp \left\{ -H_{\text{free}} \alpha_t - \frac{\alpha_t}{2} \sum_{\vec{n}, \vec{m}} \rho(\vec{n}) V(\vec{n} - \vec{m}) \rho(\vec{m}) \right\} :$$

We will couple an auxiliary field  $s$  to the total density

$$M(s, n_t) =: \exp \left\{ -H_{\text{free}} \alpha_t + \alpha_t \sum_{\vec{n}} s(\vec{n}, n_t) \rho(\vec{n}) \right\} :$$

in our auxiliary field transfer matrix. More details on the next slide.

The amplitude we want to calculate is

$$Z(L_t) = \langle f_1, \dots, f_A | M^{L_t} | f_1, \dots, f_A \rangle$$

$$M =: \exp \left\{ -H_{\text{free}} \alpha_t - \frac{\alpha_t}{2} \sum_{\vec{n}, \vec{m}} \rho(\vec{n}) V(\vec{n} - \vec{m}) \rho(\vec{m}) \right\} :$$

Using the auxiliary field formalism we can also write as

$$Z(L_t) = \int Ds \, e^{-S(s)} \det \mathbf{Z}(s, L_t)$$

$$S(s) = \frac{\alpha_t}{2} \sum_{n_t} \sum_{\vec{n}, \vec{n}'} s(\vec{n}, n_t) V^{-1}(\vec{n} - \vec{n}') s(\vec{n}', n_t)$$

$$\mathbf{Z}_{i,j}(s, L_t) = \langle f_i | M(s, L_t - 1) \cdots M(s, 0) | f_j \rangle$$

$$M(s, n_t) =: \exp \left\{ -H_{\text{free}} \alpha_t + \alpha_t \sum_{\vec{n}} s(\vec{n}, n_t) \rho(\vec{n}) \right\} :$$

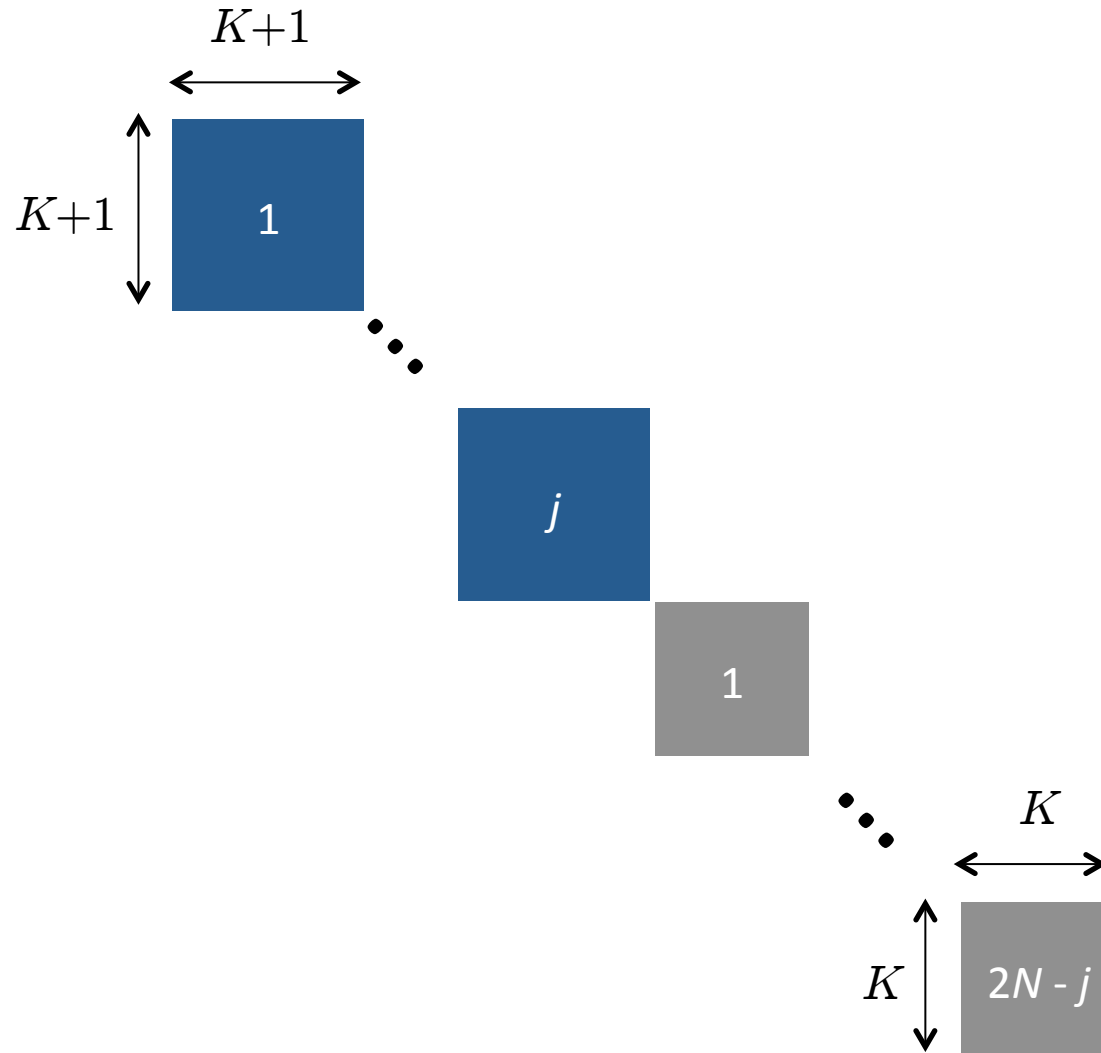
where  $V^{-1}$  is the inverse of the potential. The normalization of  $Ds$  is chosen to make this identity hold.

We choose an initial state where there are  $K + 1$  particles for the first  $j$  species and  $K$  particles for the remaining  $2N - j$  species.

$$\begin{array}{ll}
 \text{Species 1:} & 1, 2, 3 \cdots K, K + 1 \\
 \text{Species 2:} & 1, 2, 3 \cdots K, K + 1 \\
 & \vdots \\
 \text{Species } j: & 1, 2, 3 \cdots K, K + 1 \\
 \text{Species } j + 1: & 1, 2, 3 \cdots K \\
 & \vdots \\
 \text{Species } 2N - 1: & 1, 2, 3 \cdots K \\
 \text{Species } 2N: & 1, 2, 3 \cdots K
 \end{array}$$



Then the matrix  $\mathbf{Z}_{i,j}(s, L_t) = \langle f_i | M(s, L_t - 1) \cdots M(s, 0) | f_j \rangle$  has the following block diagonal structure:



The path integral over auxiliary fields is then

$$Z_{j,K+1;2N-j,K} = \int Ds e^{-S(s)} \left[ \det \mathbf{Z}_{(K+1) \times (K+1)}(s) \right]^j \left[ \det \mathbf{Z}_{K \times K}(s) \right]^{2N-j}$$

Let  $n_1$  and  $n_2$  be integers such that  $0 \leq 2n_1 \leq j \leq 2n_2 \leq 2N$ . Let us define a new positive-definite integral measure

$$\tilde{D}s = Ds e^{-S(s)} \left[ \det \mathbf{Z}_{(K+1) \times (K+1)}(s) \right]^{2n_1} \left[ \det \mathbf{Z}_{K \times K}(s) \right]^{2N-2n_2}$$

Then the amplitude can be rewritten as

$$Z_{j,K+1;2N-j,K} = \int \tilde{D}s \left[ \det \mathbf{Z}_{(K+1) \times (K+1)}(s) \right]^{j-2n_1} \left[ \det \mathbf{Z}_{K \times K}(s) \right]^{2n_2-j}$$

The Hölder inequality states that for any positive  $p, q$  satisfying

$$1/p + 1/q = 1$$

we must have

$$\int dx \, |f(x)g(x)| \leq \left[ \int dx \, |f(x)|^p \right]^{1/p} \times \left[ \int dx \, |g(x)|^q \right]^{1/q}$$

We now apply the Hölder inequality with

$$p = \frac{2n_2 - 2n_1}{j - 2n_1}, \quad q = \frac{2n_2 - 2n_1}{2n_2 - j}$$

$$\begin{aligned}
& |Z_{j,K+1;2N-j,K}| \\
&= \left| \int \tilde{D}s \left[ \det \mathbf{Z}_{(K+1) \times (K+1)}(s) \right]^{j-2n_1} \left[ \det \mathbf{Z}_{K \times K}(s) \right]^{2n_2-j} \right| \\
&\leq \left\{ \int \tilde{D}s \left| \det \mathbf{Z}_{(K+1) \times (K+1)}(s) \right|^{2n_2-2n_1} \right\}^{\frac{j-2n_1}{2n_2-2n_1}} \\
&\quad \cdot \left\{ \int \tilde{D}s \left| \det \mathbf{Z}_{K \times K}(s) \right|^{2n_2-2n_1} \right\}^{\frac{2n_2-j}{2n_2-2n_1}} \\
&\leq \left\{ \int Ds e^{-S(s)} \left| \det \mathbf{Z}_{(K+1) \times (K+1)}(s) \right|^{2n_2} \left| \det \mathbf{Z}_{K \times K}(s) \right|^{2N-2n_2} \right\}^{\frac{j-2n_1}{2n_2-2n_1}} \\
&\quad \cdot \left\{ \int Ds e^{-S(s)} \left| \det \mathbf{Z}_{(K+1) \times (K+1)}(s) \right|^{2n_1} \left| \det \mathbf{Z}_{K \times K}(s) \right|^{2N-2n_1} \right\}^{\frac{2n_2-j}{2n_2-2n_1}}
\end{aligned}$$

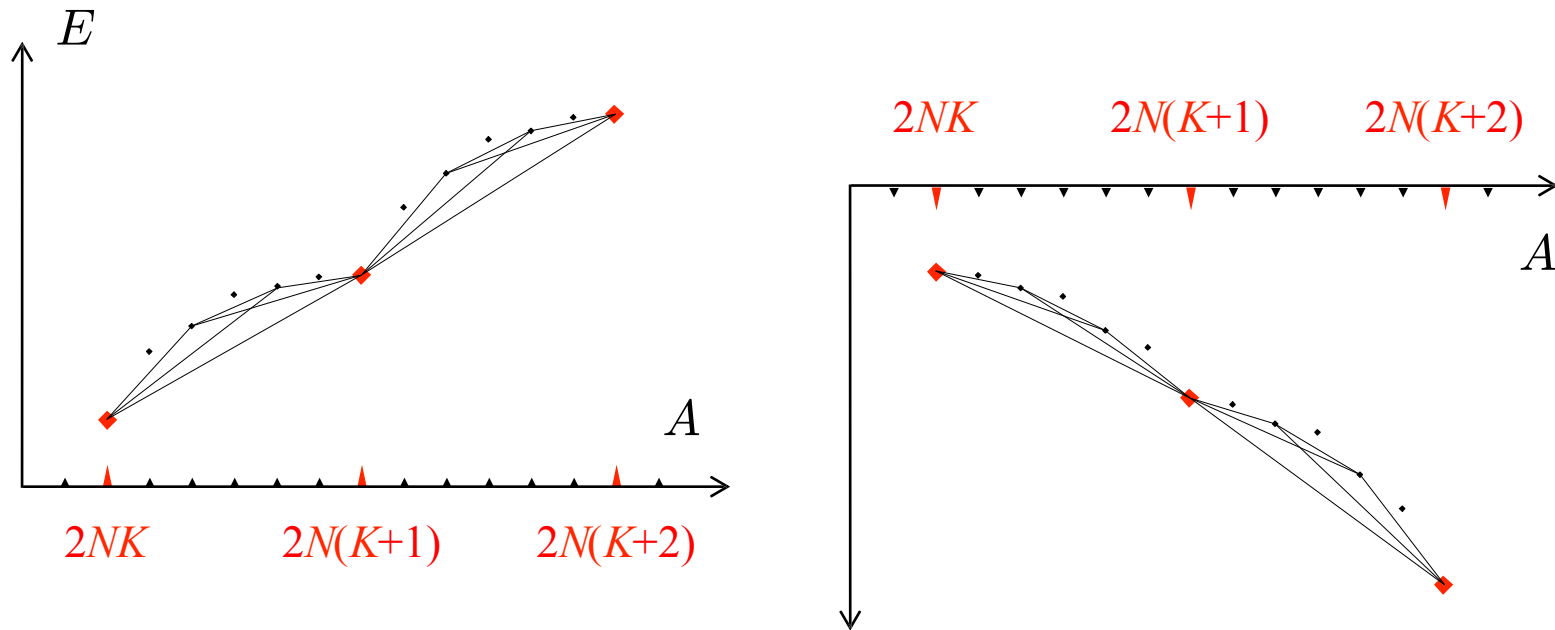
This is an inequality for the path integrals of systems with different numbers of particles. This can be written as

$$Z_{j,K+1;2N-j,K} \leq [Z_{2n_2,K+1;2N-2n_2,K}]^{\frac{j-2n_1}{2n_2-2n_1}} \times [Z_{2n_1,K+1;2N-2n_1,K}]^{\frac{2n_2-j}{2n_2-2n_1}}$$

We now take the limit of large Euclidean time. This gives us convexity bounds for the ground state energies of the systems with different numbers of particles.

$$E_{j,K+1;2N-j,K}^0 \geq \frac{j-2n_1}{2n_2-2n_1} E_{2n_2,K+1;2N-2n_2,K}^0 + \frac{2n_2-j}{2n_2-2n_1} E_{2n_1,K+1;2N-2n_1,K}^0$$

D.L., PRL 98 (2007) 182501



For similar convexity bounds applied to entanglement entropy bounds:

Drut, Porter, PRL 114, 050402 (2015)

## A tale of two interactions

Two LO interactions, A and B, have nearly identical nucleon-nucleon phase shifts and well as three- and four-nucleon bound states

Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
$^8\text{Be}$	$-58.61(14)$	$-59.73(6)$	$-56.51(14)$	$-57.29(7)$	$-56.591$
$^{12}\text{C}$	$-88.2(3)$	$-95.0(5)$	$-84.0(3)$	$-89.9(5)$	$-92.162$
$^{16}\text{O}$	$-117.5(6)$	$-135.4(7)$	$-110.5(6)$	$-126.0(7)$	$-127.619$
$^{20}\text{Ne}$	$-148(1)$	$-178(1)$	$-137(1)$	$-164(1)$	$-160.645$

Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak,  
PRL 117, 132501 (2016)

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$$\frac{E_{8\text{Be}}}{E_{4\text{He}}} = 1.997(6)$$

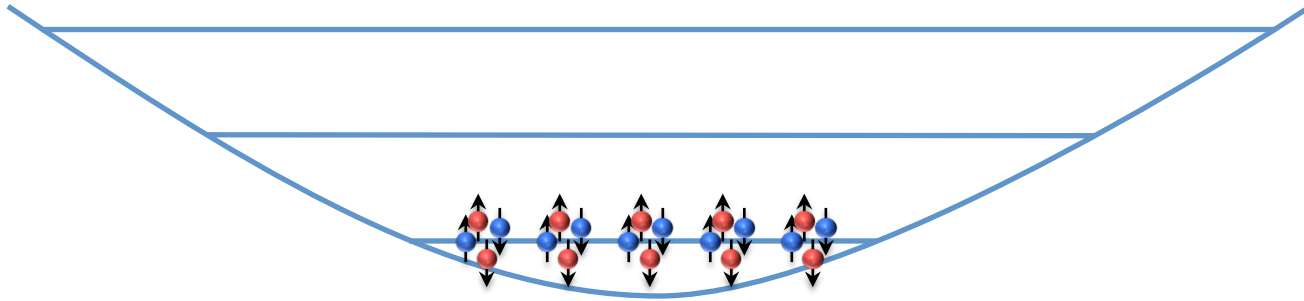
$$\frac{E_{12\text{C}}}{E_{4\text{He}}} = 3.00(1)$$

$$\frac{E_{16\text{O}}}{E_{4\text{He}}} = 4.00(2)$$

$$\frac{E_{20\text{Ne}}}{E_{4\text{He}}} = 5.03(3)$$



# Bose condensate of alpha particles!



Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
$^8\text{Be}$	-58.61(14)	-59.73(6)	-56.51(14)	-57.29(7)	-56.591
$^{12}\text{C}$	-88.2(3)	-95.0(5)	-84.0(3)	-89.9(5)	-92.162
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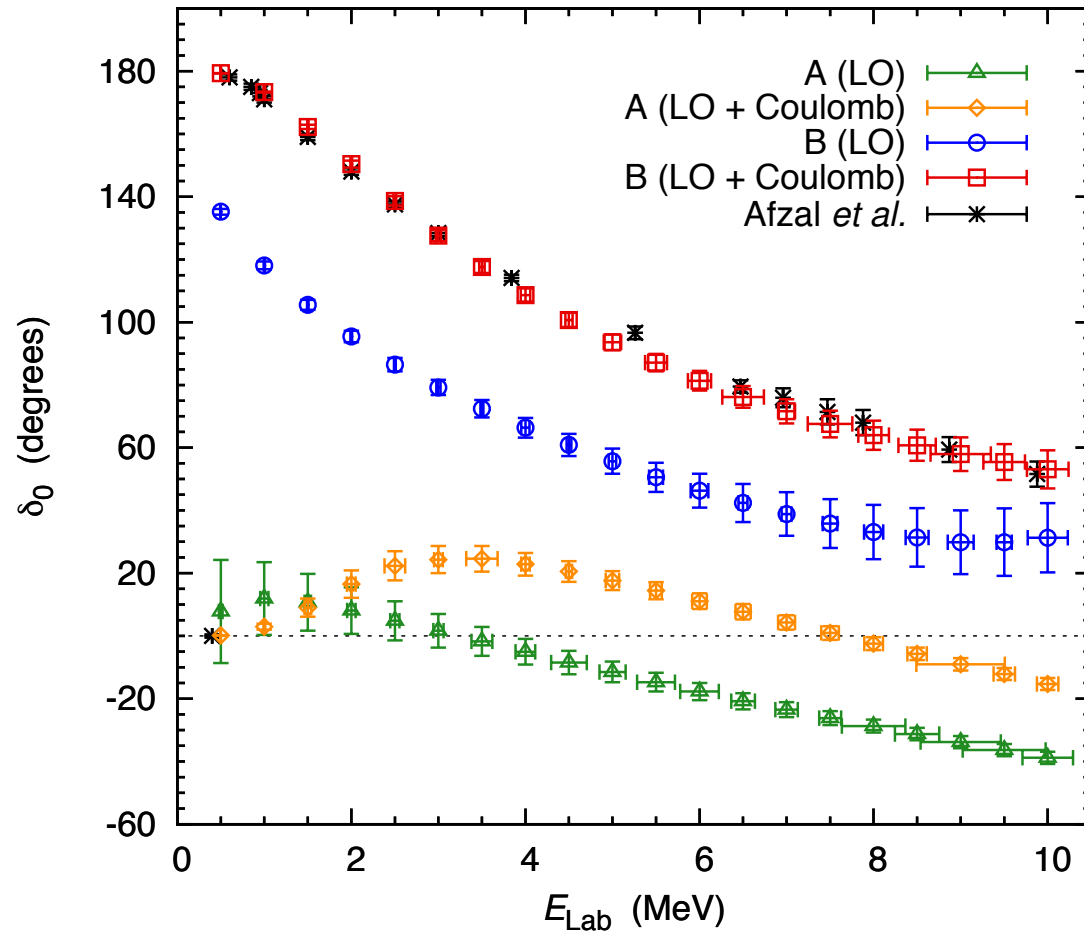
$$\frac{E_{8\text{Be}}}{E_{4\text{He}}} = 1.997(6)$$

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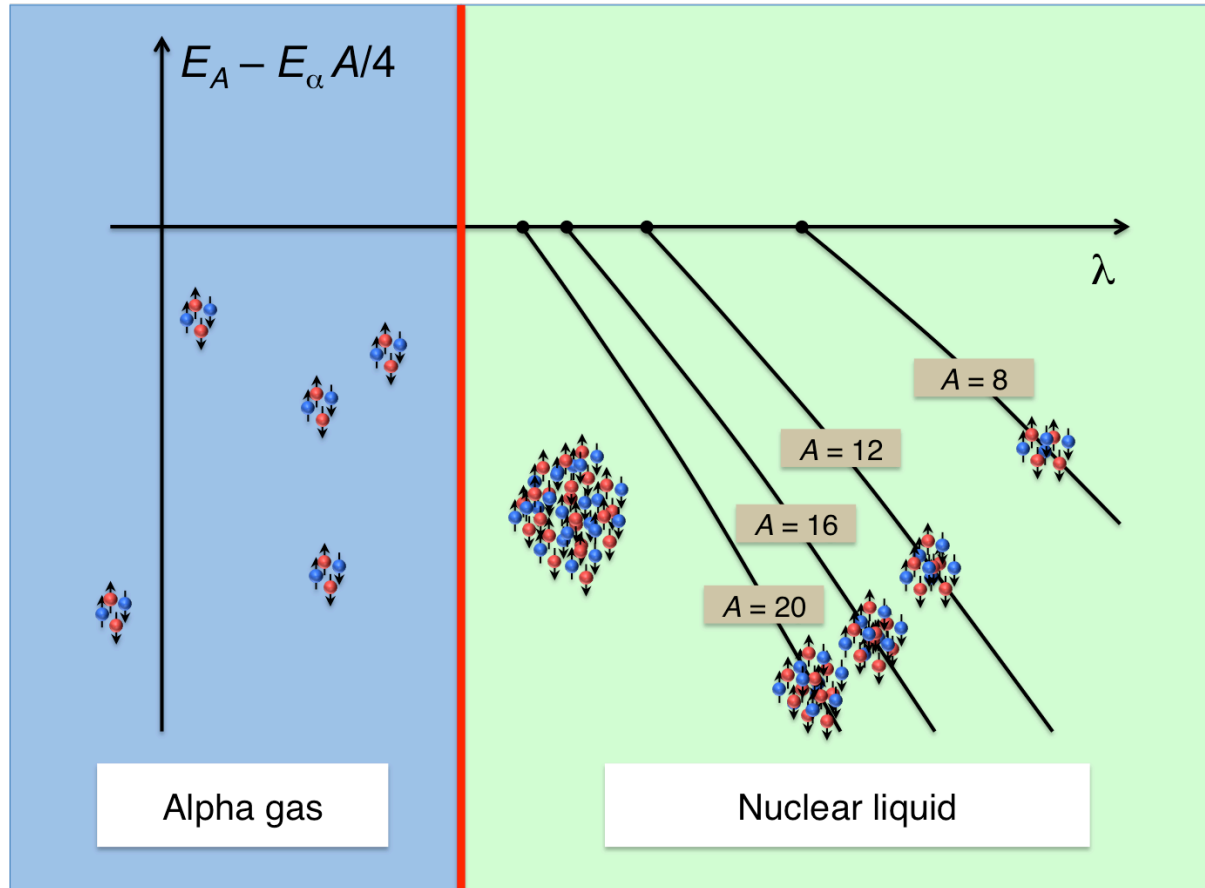
$$\frac{E_{20\text{Ne}}}{E_{4\text{He}}} = 5.03(3)$$

## Alpha-alpha scattering



Alpha-alpha interaction not uniquely determined by low-energy few-body data

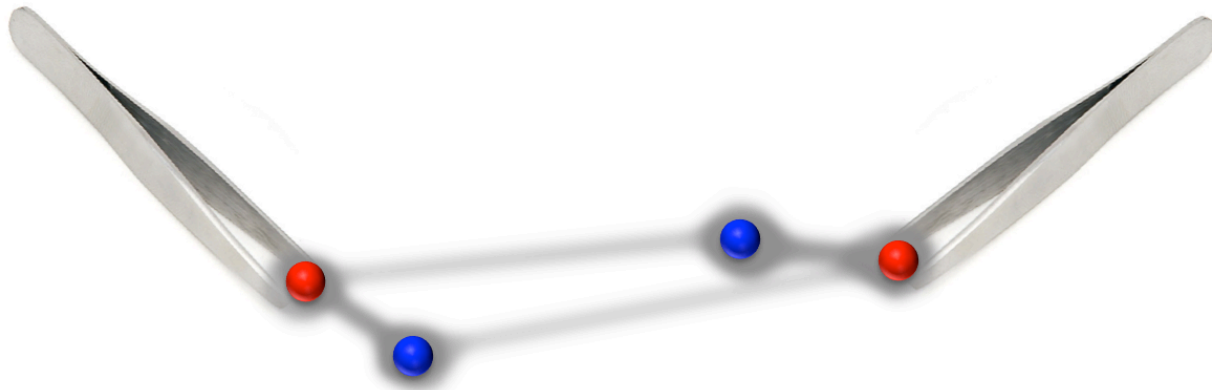
Control parameters: Sensitivity to interaction range and locality



Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

## Effective forces between bound states

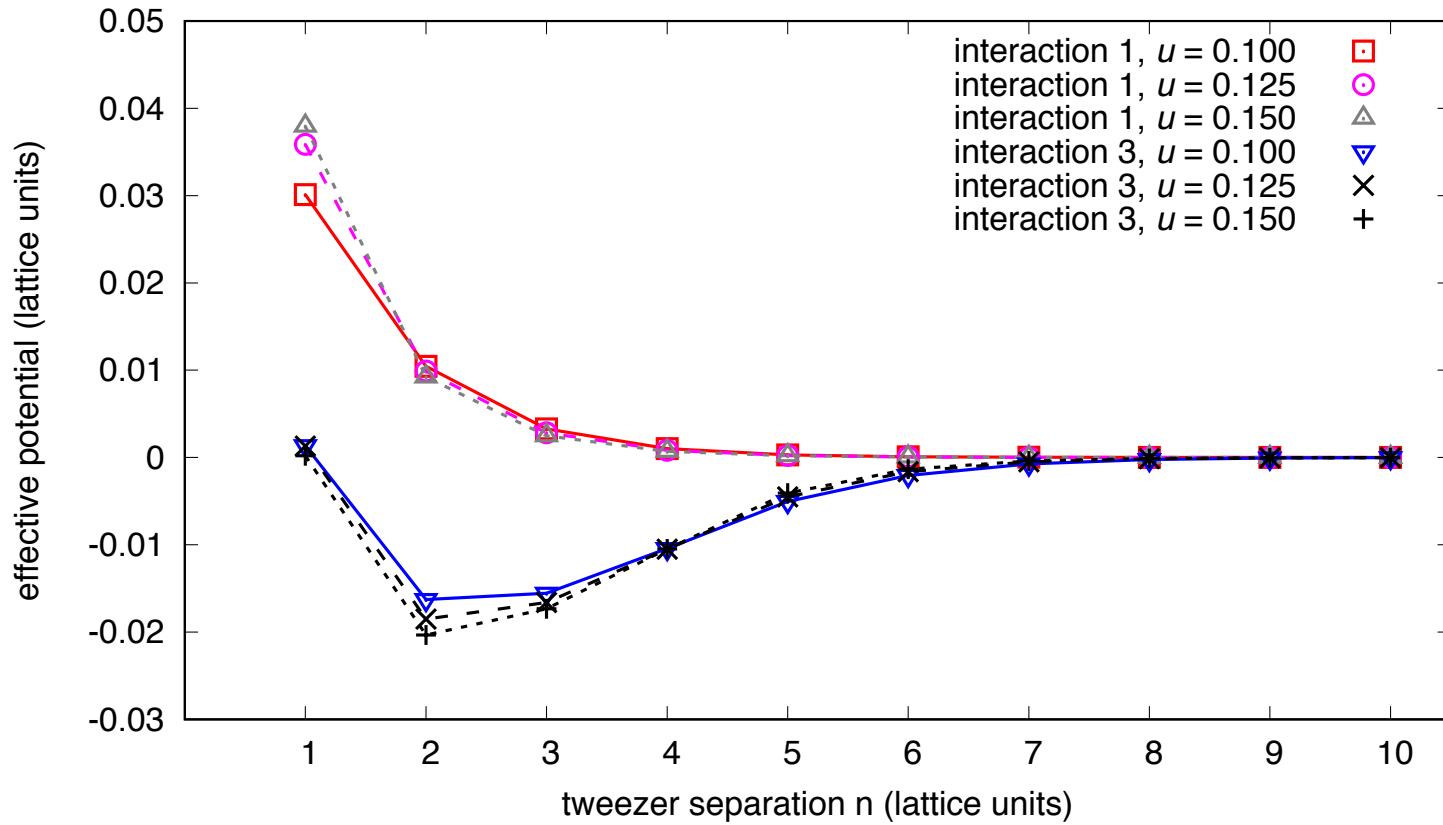
Numerical tweezers are used to probe the relation between particle-particle interactions and the induced interaction between bound states



Rokash, Epelbaum, Krebs, D.L., Rupak, Phys. Rev. Lett. 118, 232502 (2017)

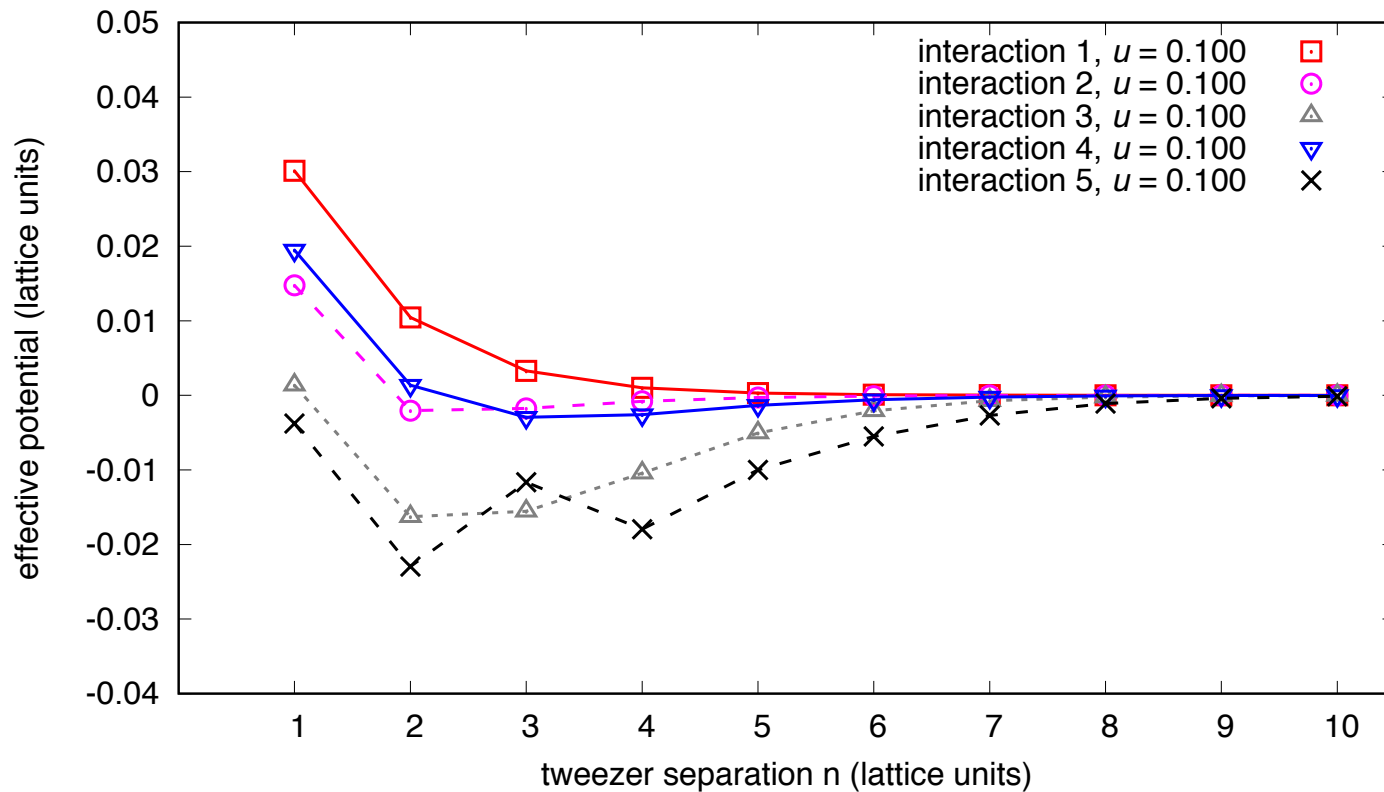
## Dimer-dimer effective potential

Dependence on tweezer trapping strength

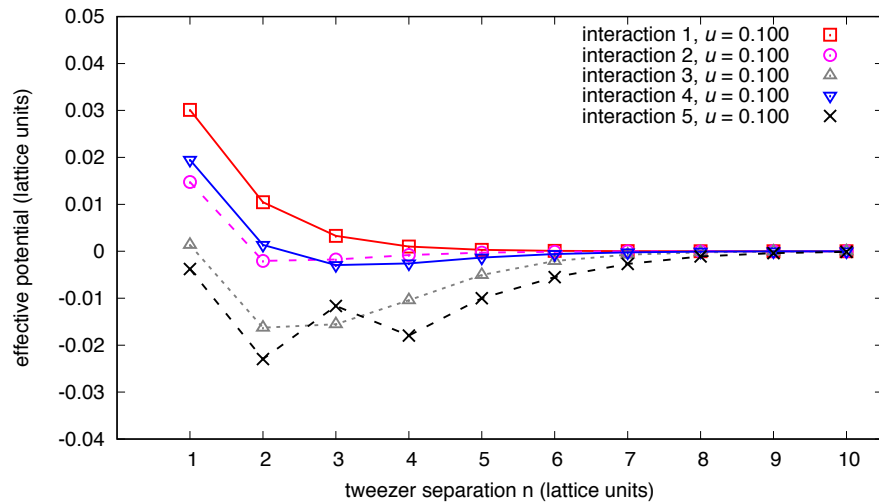


## Dimer-dimer effective potential

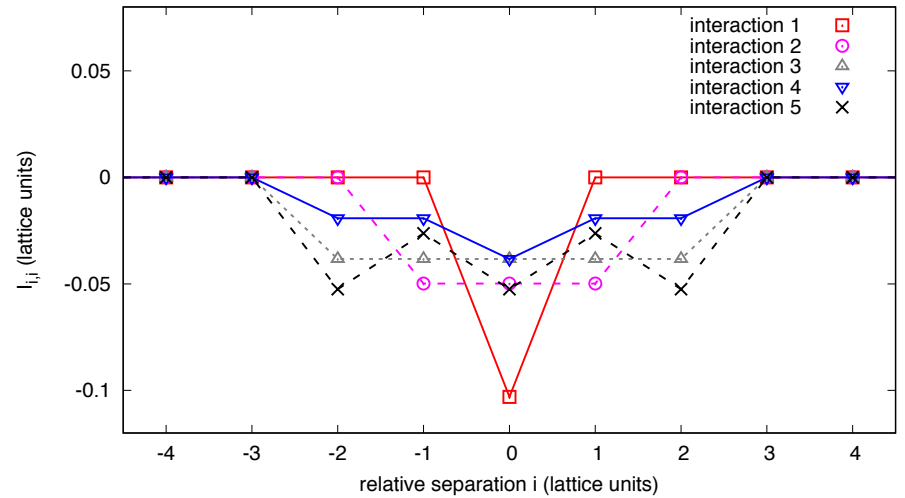
Control parameters: Sensitivity to interaction range and locality



Dimer-dimer effective potential



Local part of particle-particle interaction  
(diagonal element in position space)



## Pinhole Algorithm

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

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

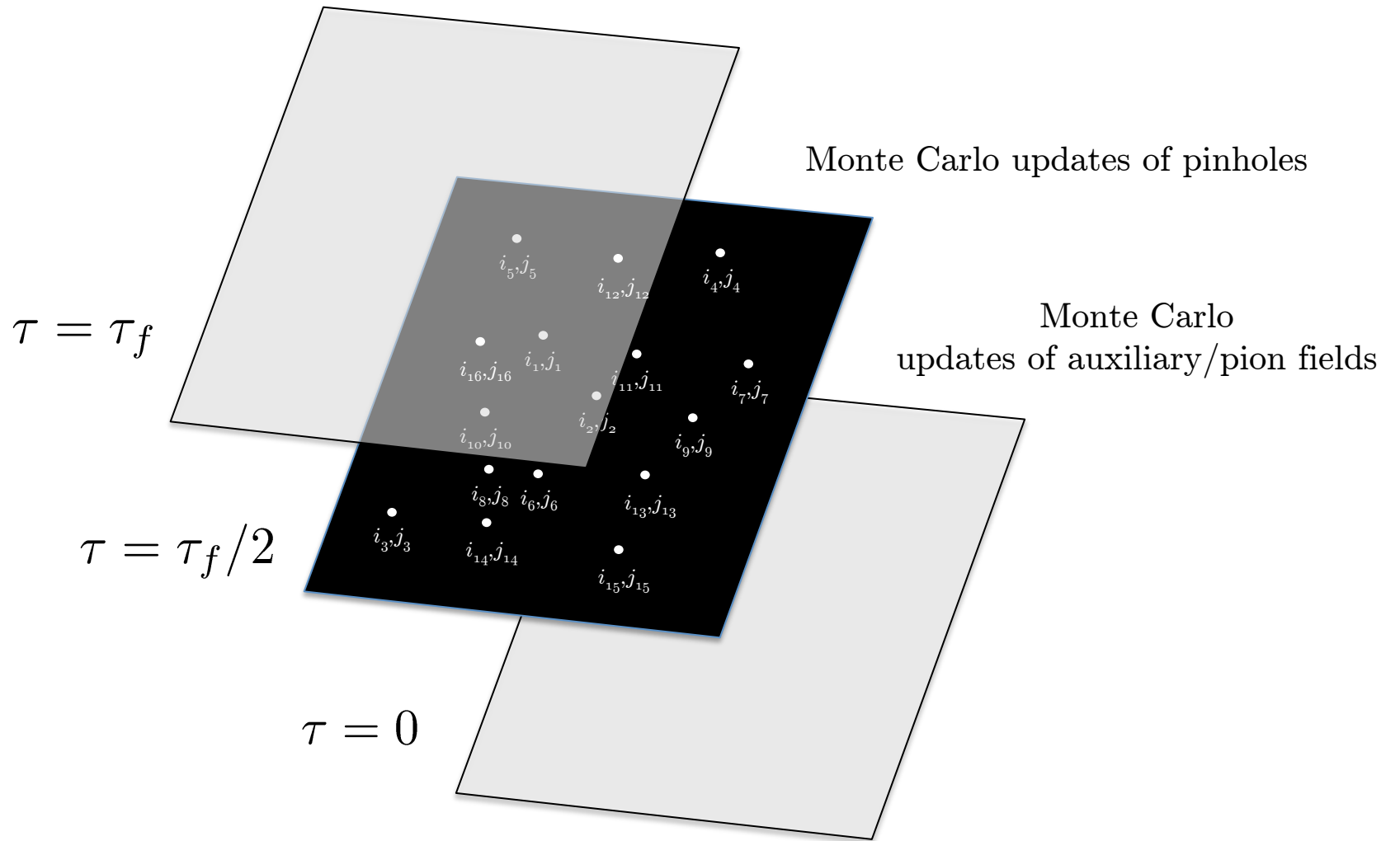
We construct the normal-ordered  $A$ -body density operator

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

In the simulations we do Monte Carlo sampling of the amplitude

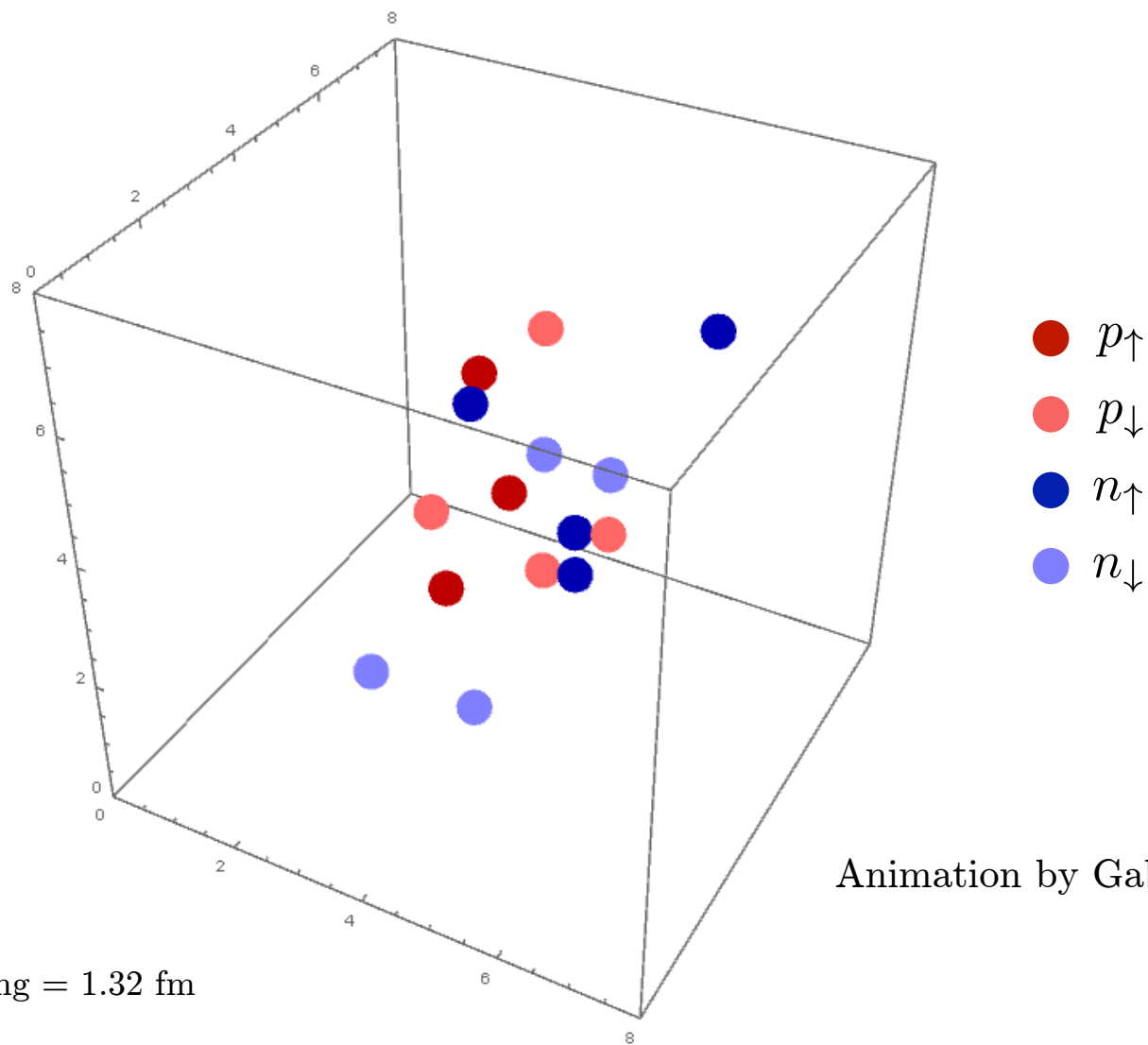
$$A_{i_1,j_1,\dots,i_A,j_A}(\mathbf{n}_1,\dots,\mathbf{n}_A,t) = \langle \Psi_I | e^{-Ht/2} \rho_{i_1,j_1,\dots,i_A,j_A}(\mathbf{n}_1,\dots,\mathbf{n}_A) e^{-Ht/2} | \Psi_I \rangle$$





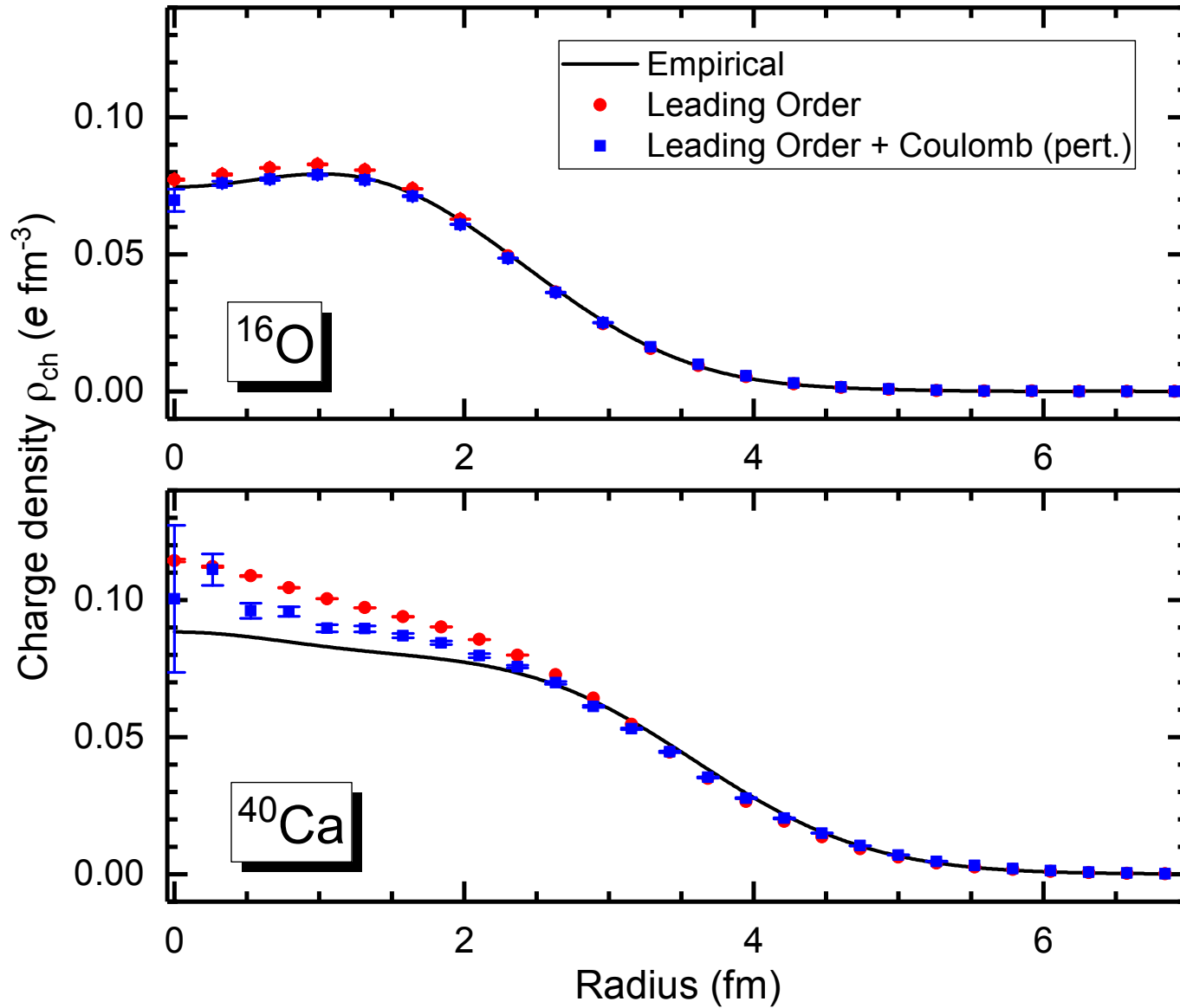
Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

# Oxygen-16



lattice spacing = 1.32 fm

Animation by Gabriel Given

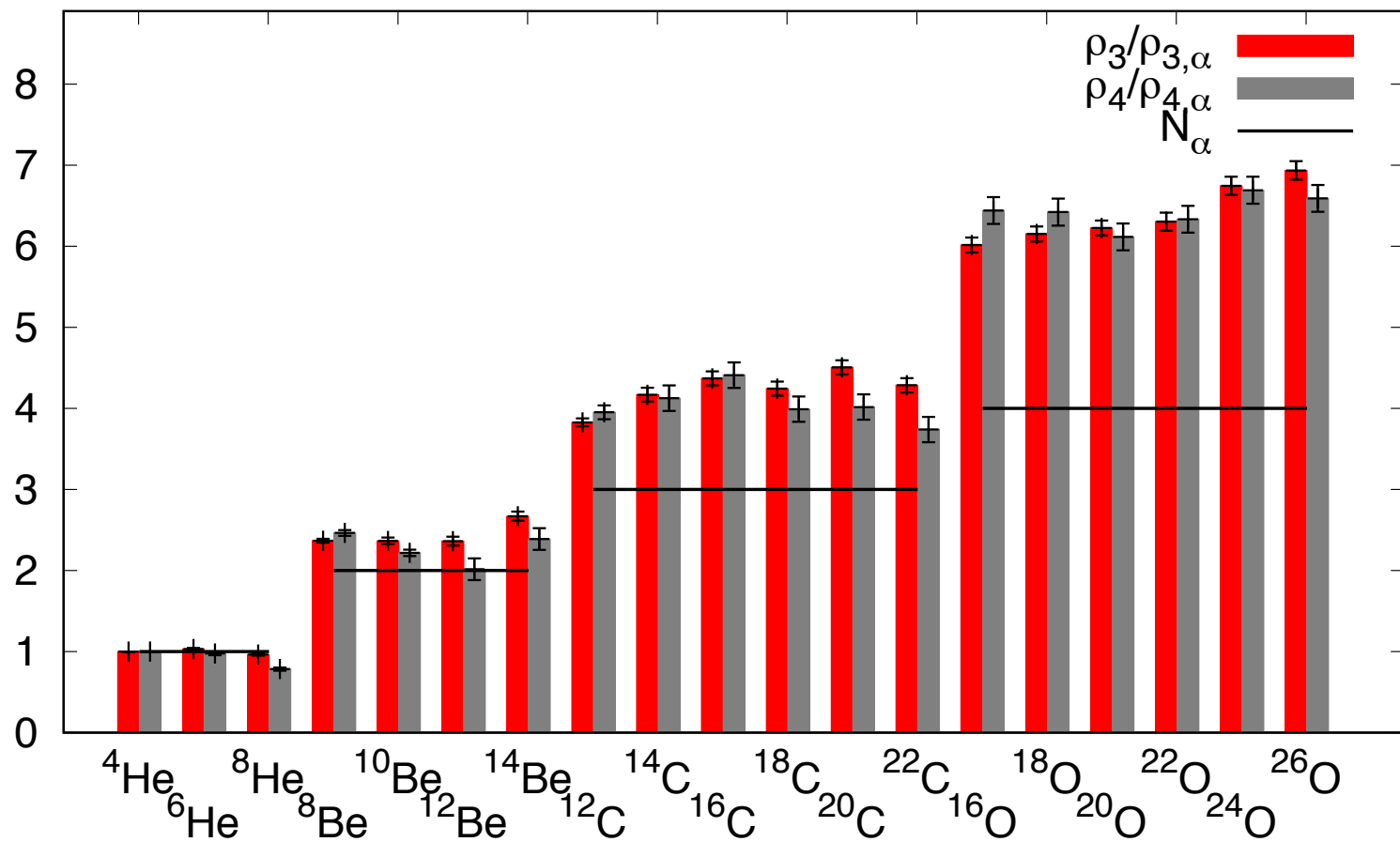


## Model-independent measure of clustering

Let  $\rho(\mathbf{n})$  be the total nucleon density operator on lattice site  $\mathbf{n}$ .  
We use local operator products as a probe of alpha clustering.

$\rho_3$  is defined as the expectation value of  $:\rho^3(\mathbf{n})/3!:$  summed over  $\mathbf{n}$ .  
 $\rho_4$  is defined as the expectation value of  $:\rho^4(\mathbf{n})/4!:$  summed over  $\mathbf{n}$ .

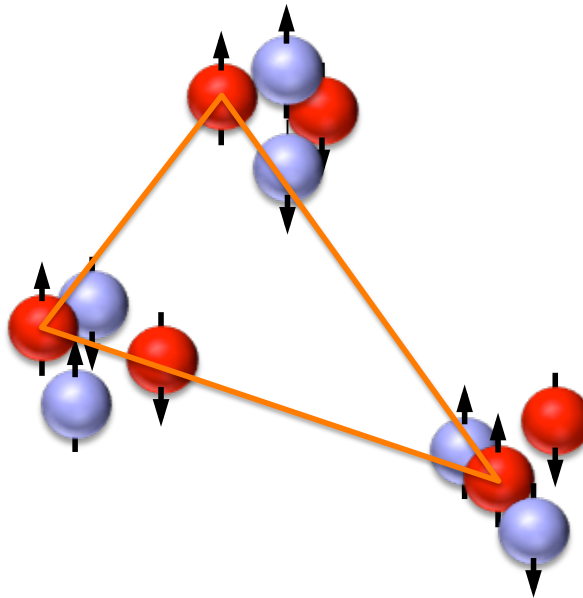
Let  $\rho_{3,\alpha}$  and  $\rho_{4,\alpha}$  be the corresponding values for the alpha particle.  
To leading order in an operator production expansion, the ratios  $\rho_3/\rho_{3,\alpha}$  and  $\rho_4/\rho_{4,\alpha}$  are model independent.

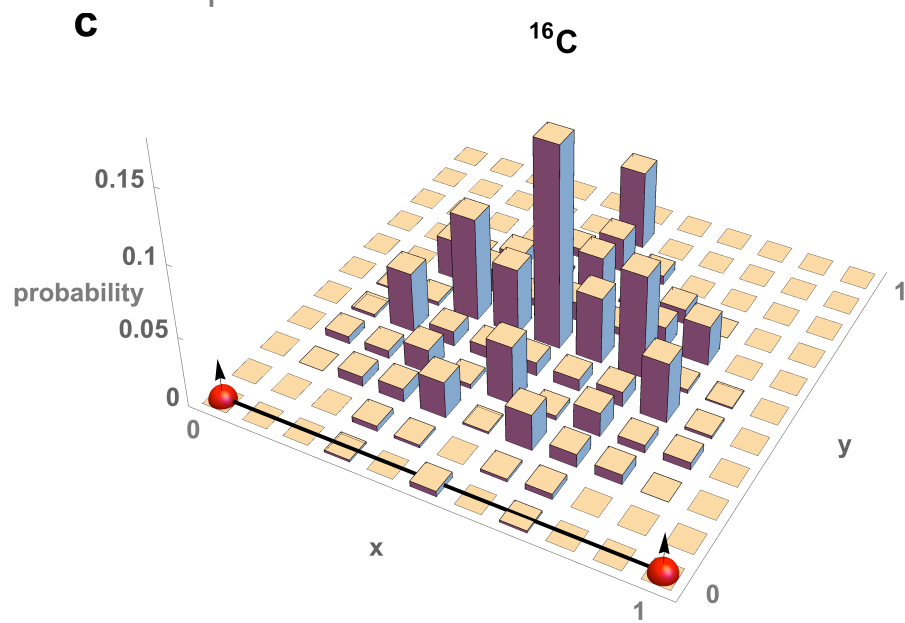
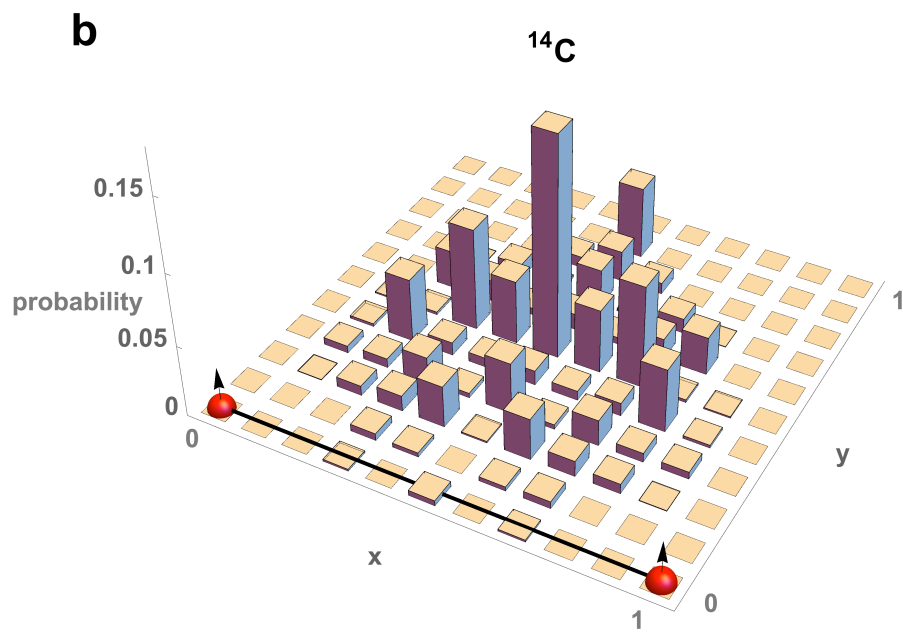
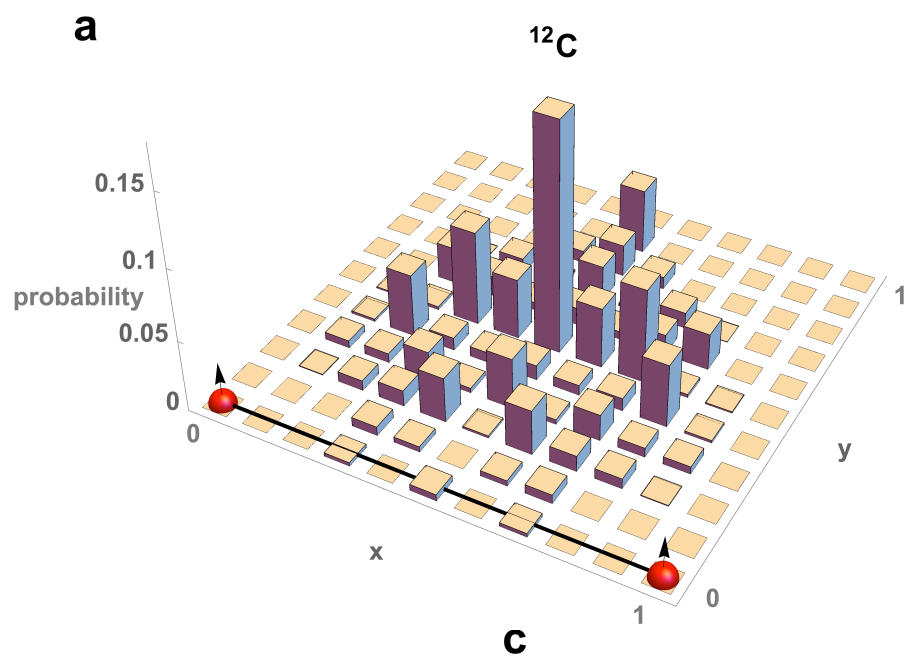


Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

## Model-independent measure of alpha cluster geometry

For the carbon isotopes, we can map out the alpha cluster geometry by computing the density correlations of the three spin-up protons. We compute these density correlations using the pinhole algorithm.





For an overview of microscopic clustering in light nuclei see the review

Freer, Horiuchi, Kanada-En'yo, D.L., Meißner, RMP 90, 035004 (2018)



## Reivew of topics

Projection Monte Carlo with auxiliary fields

Chiral effective field theory at leading order

Spectral convexity and clustering

A tale of two different interactions

Effective forces between bound states

Pinhole algorithm

Model independent probes of clustering