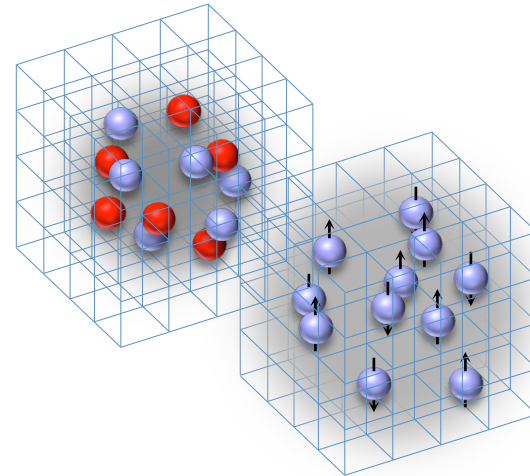


New algorithms and interactions for nuclear lattice simulations



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Progress in Ab Initio Techniques in Nuclear Physics
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Outline

Lattice chiral effective field theory

New interactions

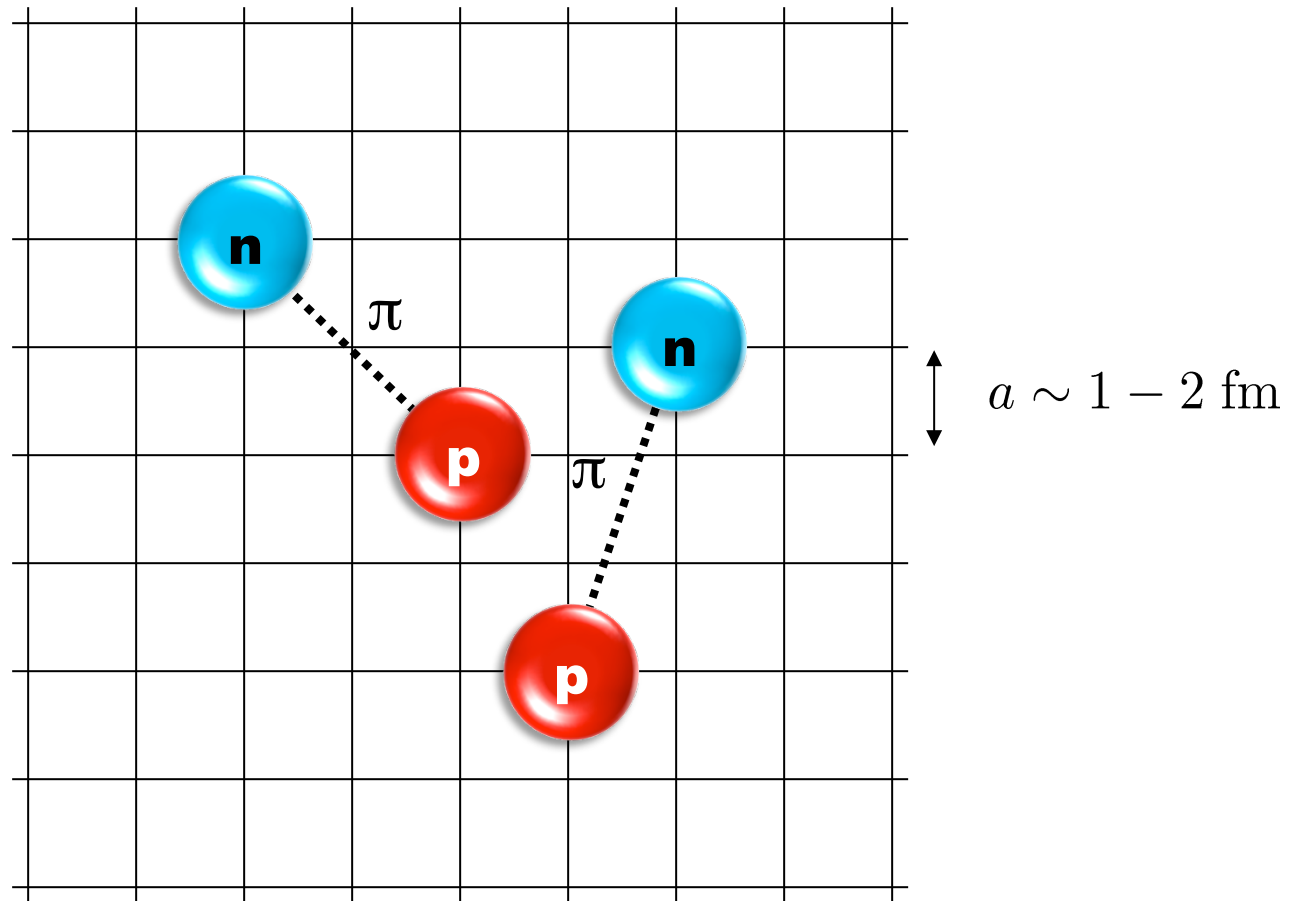
Model-independent measure of clustering

Pinhole algorithm

Model-independent measure of alpha cluster geometry

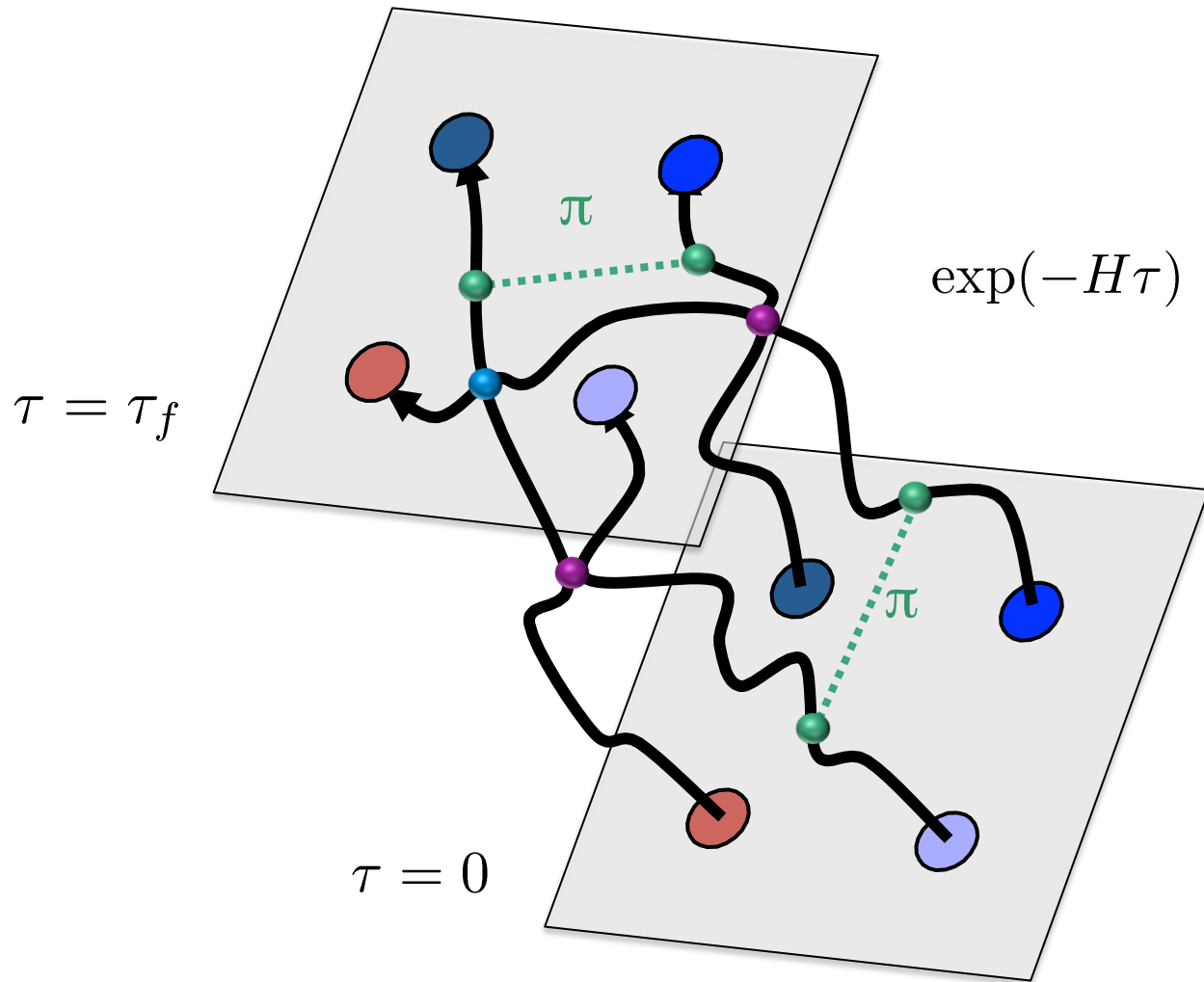
Summary and outlook

Lattice chiral effective field theory



Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)
TALENT summer school lectures: qmc2016.wordpress.ncsu.edu

Euclidean time projection

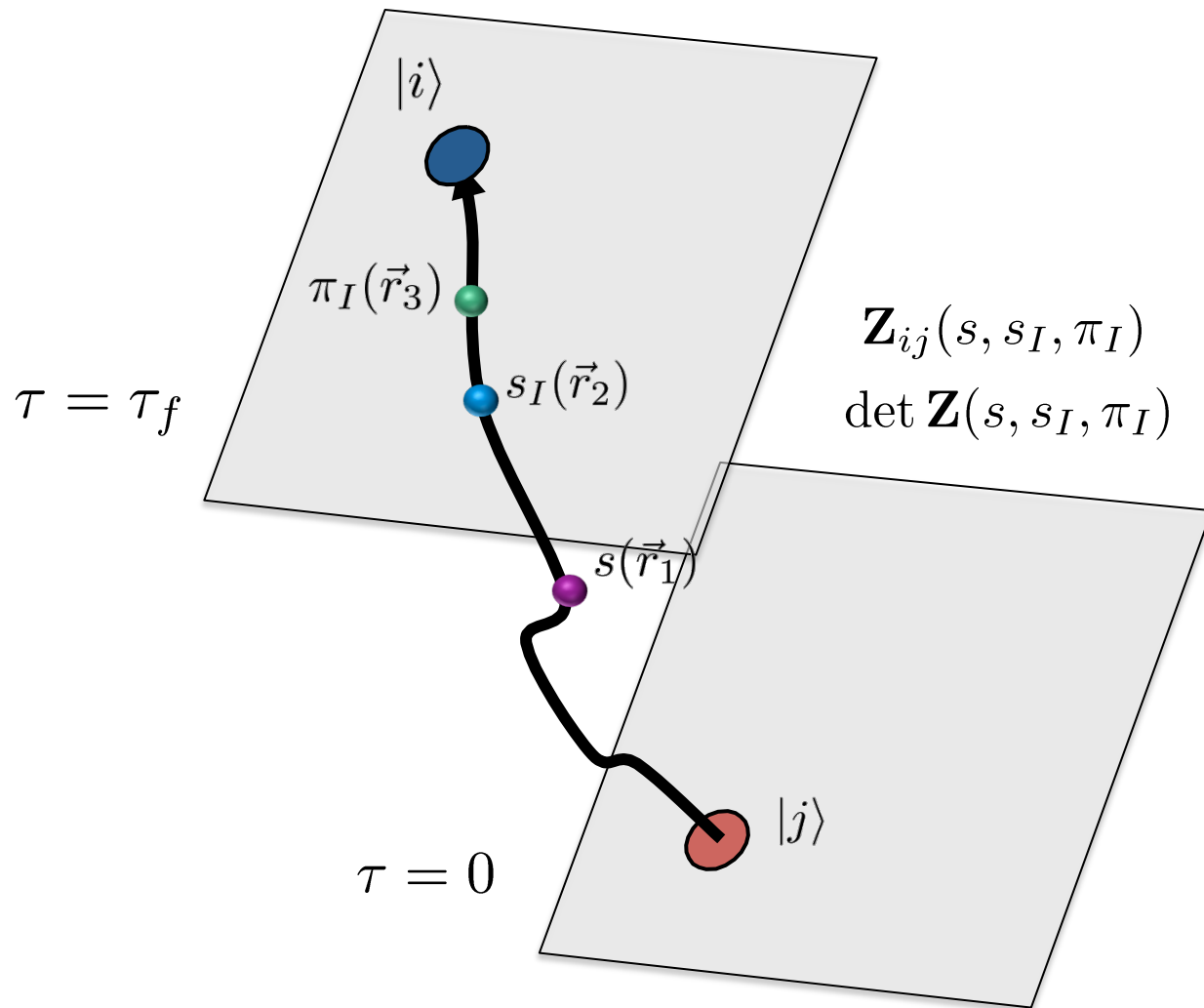


Auxiliary field method

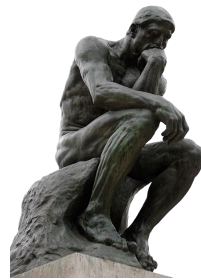
We can write exponentials of the interaction using a Gaussian integral identity

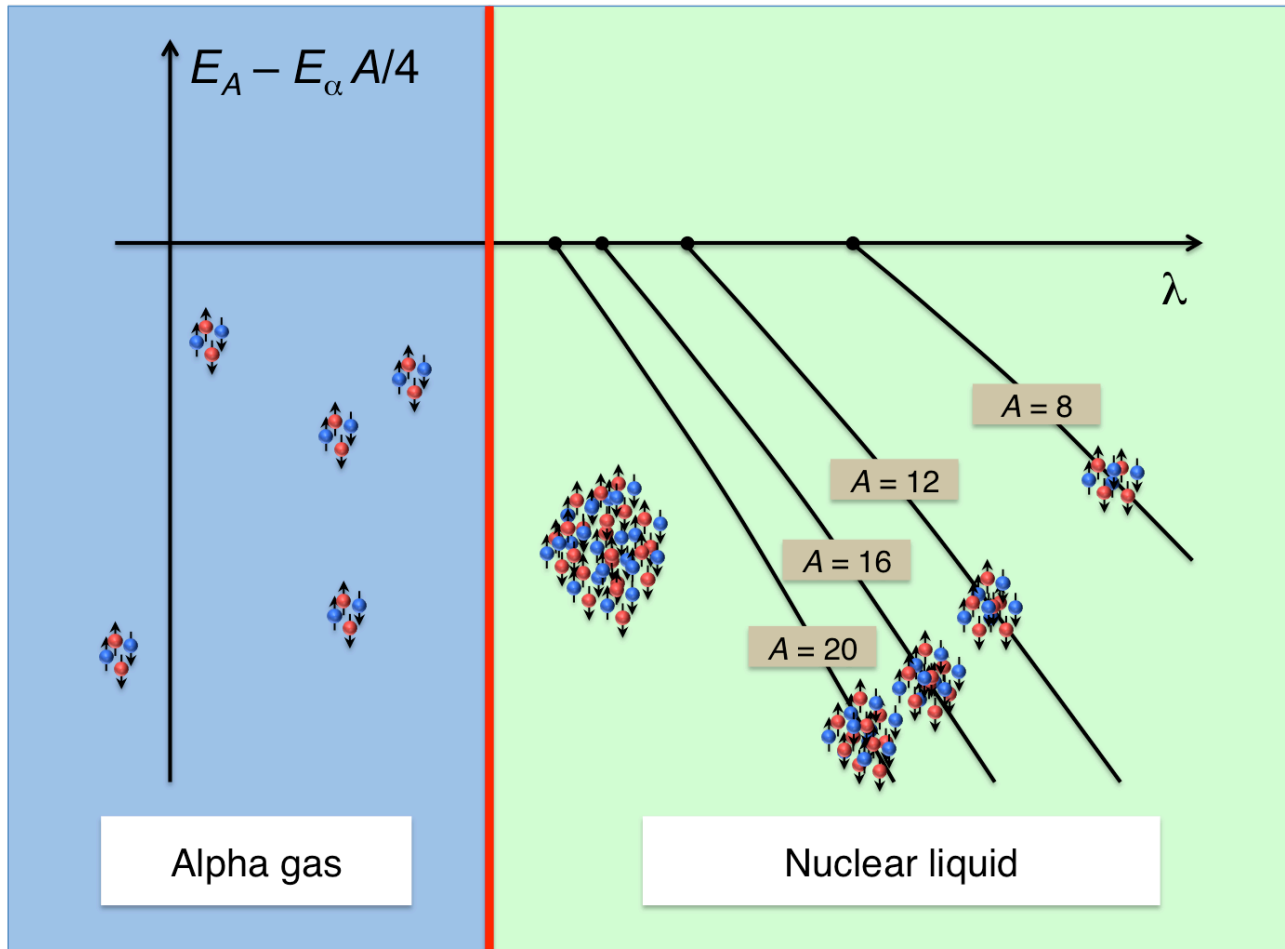
$$\begin{aligned} & \exp \left[-\frac{C}{2} (N^\dagger N)^2 \right] \quad \times \quad (N^\dagger N)^2 \\ &= \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} ds \exp \left[-\frac{1}{2} s^2 + \sqrt{-C} s (N^\dagger N) \right] \quad \rangle \quad s N^\dagger N \end{aligned}$$

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.



Unfortunately so far lattice simulations have mostly been restricted to nuclei with $N = Z$ due to Monte Carlo sign oscillations.





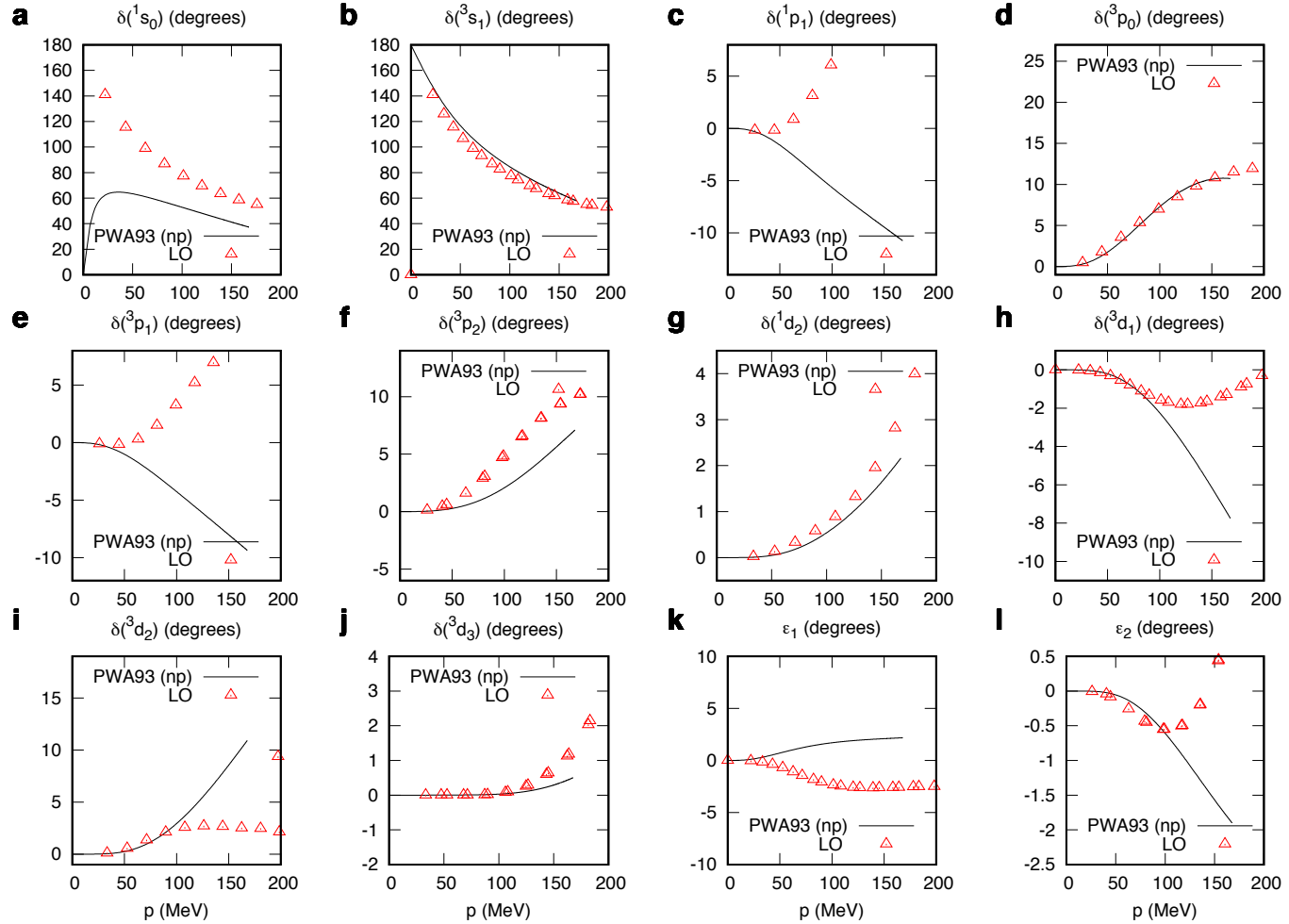
Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

Rokash, Epelbaum, Krebs, D.L., arXiv:1612:08004

Fit three parameters at leading order

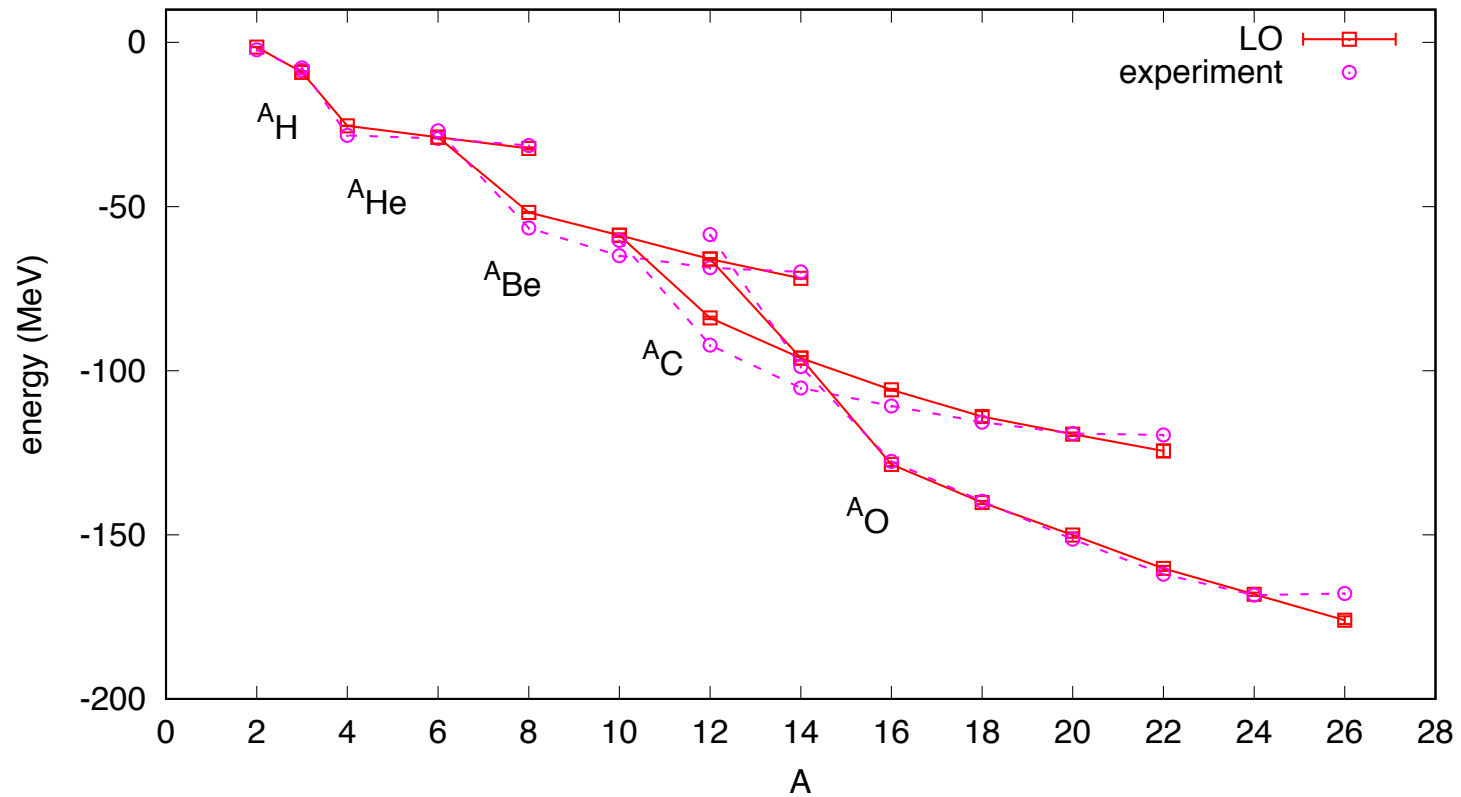
average nucleon-nucleon s -wave scattering length
average nucleon-nucleon s -wave effective range
alpha-alpha s -wave scattering length

New leading-order interactions



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

Ground state energies



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

Model-independent measure of clustering

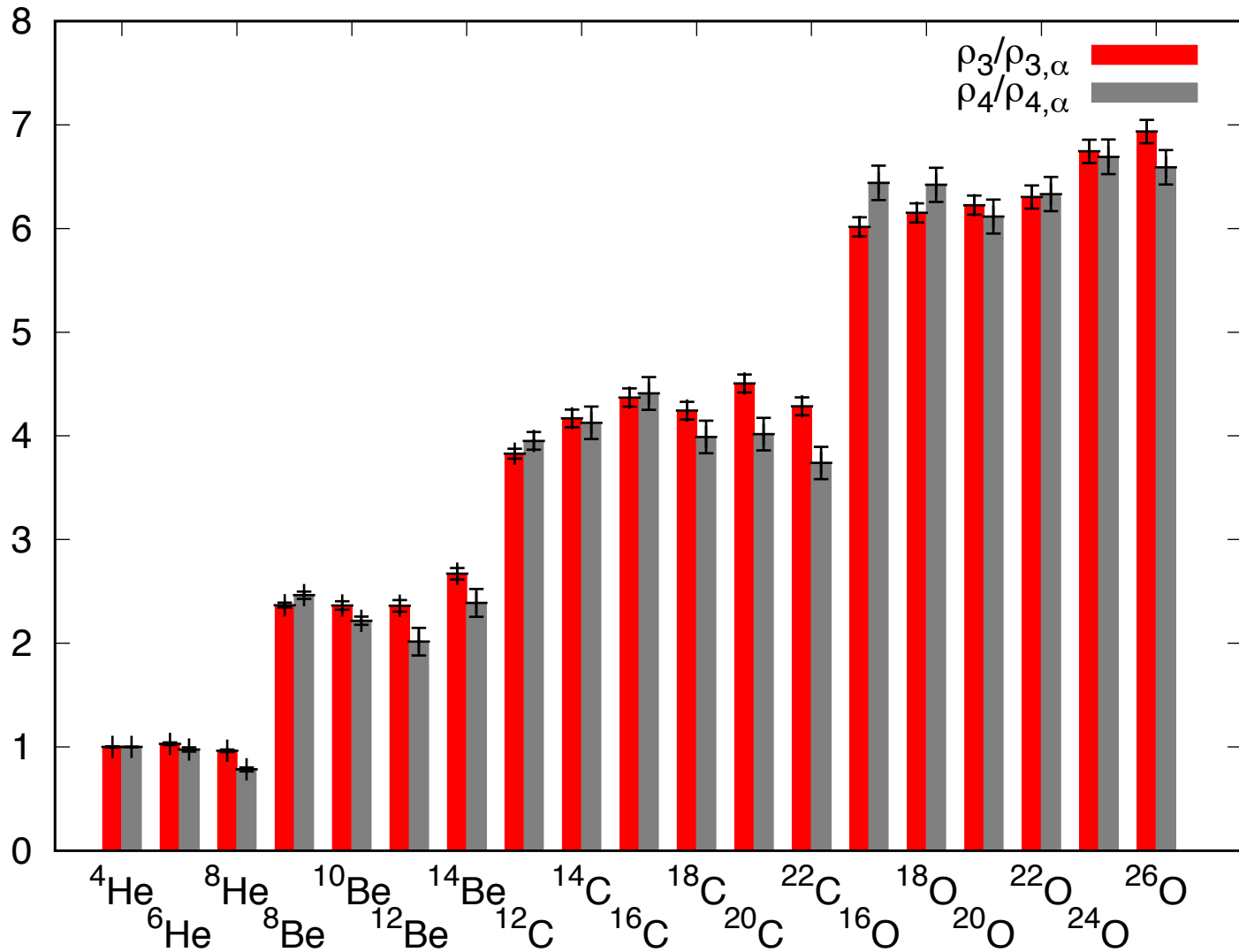
Let $\rho(\mathbf{n})$ be the total nucleon density operator on lattice site \mathbf{n} . To construct a probe for alpha clusters, we define ρ_4 as the expectation value of $:\rho^4(\mathbf{n})/4!:$ summed over \mathbf{n} .

For nuclei with even Z and even N , there are likely no well-defined ${}^3\text{H}$ or ${}^3\text{He}$ clusters since their formation is not energetically favorable.

Therefore we can use short-distance three-nucleon operators as a second probe of alpha clusters. We define ρ_3 as the expectation value of $:\rho^3(\mathbf{n})/3!:$ summed over \mathbf{n} .

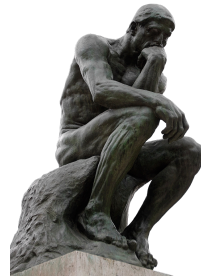
Due to divergences at short distances, ρ_3 and ρ_4 will depend on the short-distance regularization scale, which in our case is the lattice spacing. However the regularization-scale dependence of ρ_3 and ρ_4 does not depend on the nucleus being considered.

Therefore if we let $\rho_{3,\alpha}$ and $\rho_{4,\alpha}$ be the corresponding values for the alpha particle, then the ratios $\rho_3/\rho_{3,\alpha}$ and $\rho_4/\rho_{4,\alpha}$ are free from short-distance divergences and are model-independent quantities up to contributions from higher-dimensional operators in an operator product expansion.



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

Unfortunately there is 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

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

We construct the normal-ordered A -body density operator

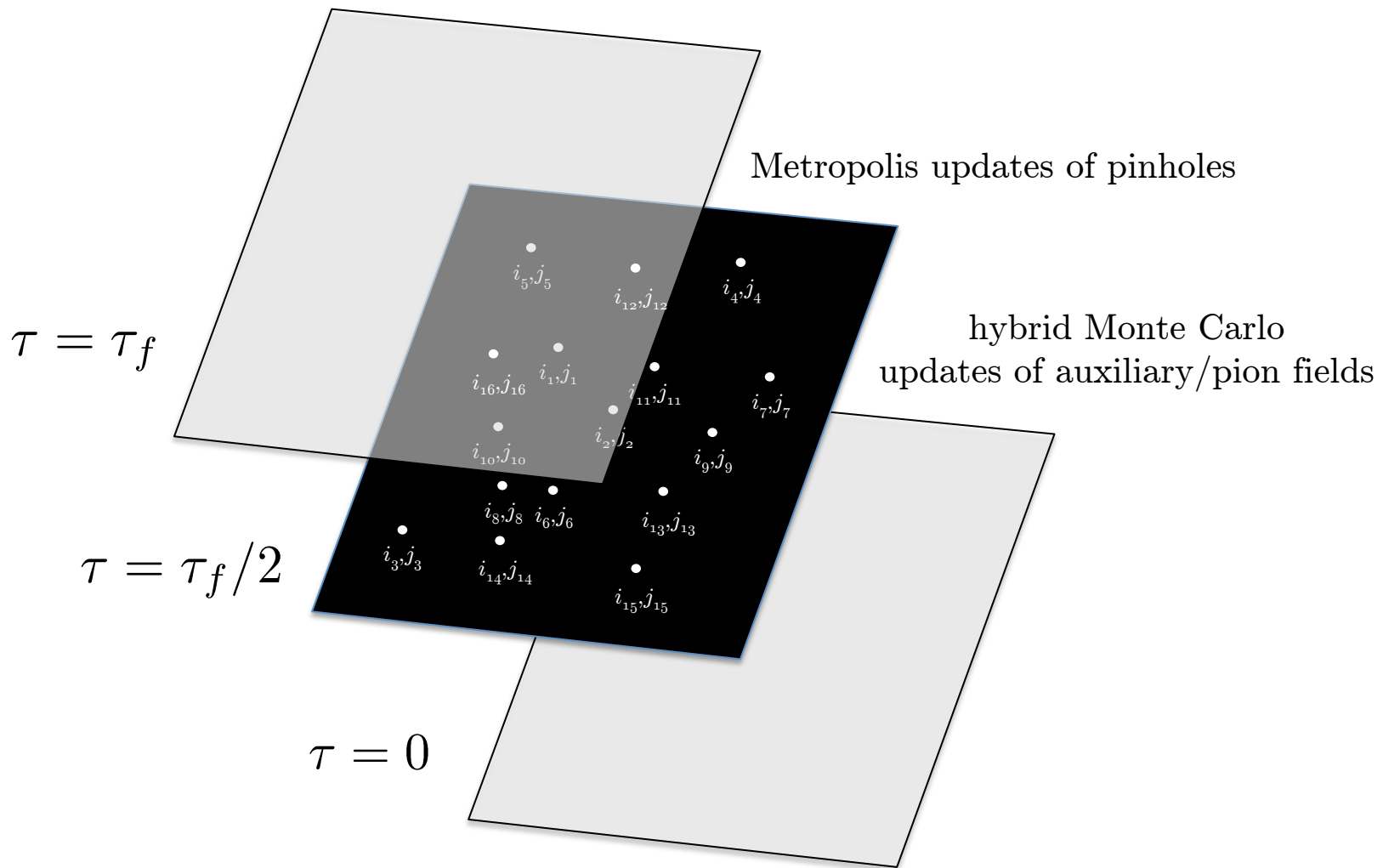
$$\rho_{i_1,j_1,\dots,i_A,j_A}(\mathbf{n}_1,\dots,\mathbf{n}_A) = : \rho_{i_1,j_1}(\mathbf{n}_1) \cdots \rho_{i_A,j_A}(\mathbf{n}_A) :$$

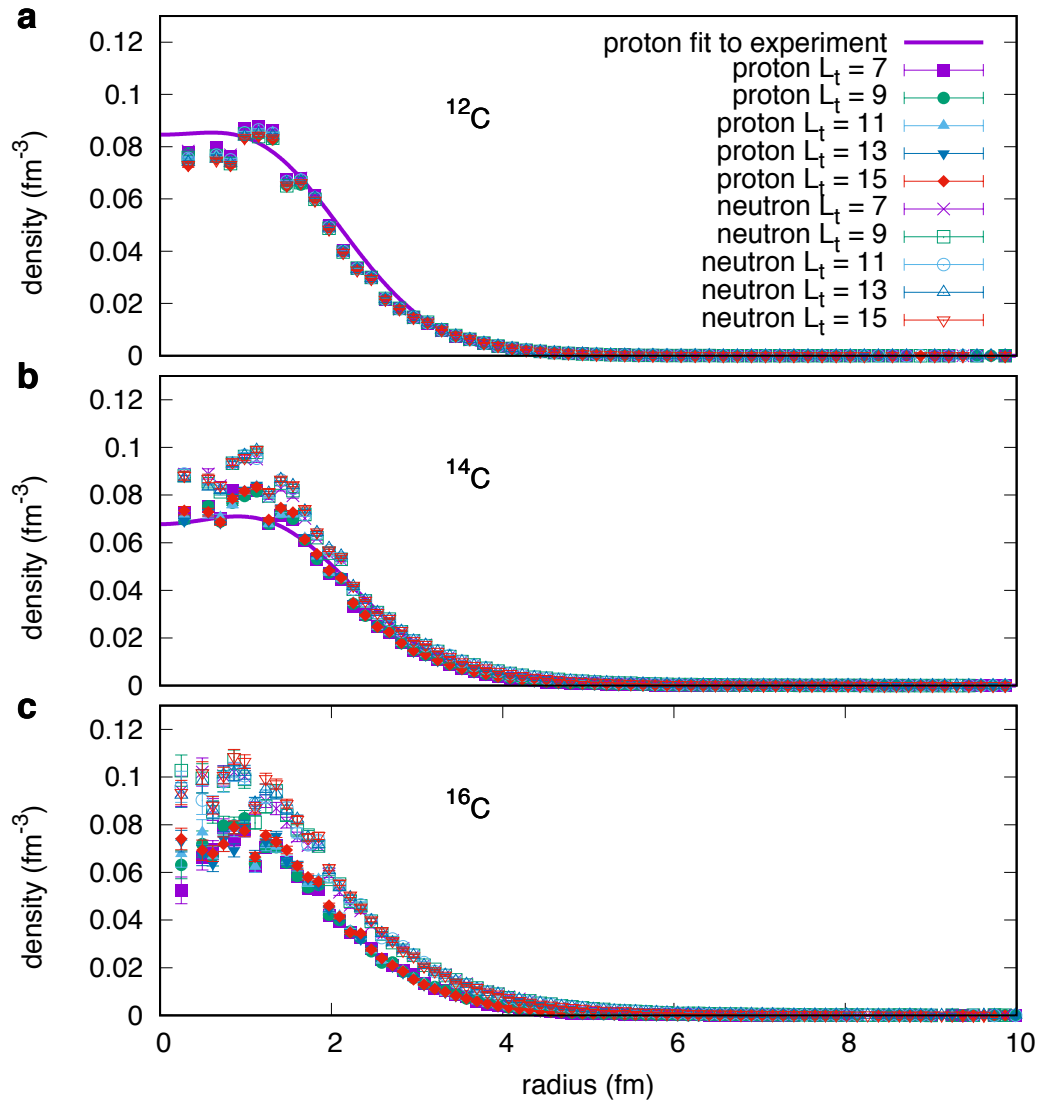
In the A -particle subspace, we have the identity

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

In the simulations we do Monte Carlo sampling of the amplitude

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



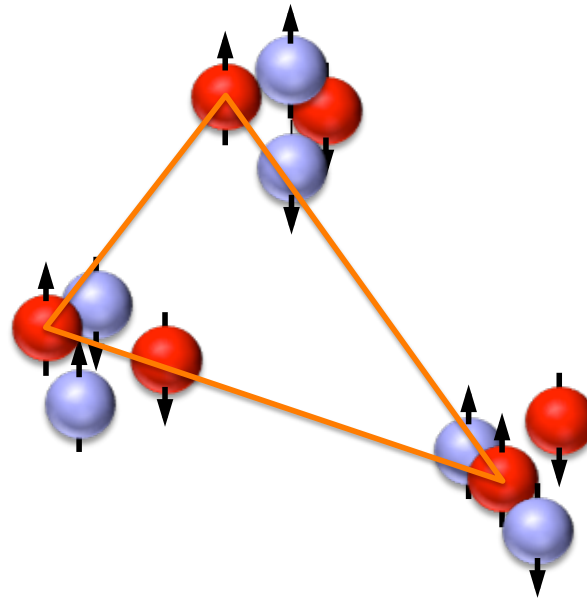


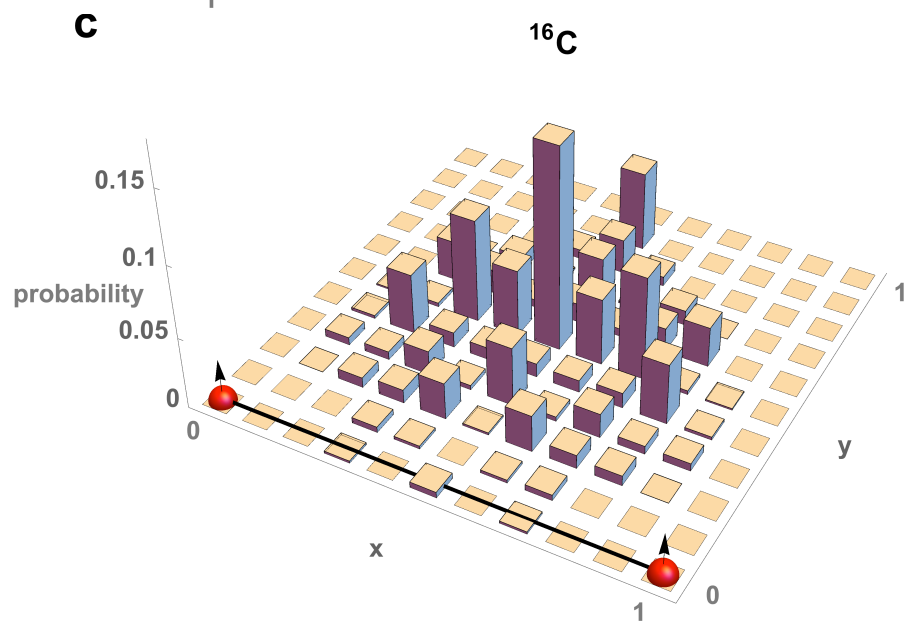
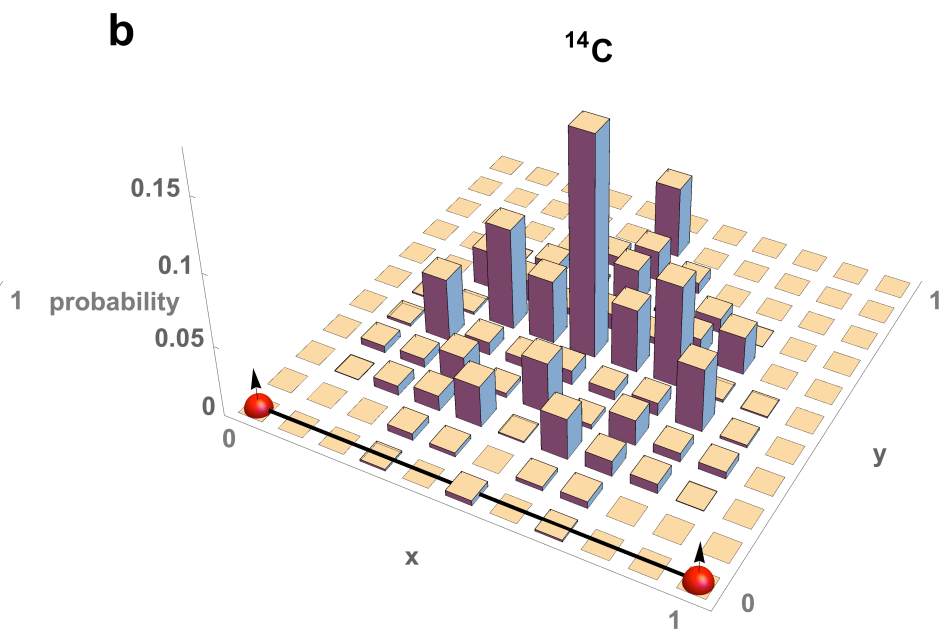
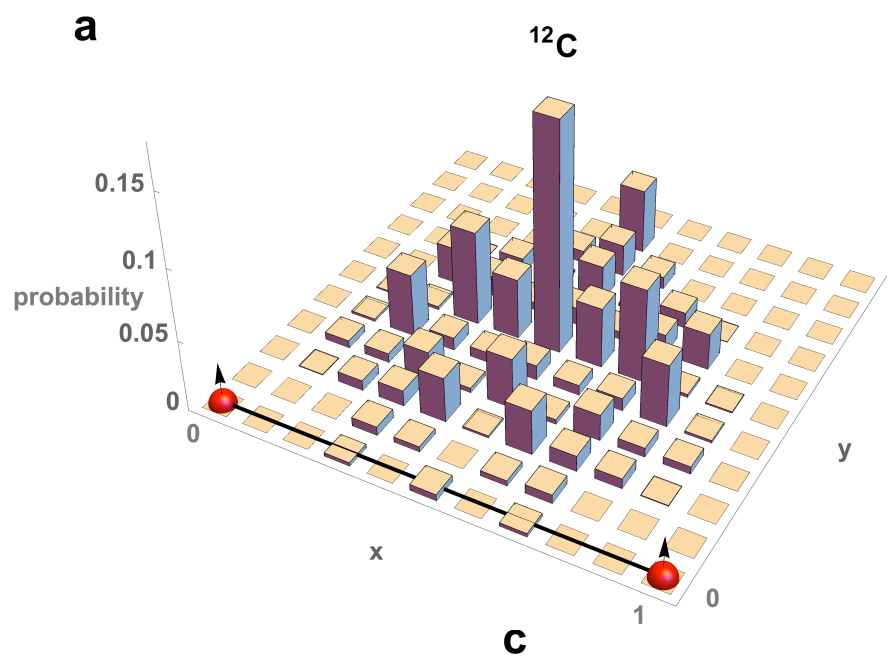
Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, arXiv:1702.05177

See also König, D.L., arXiv:1701.00279 for discussion of asymptotic properties

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.





Given the rich cluster structure of the excited states of ^{12}C , this raises the interesting possibility of similar cluster states appearing in ^{14}C and ^{16}C .

In particular, the bound 0_2^+ state at 6.59 MeV above the ground state of ^{14}C may be a bound-state analog to the Hoyle state resonance in ^{12}C at 7.65 MeV. It may also have a clean experimental signature since low-lying neutron excitations are suppressed by the shell closure at eight neutrons.

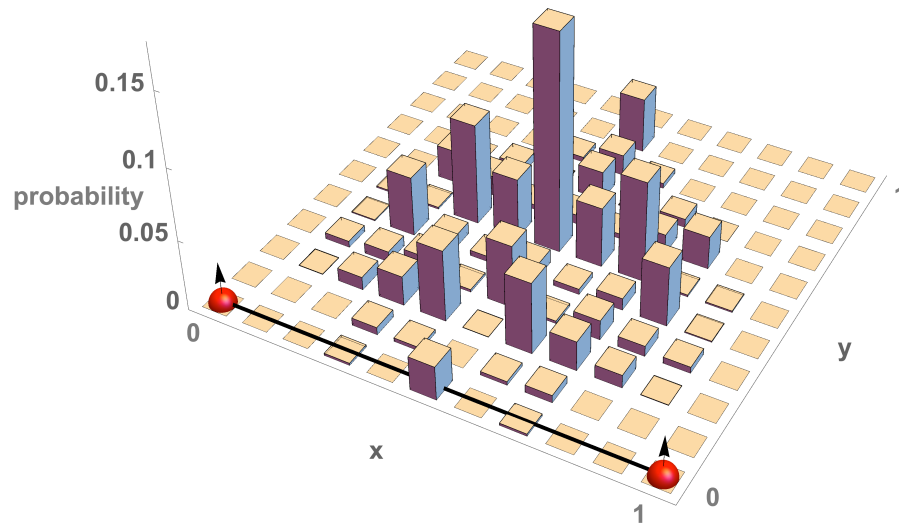
There is also a bound 0_2^+ in ^{16}C , however in this case one expects low-lying two-neutron excitations to be important, thereby making the analysis more complicated.

We can make a simple Gaussian lattice model of the distribution of the spin-up protons. We consider a probability distribution $P(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ on our lattice grid for the positions of the protons \vec{r}_1 , \vec{r}_2 , and \vec{r}_3 .

We take the probability distribution to be a product of Gaussians with root-mean-square radius 2.6 fm (charge radius of ^{14}C) and unit step functions which vanish if the magnitude of $\vec{r}_1 - \vec{r}_2$, $\vec{r}_2 - \vec{r}_3$, or $\vec{r}_3 - \vec{r}_1$ is smaller than 1.7 fm (charge radius of ^4He).

We can factor out the center-of-mass distribution of the three spin-up protons and recast the Gaussian factors as a product of Gaussians for the separation vectors $\vec{r}_1 - \vec{r}_2$, $\vec{r}_2 - \vec{r}_3$, and $\vec{r}_3 - \vec{r}_1$ with root-mean-square radius 4.5 fm.

Gaussian model



Summary and outlook

These are exciting times for *ab initio* nuclear theory. In lattice EFT, we have new projects in motion which are pushing the theoretical and computational frontiers beyond what was previously possible.

One development is our improved understanding of the connection between nuclear forces and nuclear structure. This has led to a more efficient set of lattice chiral EFT interactions that should have better order-by-order convergence for a wide range of nuclear masses and also reduce the Monte Carlo sign oscillations.

Another development is the pinhole method for calculating A -body densities with applications to density distributions, matrix elements of electric and magnetic multipole operators, form factors, and radiative capture reactions.

We now also have model-independent measures of clustering and the geometry of alpha clusters.