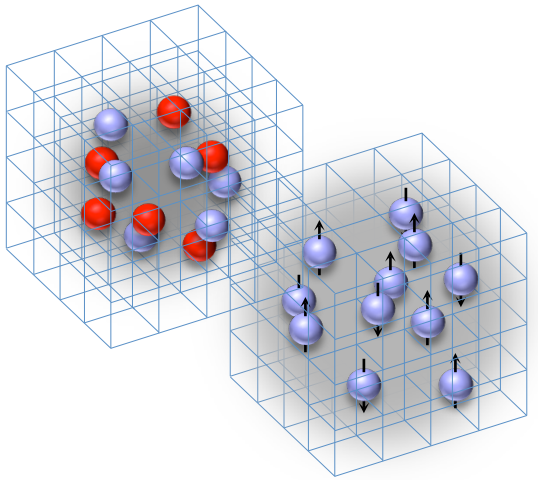
Nuclear binding near a quantum phase transition

Dean Lee
North Carolina State University
Nuclear Lattice EFT Collaboration



First Tsukuba-CCS-RIKEN Joint Workshop on
Microscopic Theories of Nuclear Structure and Dynamics
December 12-16, 2016

Outline

Lattice chiral effective field theory

Adiabatic projection method

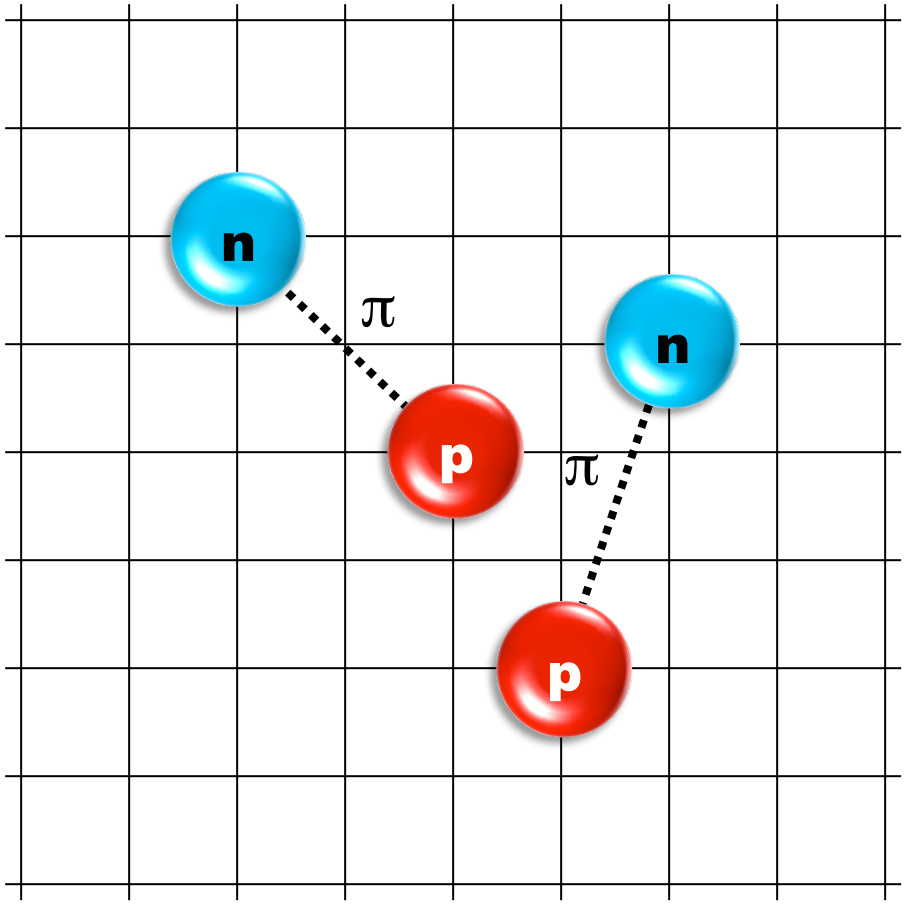
Pinhole algorithm

Nuclear binding near a quantum phase transition

Lattice chiral EFT interactions revisited

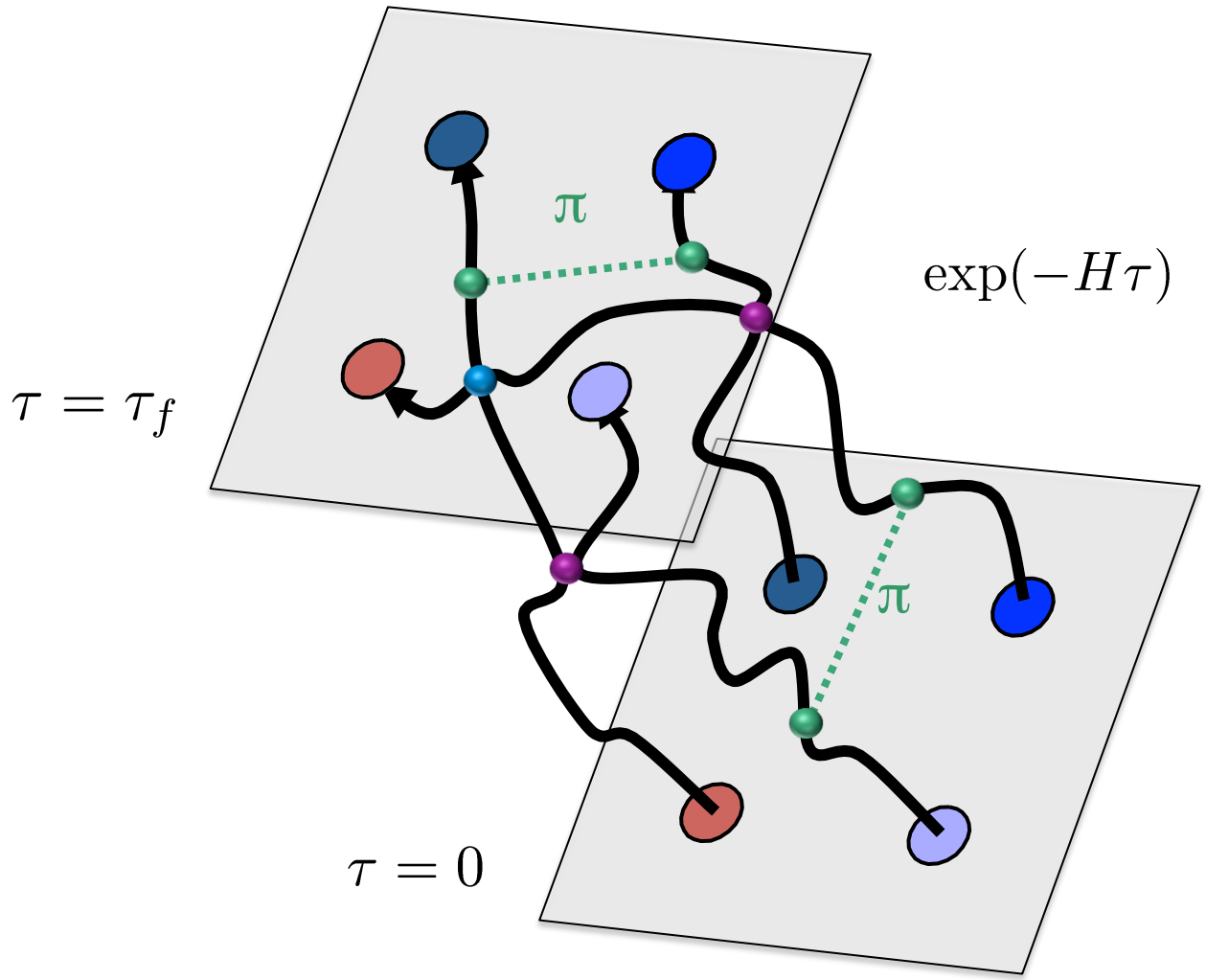
Summary and outlook

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



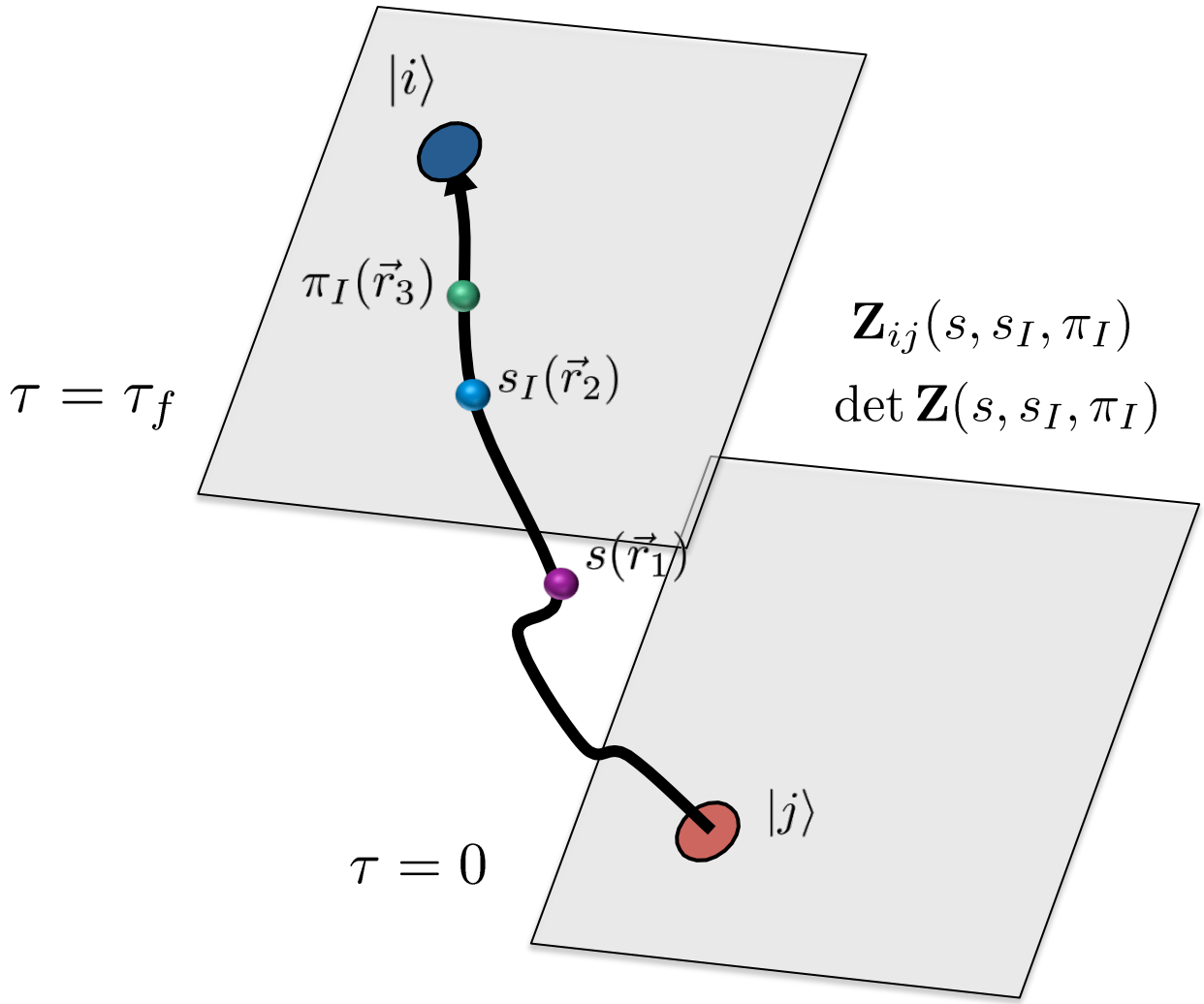
Auxiliary field method

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

$$\exp\left[-\frac{C}{2}(N^\dagger N)^2\right] \qquad \times \quad (N^\dagger N)^2$$

$$= \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-C}\, s(N^\dagger N)\right] \qquad \rangle \bullet \quad sN^\dagger N$$

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


$|i\rangle$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$s(\vec{r}_1)$
$|j\rangle$
$\tau = \tau_f$
$\tau = 0$
$\mathbf{Z}_{ij}(s, s_I, \pi_I)$
$\det \mathbf{Z}(s, s_I, \pi_I)$

Adiabatic projection method

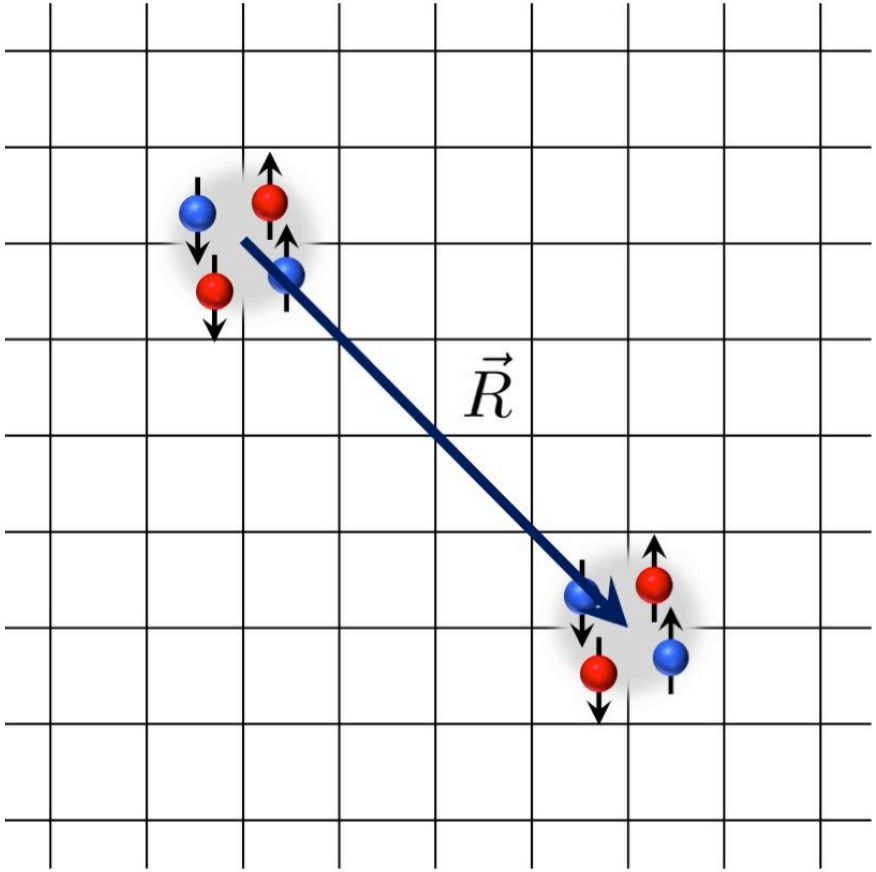
The adiabatic projection method a first principles method for scattering and reactions. It computes enough scattering information to construct an effective Hamiltonian.

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.

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 $\vec{R}$

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



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

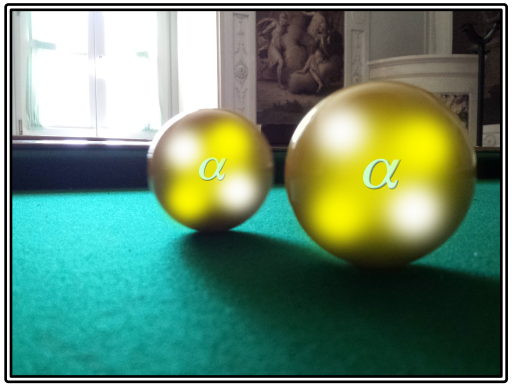
$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

Distortion and polarization of the nuclear wave functions are automatically produced by the Euclidean time projection.

As we increase the projection time, the adiabatic Hamiltonian exactly reproduces the low-energy spectrum of the full microscopic Hamiltonian. We can read off the scattering phase shifts for the asymptotic long-distance properties of the scattering wave functions.

Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, PRC 106, 054612, 2015
Elhatisari, D.L., PRC 90, 064001, 2014

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

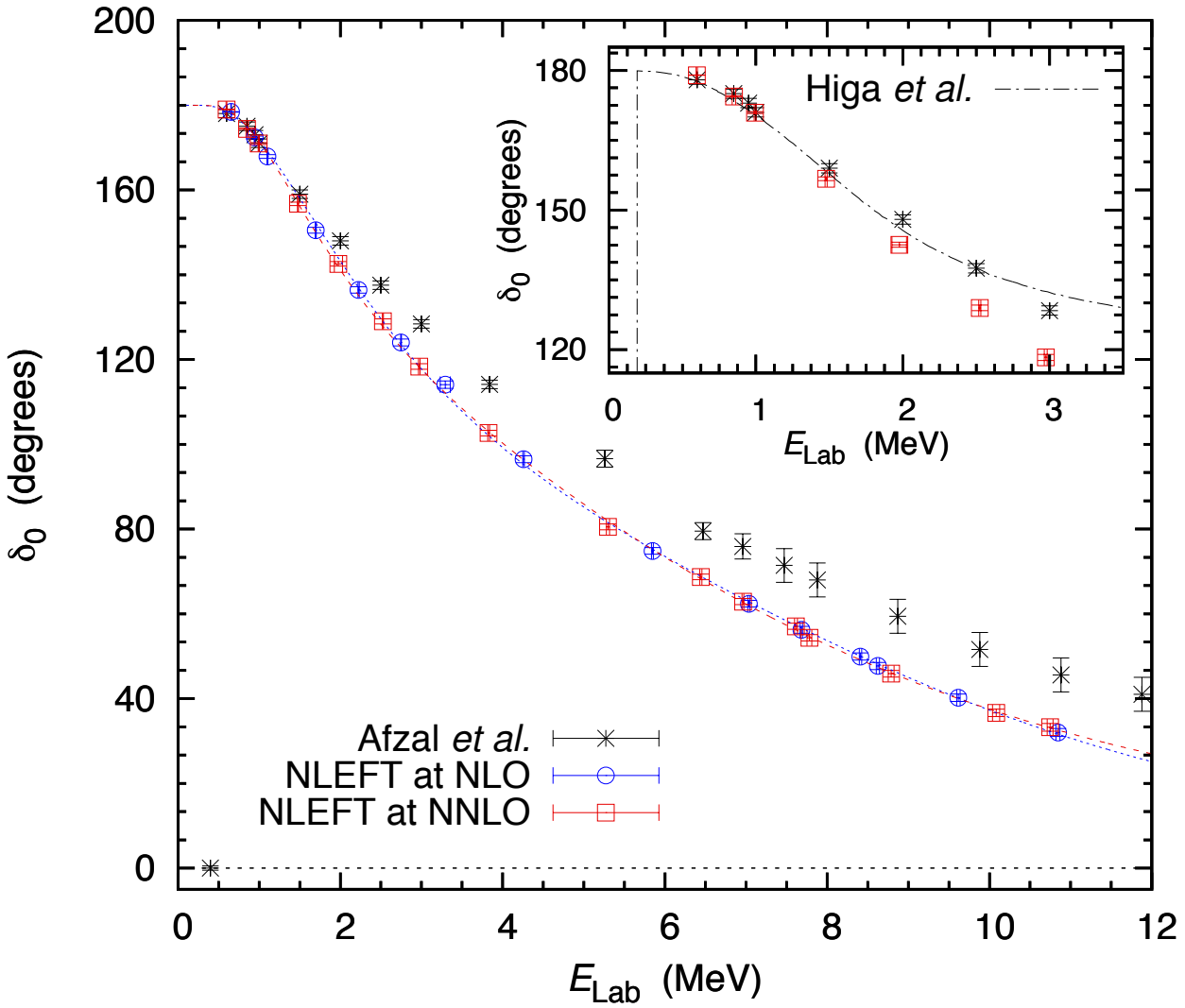


We present *ab initio* results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.

Using the adiabatic projection method, we performed lattice simulations for the S-wave and D-wave channels.

Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)

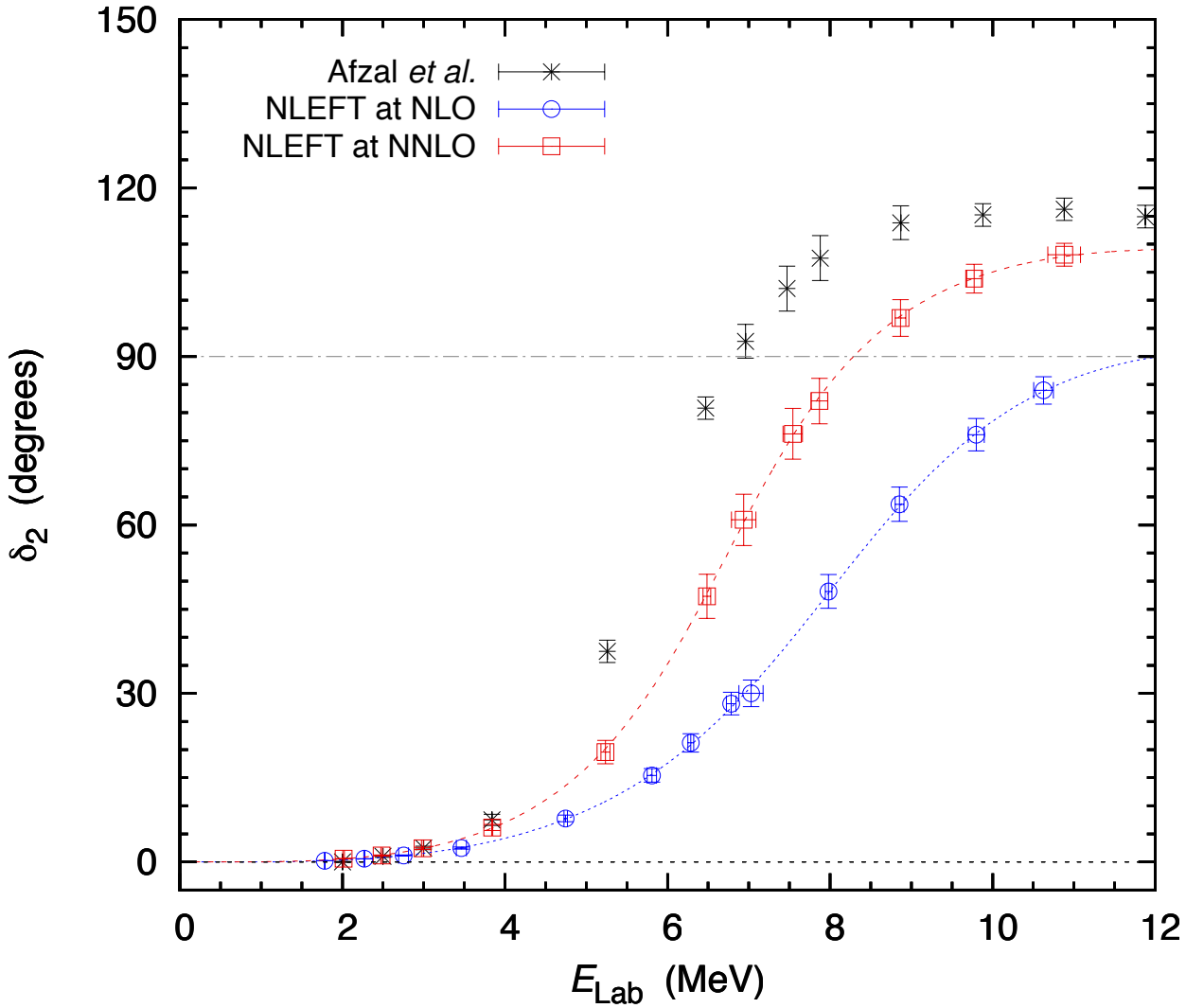
S-wave scattering



Afzal, Ahmad, Ali, RMP 41 247 (1969)

Higa, Hammer, van Kolck, NPA 809 171(2008)

D-wave scattering



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

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

We construct the normal-ordered A-body density operator

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

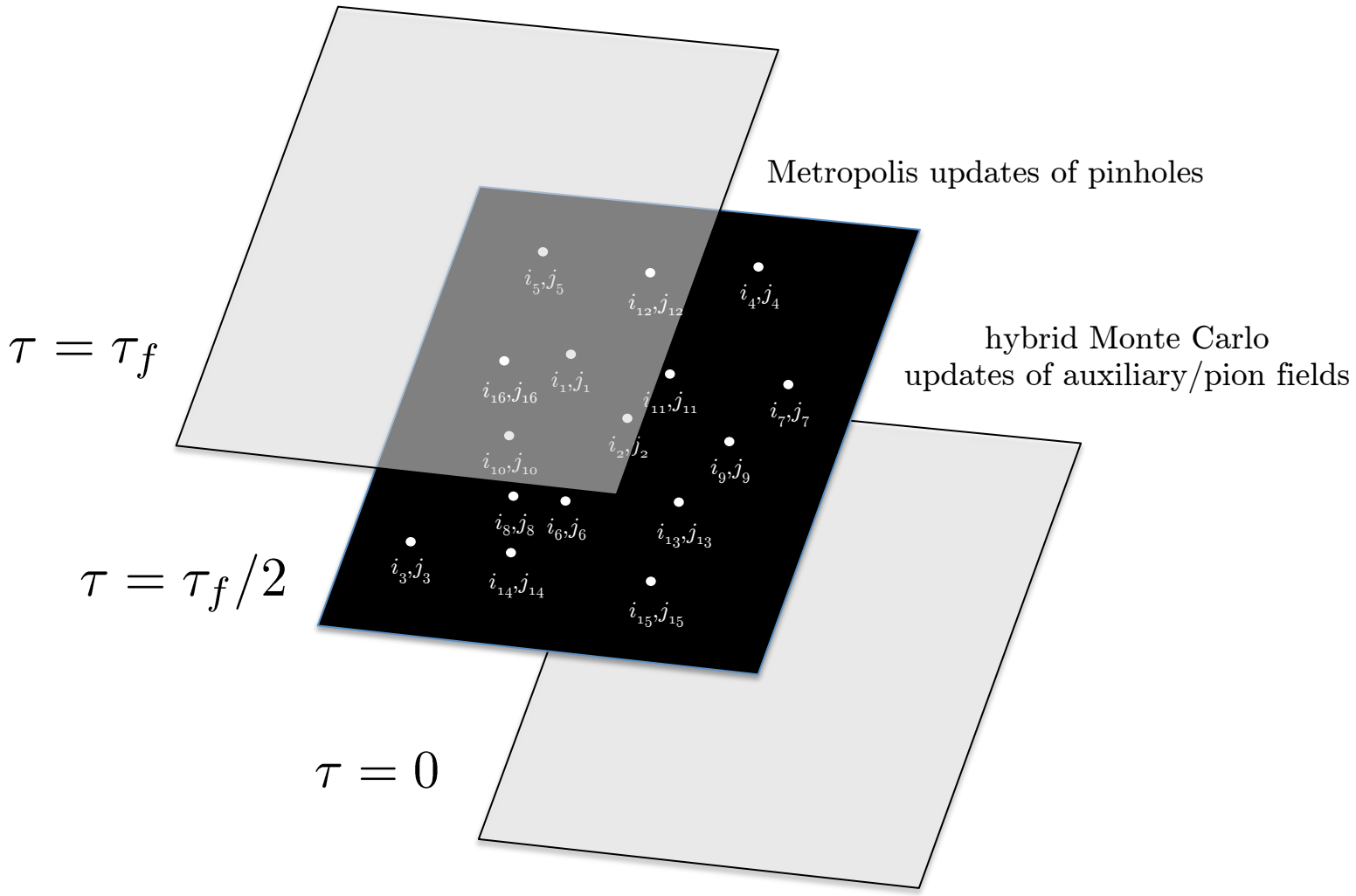
In the A-particle subspace, we have the identity

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

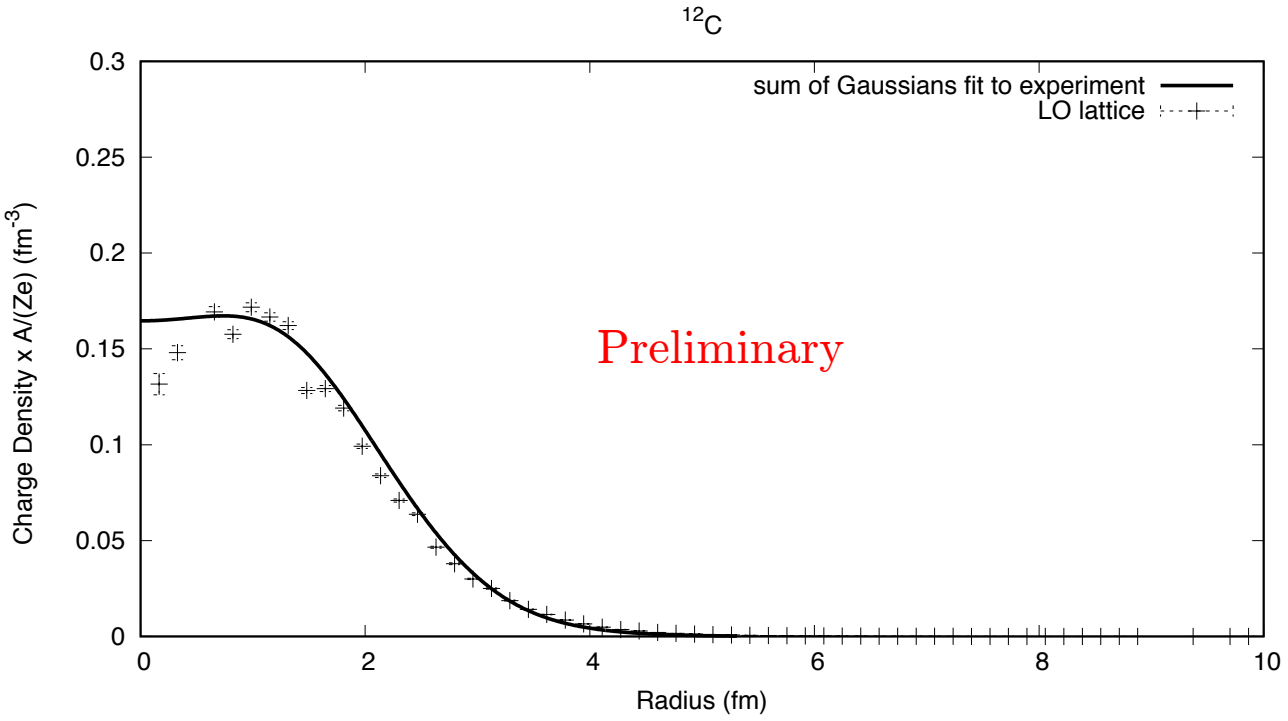
In the simulations we do Monte Carlo sampling of the amplitude

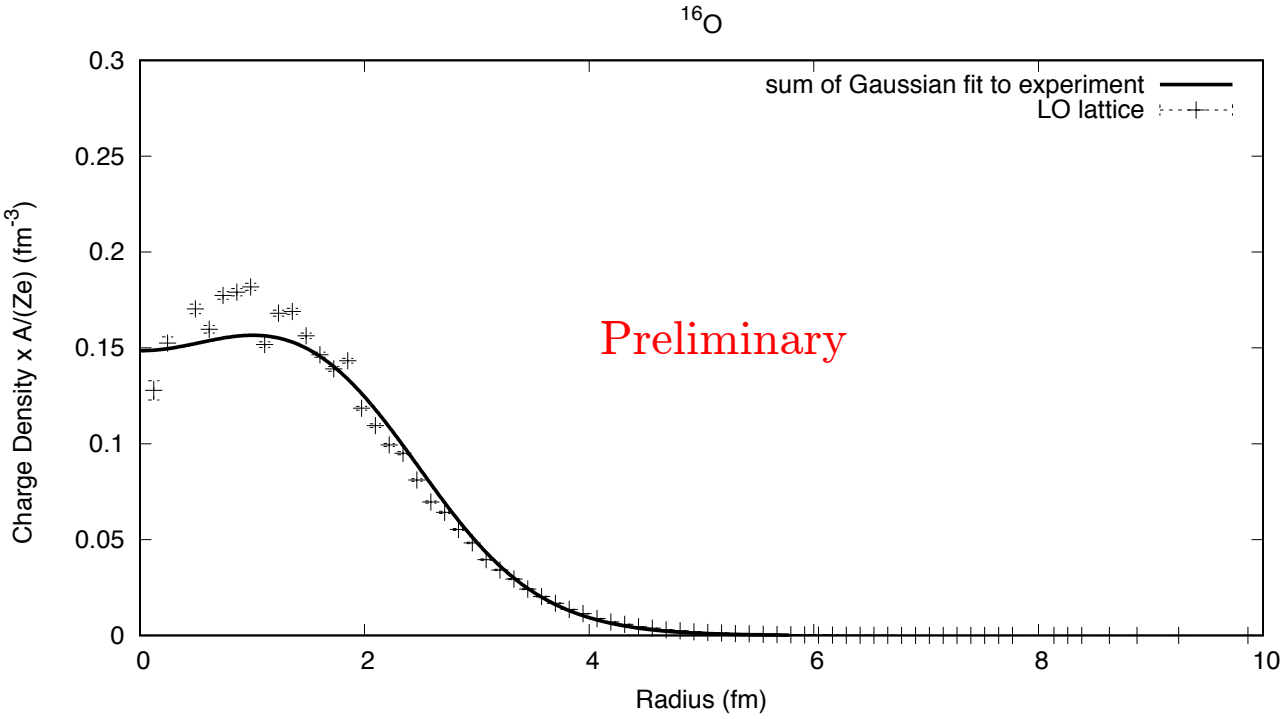
$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A, L_t) = \langle \Psi_I | M^{L_t/2} \rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) M^{L_t/2} | \Psi_I \rangle$$

Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Luu, Meißner, Rupak, in progress



Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Luu, Meißner, Rupak, in progress


^{12}C
sum of Gaussians fit to experiment
LO lattice
Preliminary
Charge Density x A/(Ze) (fm^{-3})
Radius (fm)
0.3
0.25
0.2
0.15
0.1
0.05
0
0
2
4
6
8
10


^{16}O
sum of Gaussian fit to experiment
LO lattice
Preliminary
Charge Density x A/(Ze) (fm^{-3})
Radius (fm)
0.3
0.25
0.2
0.15
0.1
0.05
0
0
2
4
6
8
10

Pinhole algorithm will be used to calculate density distributions, matrix elements of electric and magnetic multipole operators, form factors, and radiative capture reactions using the adiabatic projection method.

Can also be used to measure more complicated density correlations such as nuclear clustering. Currently working on a three-dimensional map of alpha clusters in the Hoyle state of ^{12}C.

Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Luu, Meißner, Rupak, in progress

Nuclear binding near a quantum phase transition

Interaction A (LO + Coulomb)

Nonlocal short-range interactions
One-pion exchange interaction
(+ Coulomb interaction)

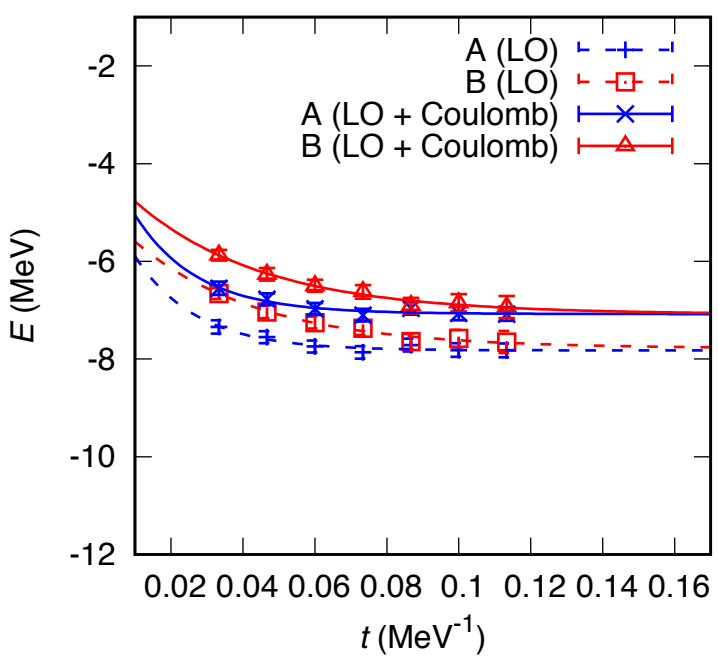
Interaction B (LO + Coulomb)

Nonlocal short-range interactions
Local short-range interactions
One-pion exchange interaction
(+ Coulomb interaction)

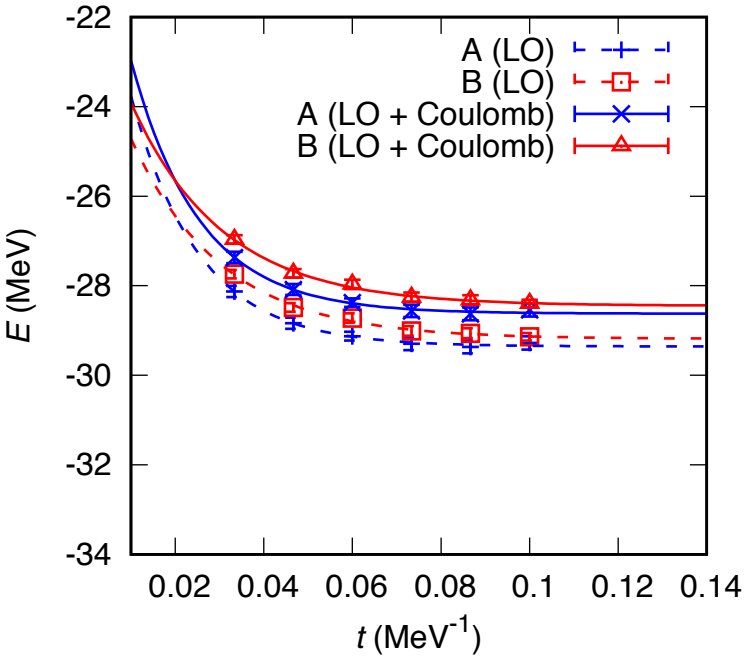
Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

Ground state energies

^{3}He

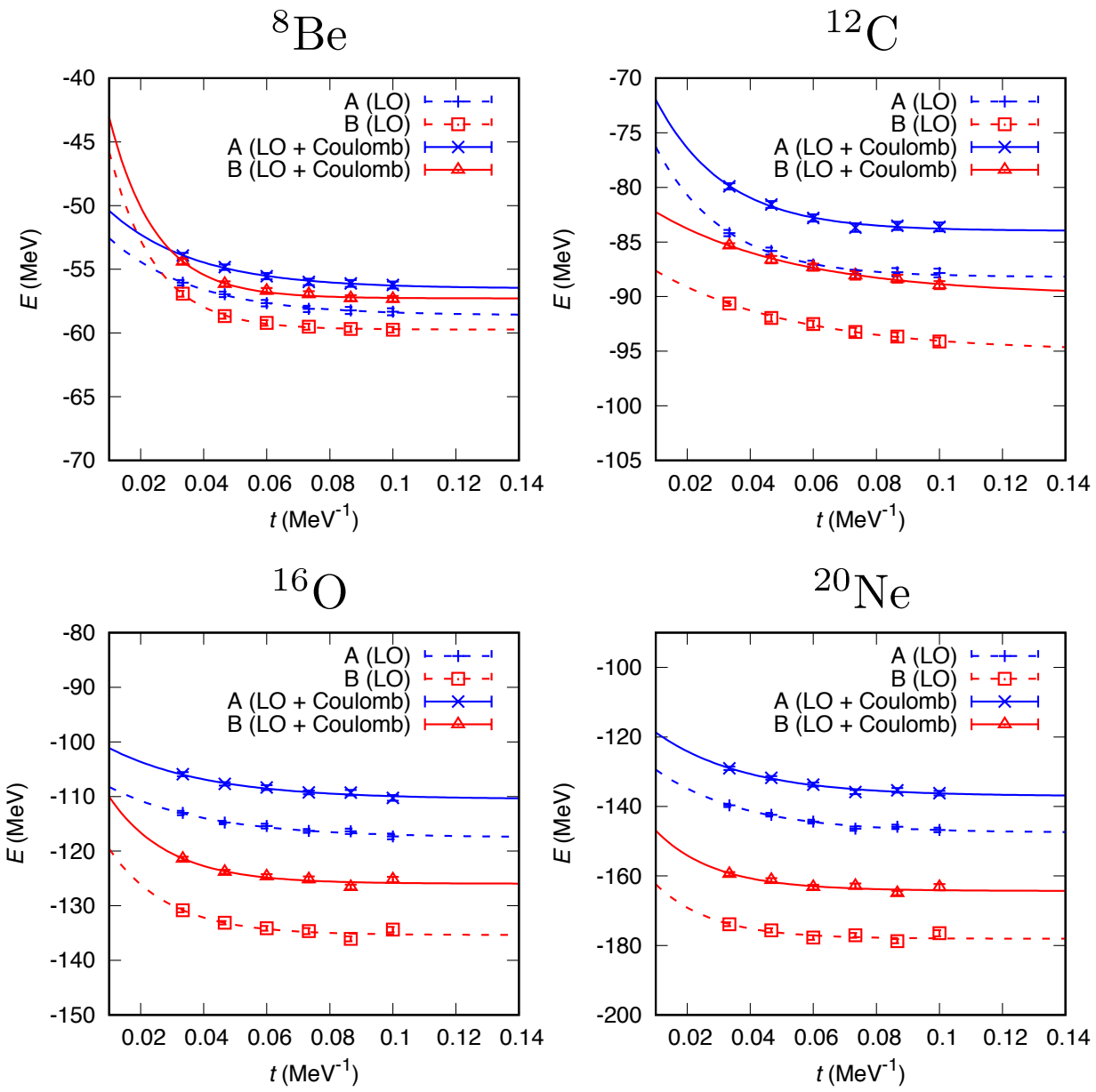


^{4}He



Both interactions significantly reduce the Monte Carlo sign oscillation problem.

Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
^{3}H	$-7.82(5)$	$-7.78(12)$	$-7.82(5)$	$-7.78(12)$	-8.482
^{3}He	$-7.82(5)$	$-7.78(12)$	$-7.08(5)$	$-7.09(12)$	-7.718
^{4}He	$-29.36(4)$	$-29.19(6)$	$-28.62(4)$	$-28.45(6)$	-28.296


^{8}Be
^{12}C
^{16}O
^{20}Ne
A (LO)
B (LO)
A (LO + Coulomb)
B (LO + Coulomb)
E (MeV)
t (MeV^{-1})

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

?

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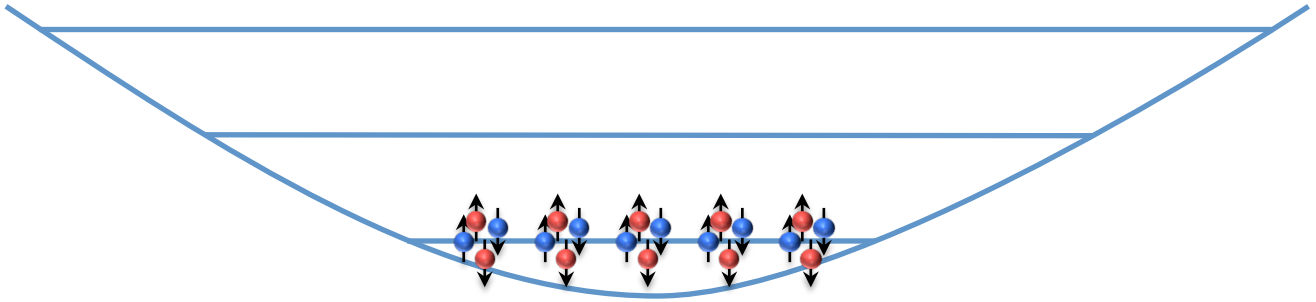
$$\frac{E_{^{8}\mathrm{Be}}}{E_{^{4}\mathrm{He}}} = 1.997(6)$$

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

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

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

Bose condensate of alpha particles!



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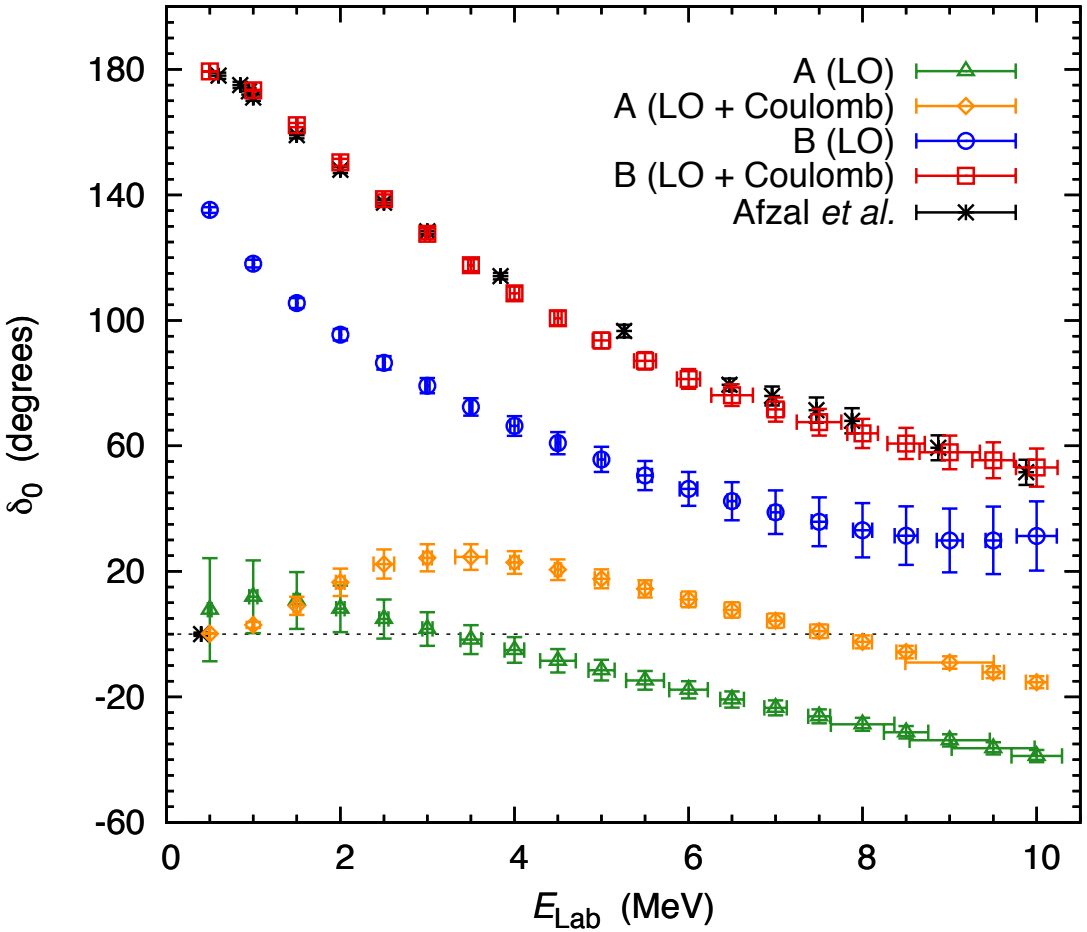
$$\frac{E_{^{20}\mathrm{Ne}}}{E_{^{4}\mathrm{He}}} = 5.03(3)$$

alpha-alpha S-wave scattering



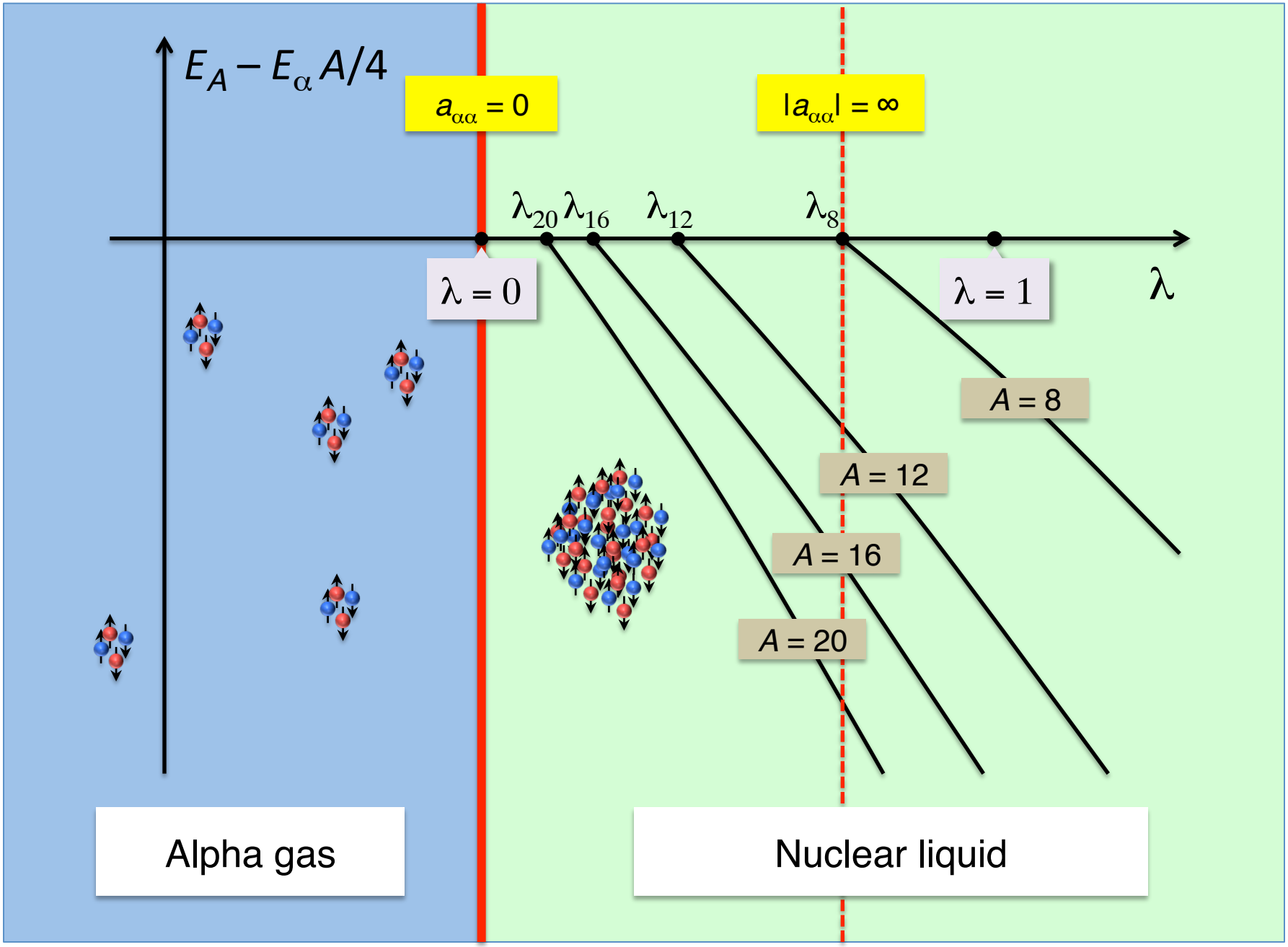
Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

Using the interactions A and B, we can define a one-parameter family of interactions

$$V_\lambda = (1-\lambda)V_\mathrm{A} + \lambda V_\mathrm{B}$$

In order to discuss the many-body limit, we turn off the Coulomb interaction and explore the zero-temperature phase diagram.

As a function of λ, there is a quantum phase transition at the point where the alpha-alpha scattering length vanishes. The transition is a first-order transition from a Bose-condensed gas of alpha particles to a nuclear liquid.


$E_A - E_\alpha A/4$
$a_{\alpha\alpha} = 0$
$|a_{\alpha\alpha}| = \infty$
λ_{20} λ_{16} λ_{12} λ_8
$\lambda = 0$
$\lambda = 1$
λ
$A = 8$
$A = 12$
$A = 16$
$A = 20$
Alpha gas
Nuclear liquid

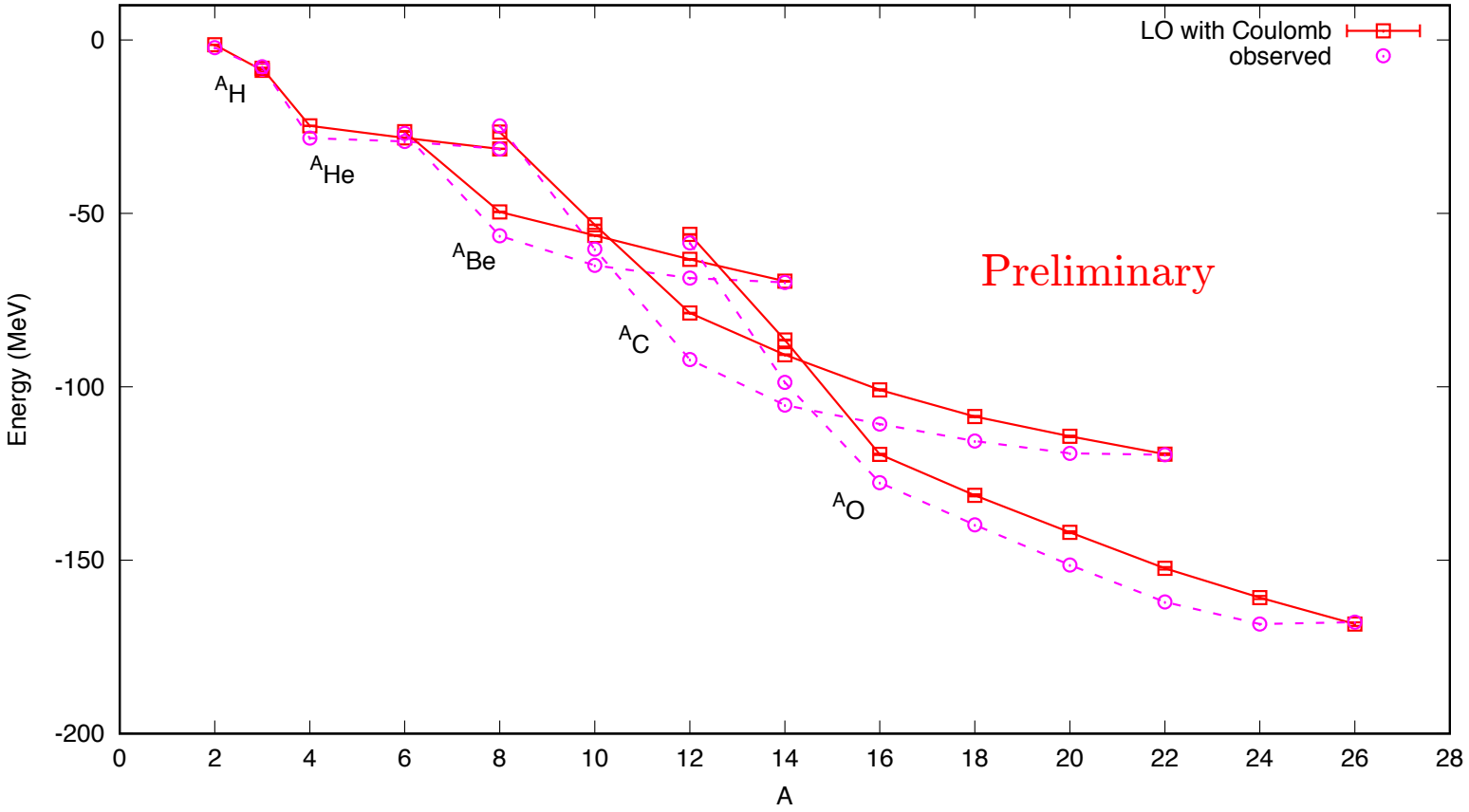
Unfortunately so far lattice simulations have mostly been restricted to nuclei with $N = Z$ due to Monte Carlo sign oscillations.

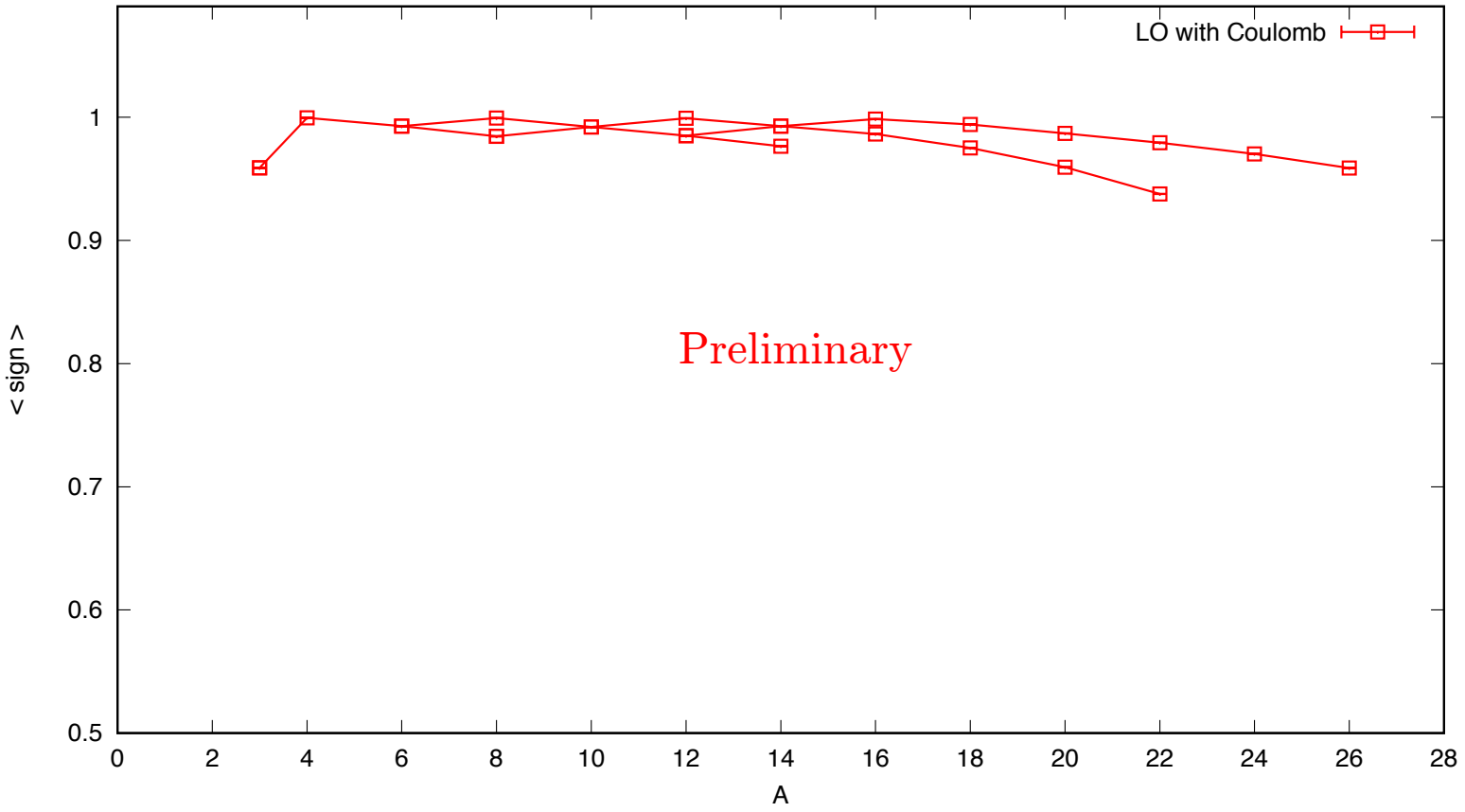
Lattice chiral EFT interactions revisited

With a better understanding of the connection between nuclear forces and nuclear structure, we are developing lattice chiral EFT interactions which should have better order-by-order convergence for a wide range of nuclear masses. We also reduce the Monte Carlo sign oscillations so that larger neutron- and proton-rich nuclei can be simulated.

We are currently coding the NN interactions up to order Q^4 and the NNN interaction up to order Q^3, with a planned extension to Q^4. But the results using only LO with Coulomb already look quite promising. At the very least, the additional corrections needed appear to be well within the domain of applicability of perturbation theory.

Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Luu, Meißner, Rupak, in progress


LO with Coulomb
observed
Preliminary
Energy (MeV)
A
0
-50
-100
-150
-200
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
AH
AHe
ABe
AC
AO


LO with Coulomb
Preliminary
< sign >
A
1
0.9
0.8
0.7
0.6
0.5
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28

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 recent development is the adiabiatic projection method for scattering and reactions. Another new 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.

Another 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.