Nuclear Structure and Reactions using Lattice Effective Field Theory

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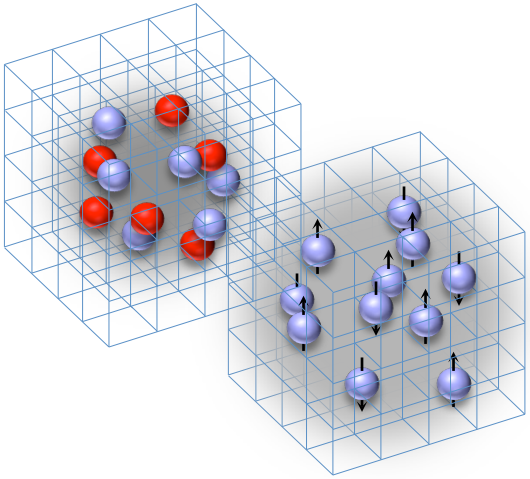
Nuclear Lattice EFT Collaboration



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Outline

Lattice effective field theory

Projection Monte Carlo with auxiliary fields

Adiabatic projection method

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

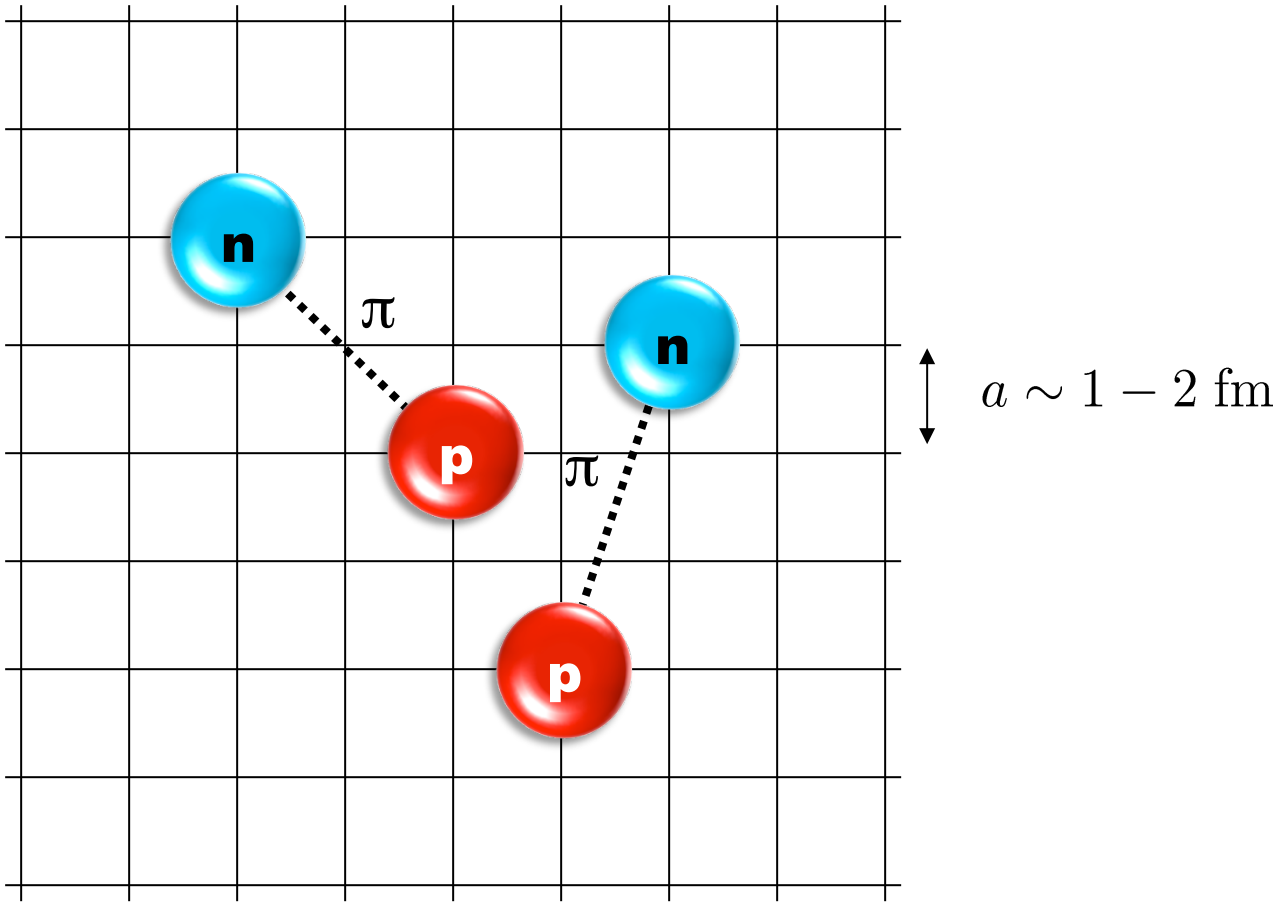
New lattice interactions

Quantum phase transition

Applications

The road forward

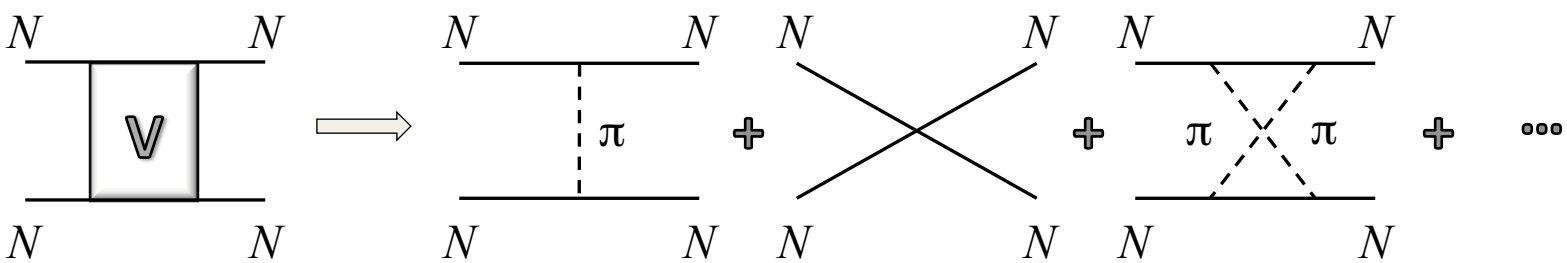
Lattice chiral effective field theory



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

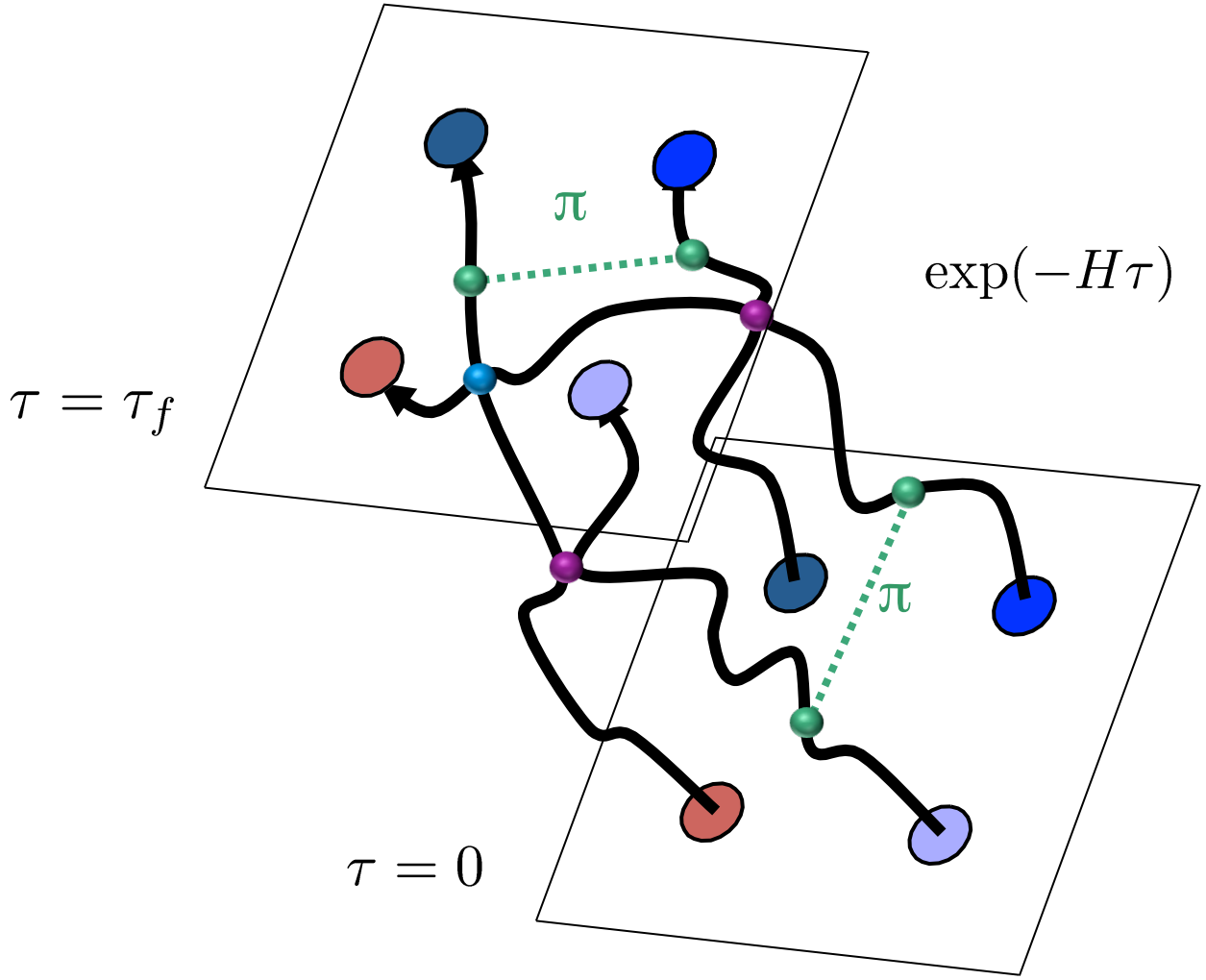
Chiral effective field theory

Construct the effective potential order by order



$$\underbrace{V^{\mathrm{OPEP}}\ \text{Contact interactions}}_{\text{Leading order (LO)}}\quad\underbrace{V^{\mathrm{TPEP}}}_{\text{Next-to-leading order (NLO)}}$$

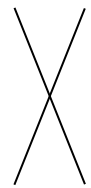
Euclidean time projection



Auxiliary field method

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

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

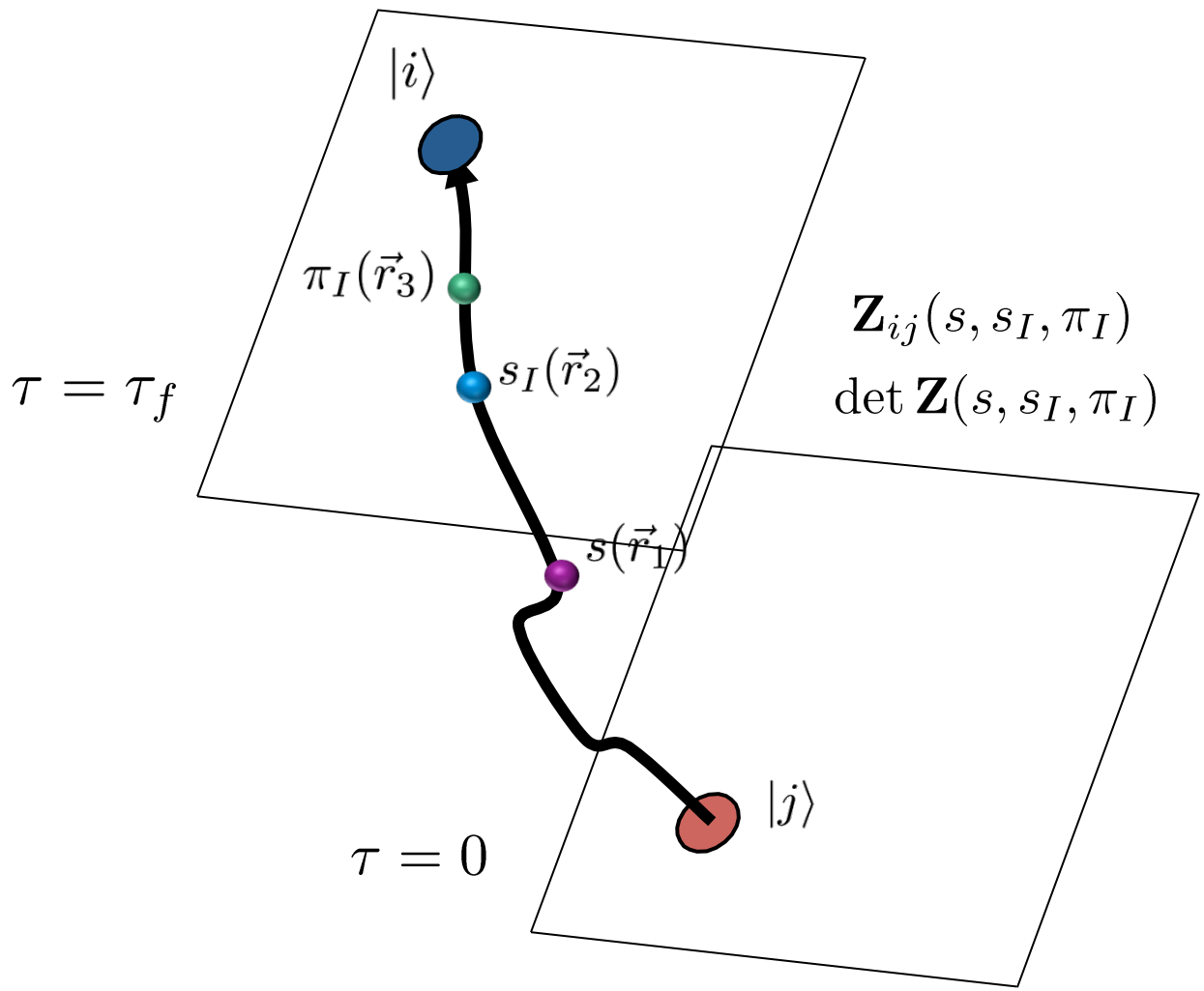


$$(N^\dagger N)^2$$

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

$$sN^\dagger N$$

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


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

Projection Monte Carlo with auxiliary fields

Let us consider a system with A particles. Projection Monte Carlo uses a given initial and final state. Often they are chosen to be the same state. The initial and final state will sandwich a product of a string of transfer matrices (normal-ordered exponential of Hamiltonian over one Euclidean time lattice spacing).

$$M =: \exp(-H\alpha_t): \quad \text{where} \quad \alpha_t = a_t/a$$

$$Z(L_t) = \langle \psi_{\text{init}} | \overbrace{\underbrace{\cdots}_{MMM}}^{\cdots} \overbrace{\underbrace{\cdots}_{MM}}^{\cdots} | \psi_{\text{init}} \rangle$$

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

$$Z(s, L_t) = \langle \psi_{\text{init}} | \overbrace{\boxed{}}^{M(s,L_t-1)M(s,L_t-2)\quad\cdots\quad M(s,1)M(s,0)} | \psi_{\text{init}} \rangle$$

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

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

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

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

In the projection Monte Carlo calculation we compute the amplitude

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

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

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

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

So now we want to compute the following ratio for large L_t:

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

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

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 reduce the noise/signal in the energy calculations, we set up a Markov chain Monte Carlo process where we importance sample according to $|Z(s, L_t)|$ and measure $Z(s, L_t - 1)$ as well as the phase of $Z(s, L_t)$. We use hybrid Monte Carlo for the updates.

For discussion: Can a similar importance sampling be used in lattice QCD calculations? Perhaps one can start with a simple observable such as the pion correlation function.

Adiabatic projection method

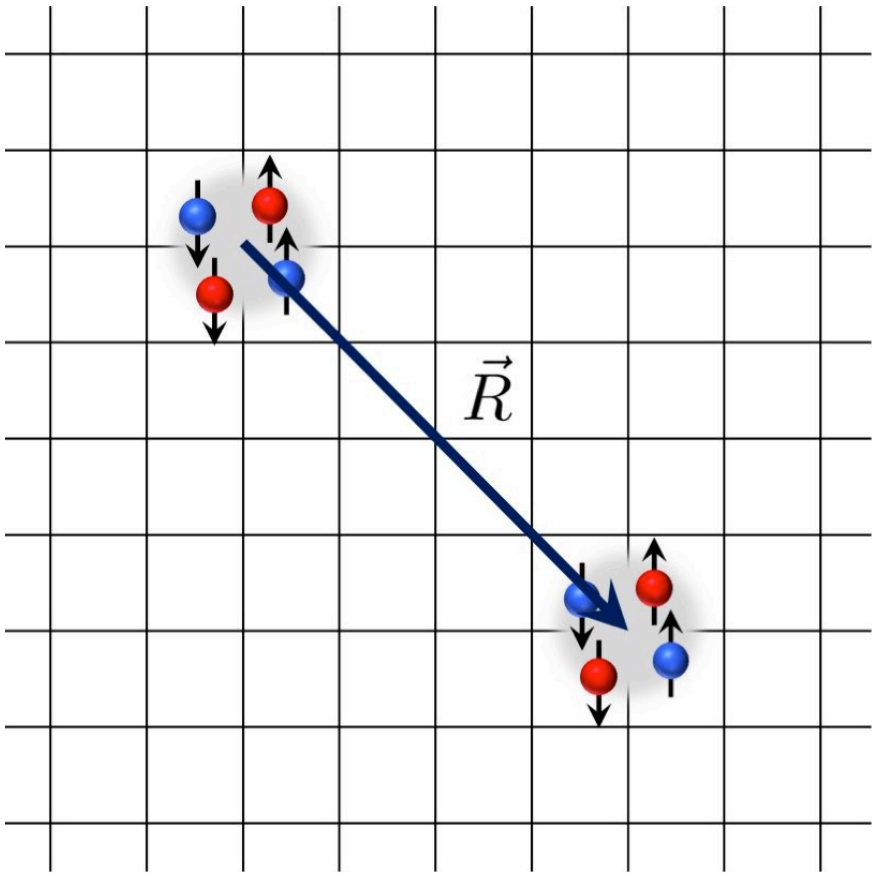
Zohreh gave a nice talk at this KITP program about Lüscher's finite volume method. The adiabatic projection method is another first principles method for scattering and reactions. It computes enough scattering information to construct an effective Hamiltonian. This makes the calculation robust when finite-volume energy differences are too small too measure accurately.

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 time 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 $\vec{R}$

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



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.

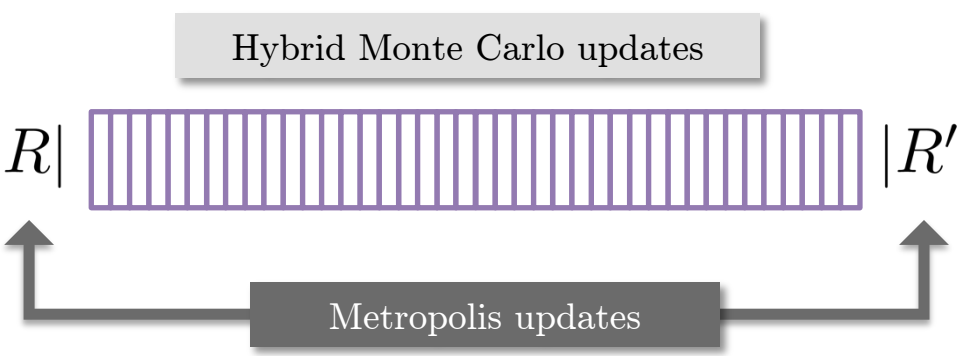
Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, PRC 106, 054612, 2015
Elhatisari, D.L., PRC 90, 064001, 2014
Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)

We use projections onto spherical harmonics defined on sets of lattice points with the same distance from the origin.

$$|R\rangle^{L,L_z} = \sum_{\vec{R}'} Y_{L,L_z}(\hat{R}')\delta_{R,|\vec{R}'|}|\vec{R}'\rangle$$

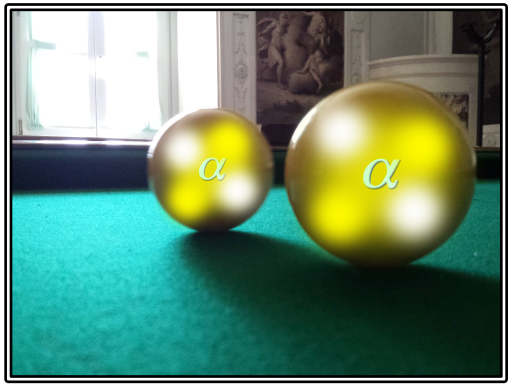
We then do auxiliary field updates as well as initial/final state Monte Carlo updates

$$[Z_{n_t,\mathrm{LO}}]^{L,L_z}_{R,R'} = {}^{L,L_z}\langle R|$$



$$|R'\rangle^{L,L_z}$$

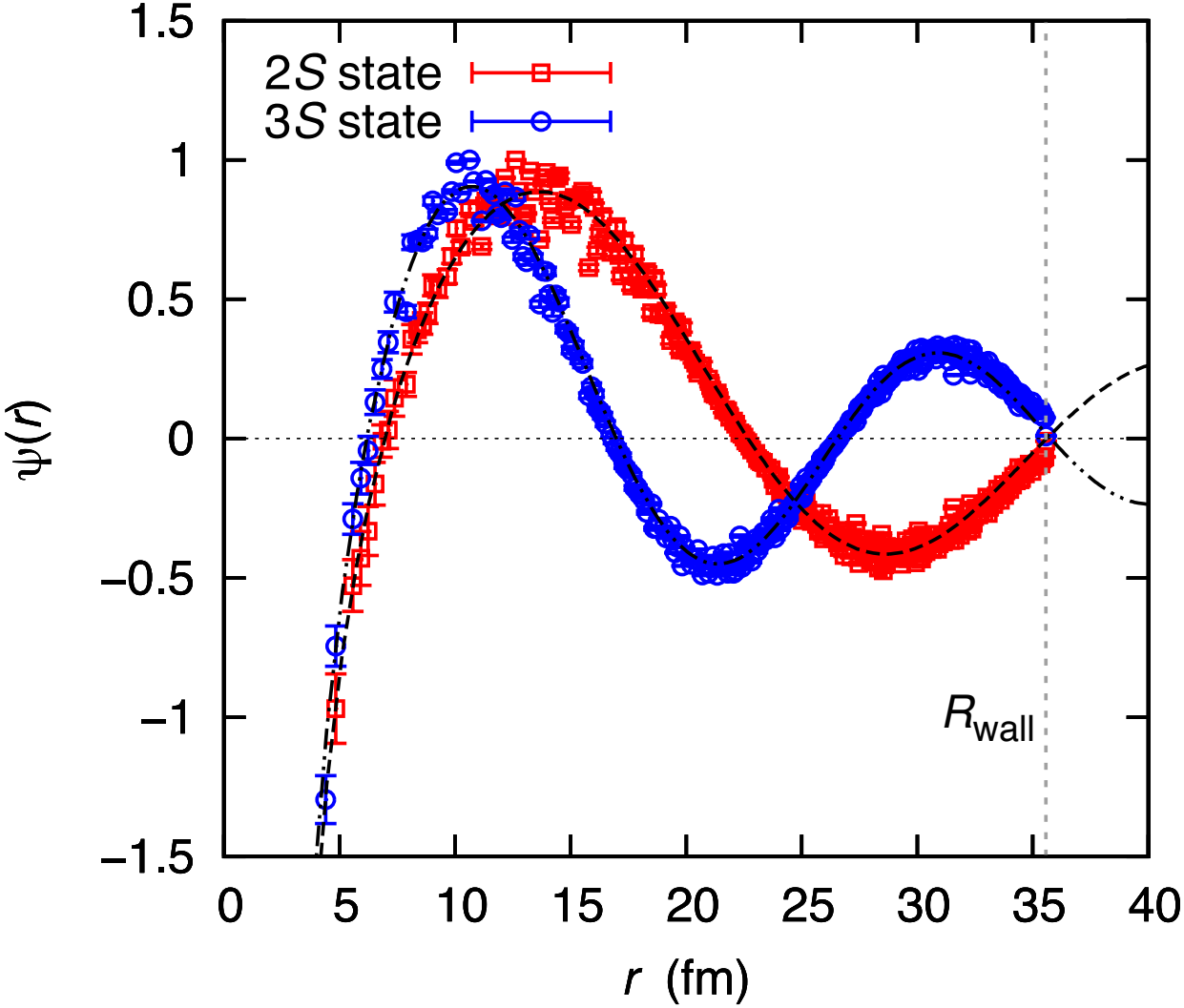
$^4\mathrm{He} + {}^4\mathrm{He} \to {}^4\mathrm{He} + {}^4\mathrm{He}$



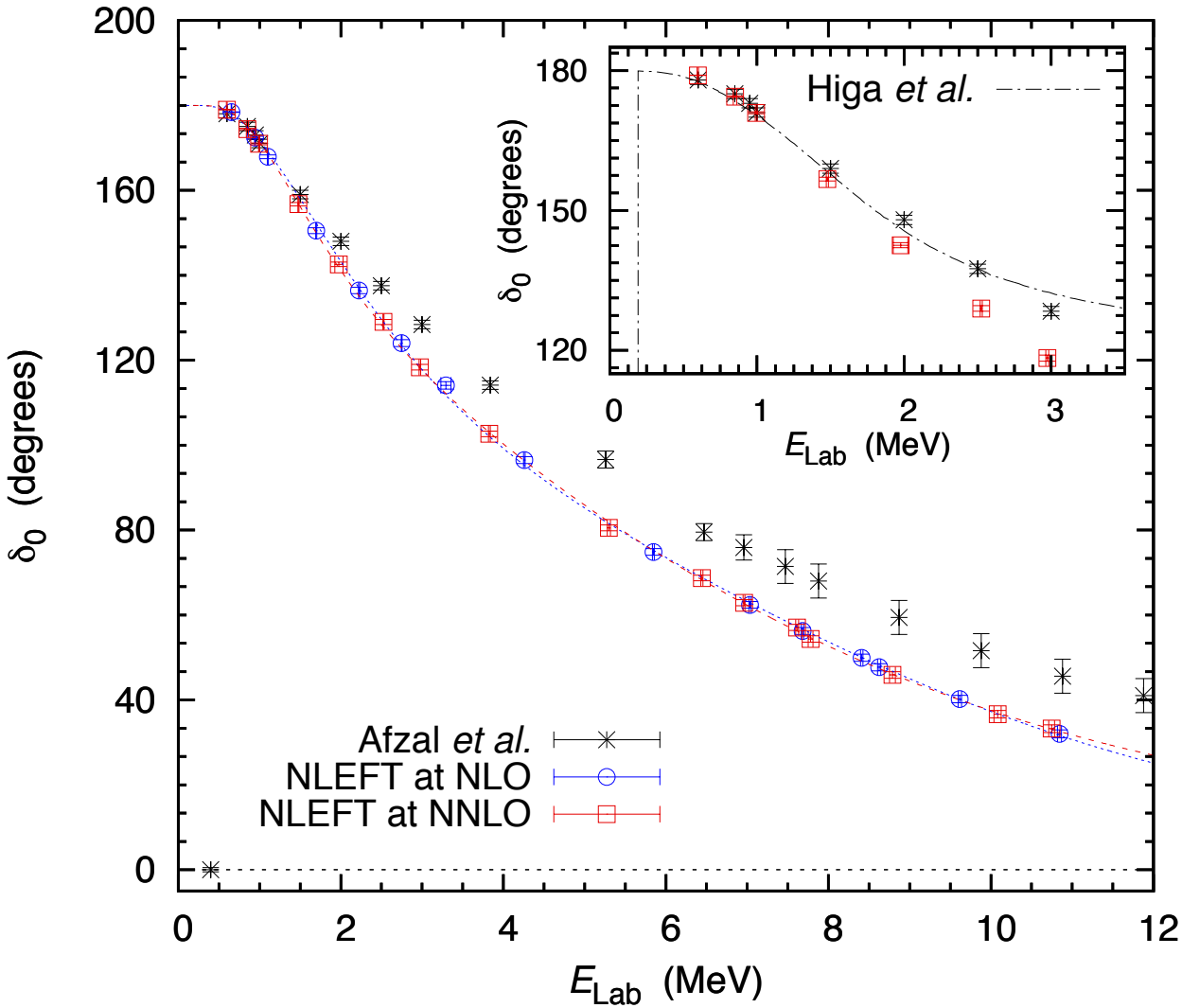
We now present *ab initio* results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.

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)


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

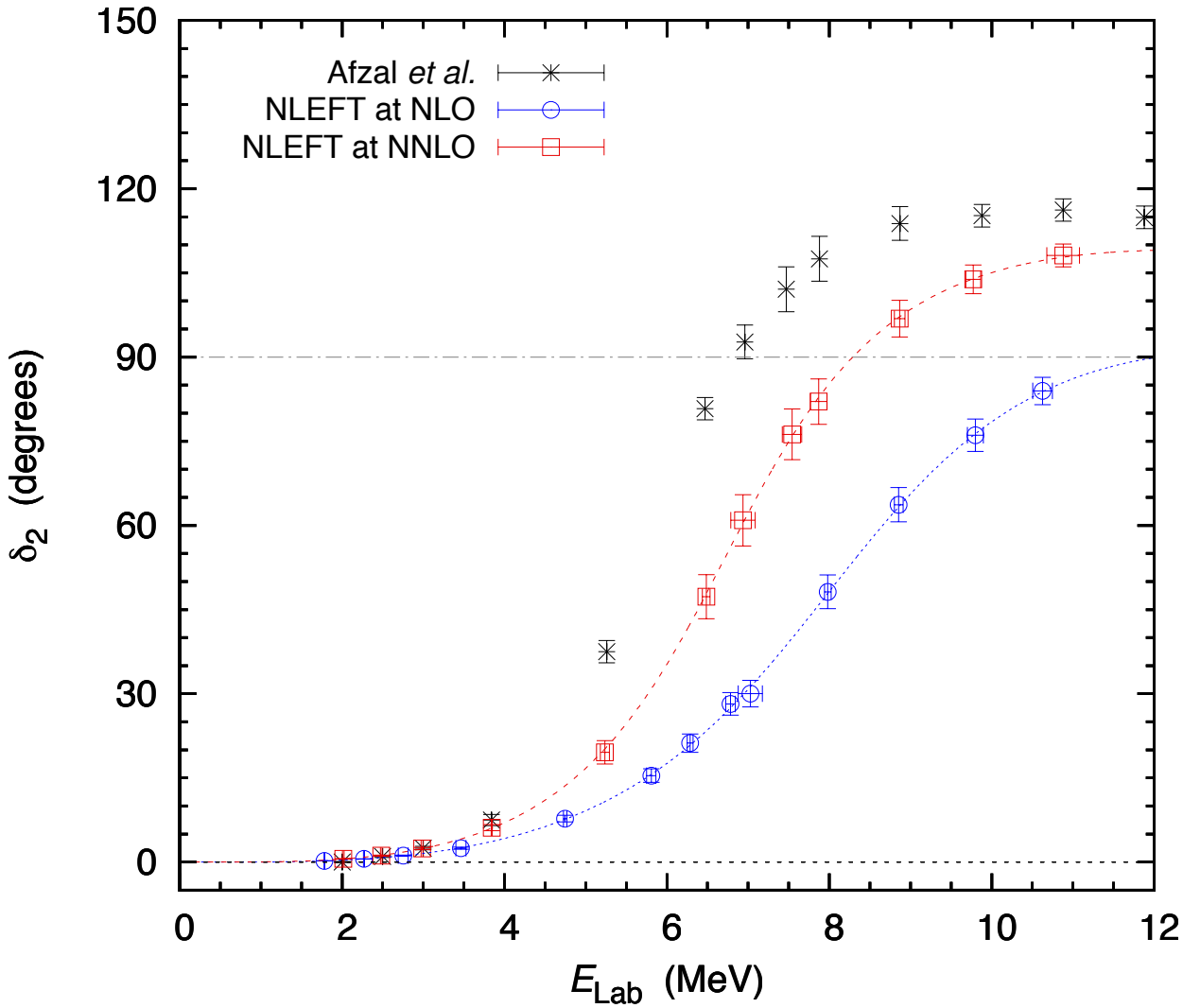
S-wave scattering



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

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

D-wave scattering



More work needs to be done. But alpha processes now appear to be in reach of *ab initio* methods.

For an A_1-body + A_2-body scattering or reaction process the computational scaling is typically $\sim (A_1 + A_2)^2$.

For mass and charge transfer processes, we do the same steps but consider coupled channel scattering. For capture reactions, we include one-photon matrix elements and compute overlaps between bound states and scattering states.

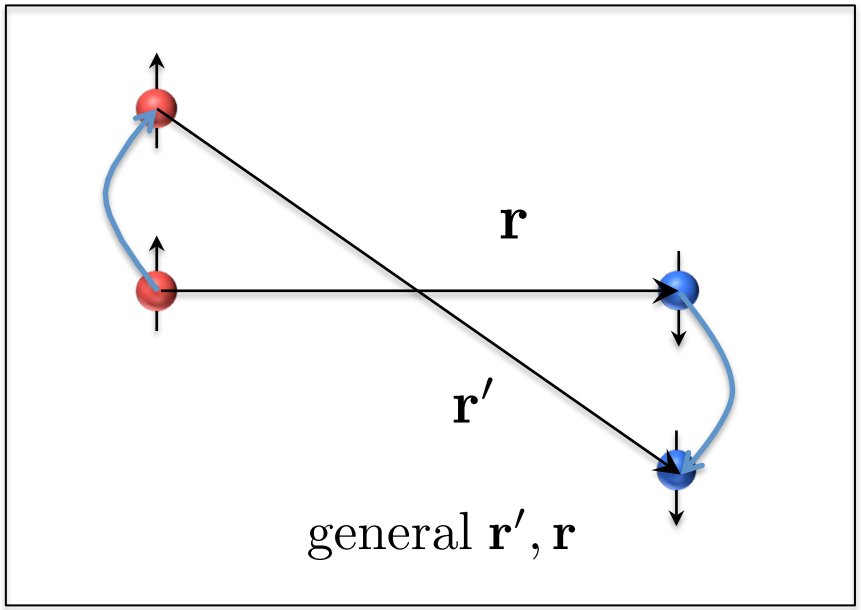
Rupak, D.L., PRL 111 032502 (2013)

For discussion: How can the adiabatic projection method be applied to lattice QCD calculations for hadronic scattering and reactions?

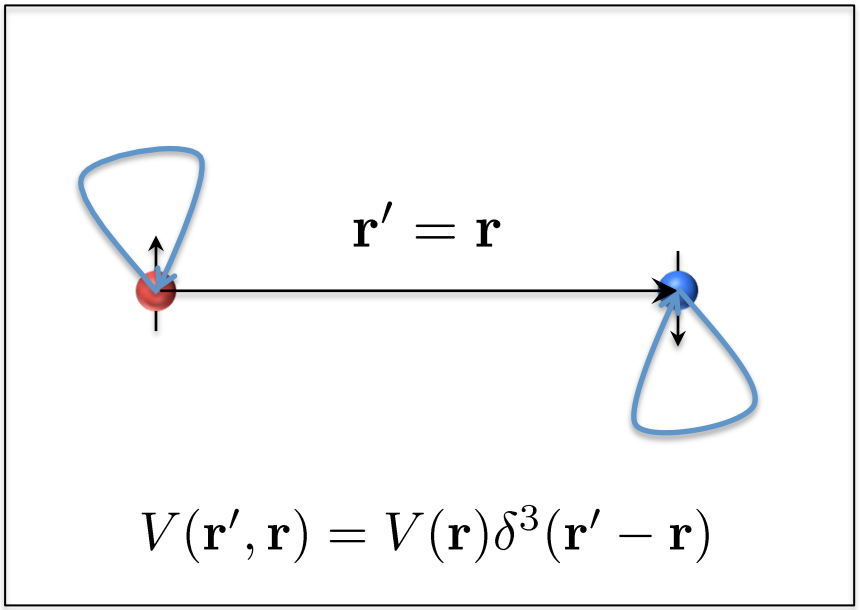
New lattice interactions

$$V(\mathbf{r}', \mathbf{r})$$

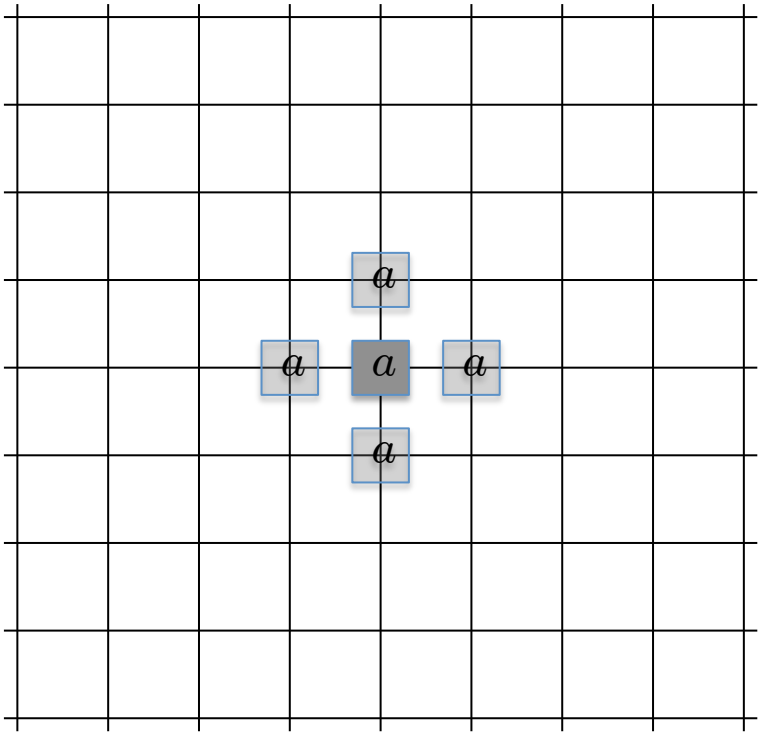
Nonlocal interaction



Local interaction



Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, arXiv:1602.04539, Phys. Rev. Lett. in press



$$a_{\mathrm{NL}}(\mathbf{n}) = a(\mathbf{n}) + s_{\mathrm{NL}} \sum_{\langle \mathbf{n}' \, \mathbf{n} \rangle} a(\mathbf{n}')$$

$$a^{\dagger}_{\mathrm{NL}}(\mathbf{n}) = a^{\dagger}(\mathbf{n}) + s_{\mathrm{NL}} \sum_{\langle \mathbf{n}' \, \mathbf{n} \rangle} a^{\dagger}(\mathbf{n}')$$

Nonlocal density operators

$$\rho_{\rm NL}(\mathbf{n}) = a^\dagger_{\rm NL}(\mathbf{n}) a_{\rm NL}(\mathbf{n})$$
$$\rho_{I,{\rm NL}}(\mathbf{n}) = a^\dagger_{\rm NL}(\mathbf{n})[\tau_I] a_{\rm NL}(\mathbf{n})$$

Nonlocal S-wave interactions

$$V_{\rm NL} = \tfrac{c_{\rm NL}}{2} \sum_{\mathbf{n}} : \rho_{\rm NL}(\mathbf{n})\rho_{\rm NL}(\mathbf{n}) : + \tfrac{c_{I,{\rm NL}}}{2} \sum_{\mathbf{n},I} : \rho_{I,{\rm NL}}(\mathbf{n})\rho_{I,{\rm NL}}(\mathbf{n}) :$$

We can simulate using auxiliary fields

$$V^s_{\rm NL} = \sqrt{-c_{\rm NL}} \sum_{\mathbf{n}} \rho_{\rm NL}(\mathbf{n}) s(\mathbf{n}) + \sqrt{-c_{I,{\rm NL}}} \sum_{\mathbf{n},I} \rho_{I,{\rm NL}}(\mathbf{n}) s_I(\mathbf{n})$$

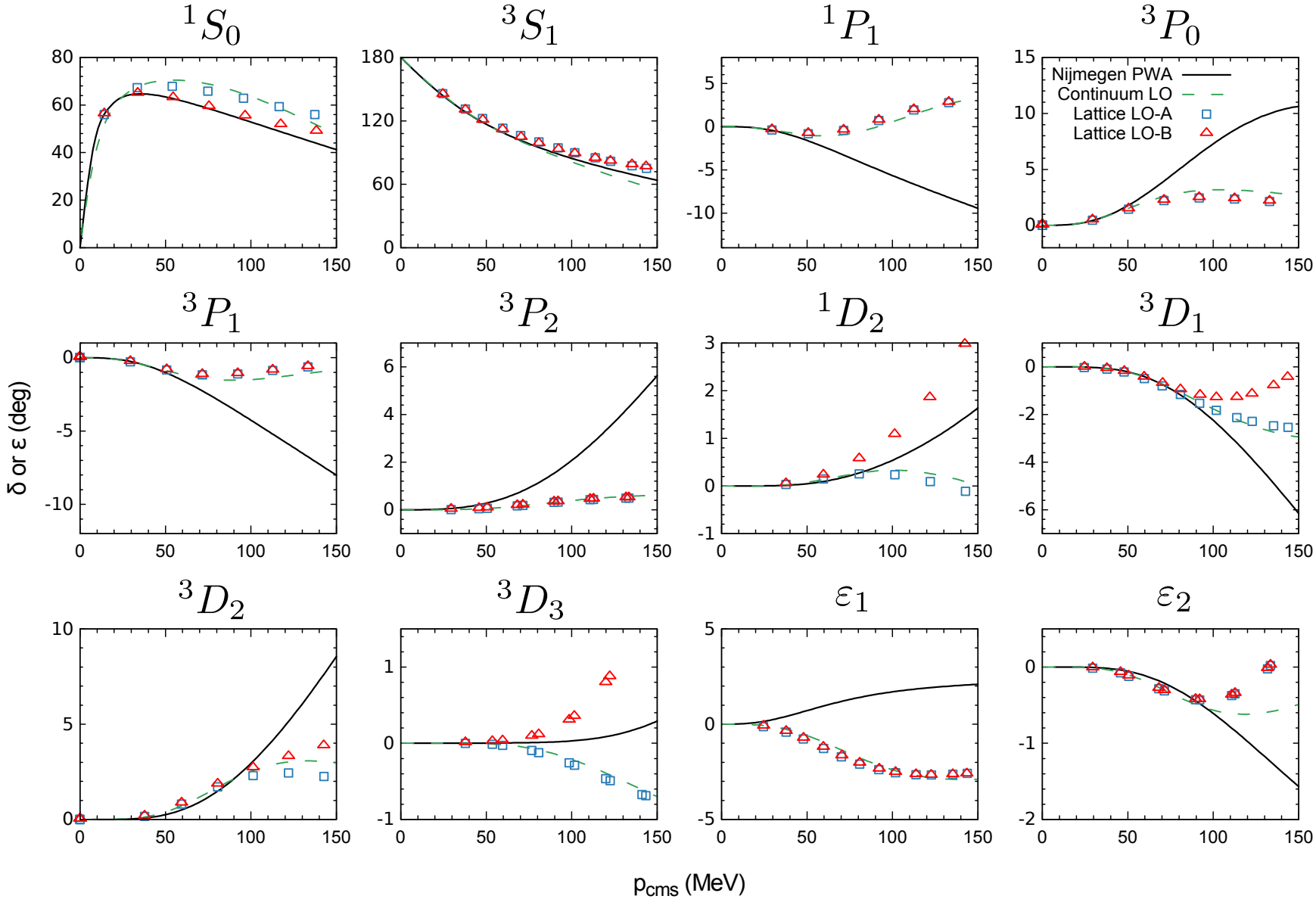
Interaction A at LO (LO + Coulomb)

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

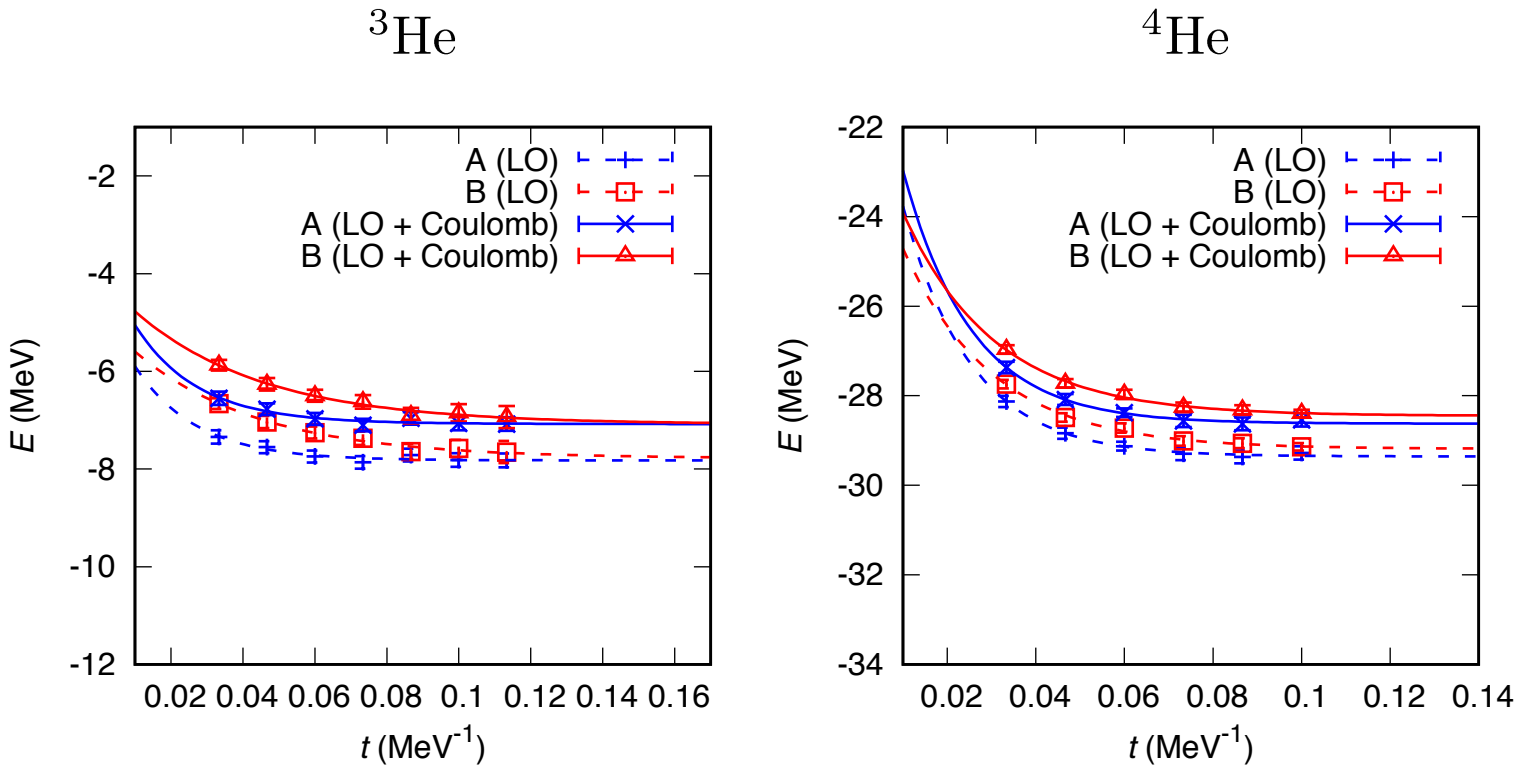
Interaction B at LO (LO + Coulomb)

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

Details of how the interactions are fitted described later in the discussion.

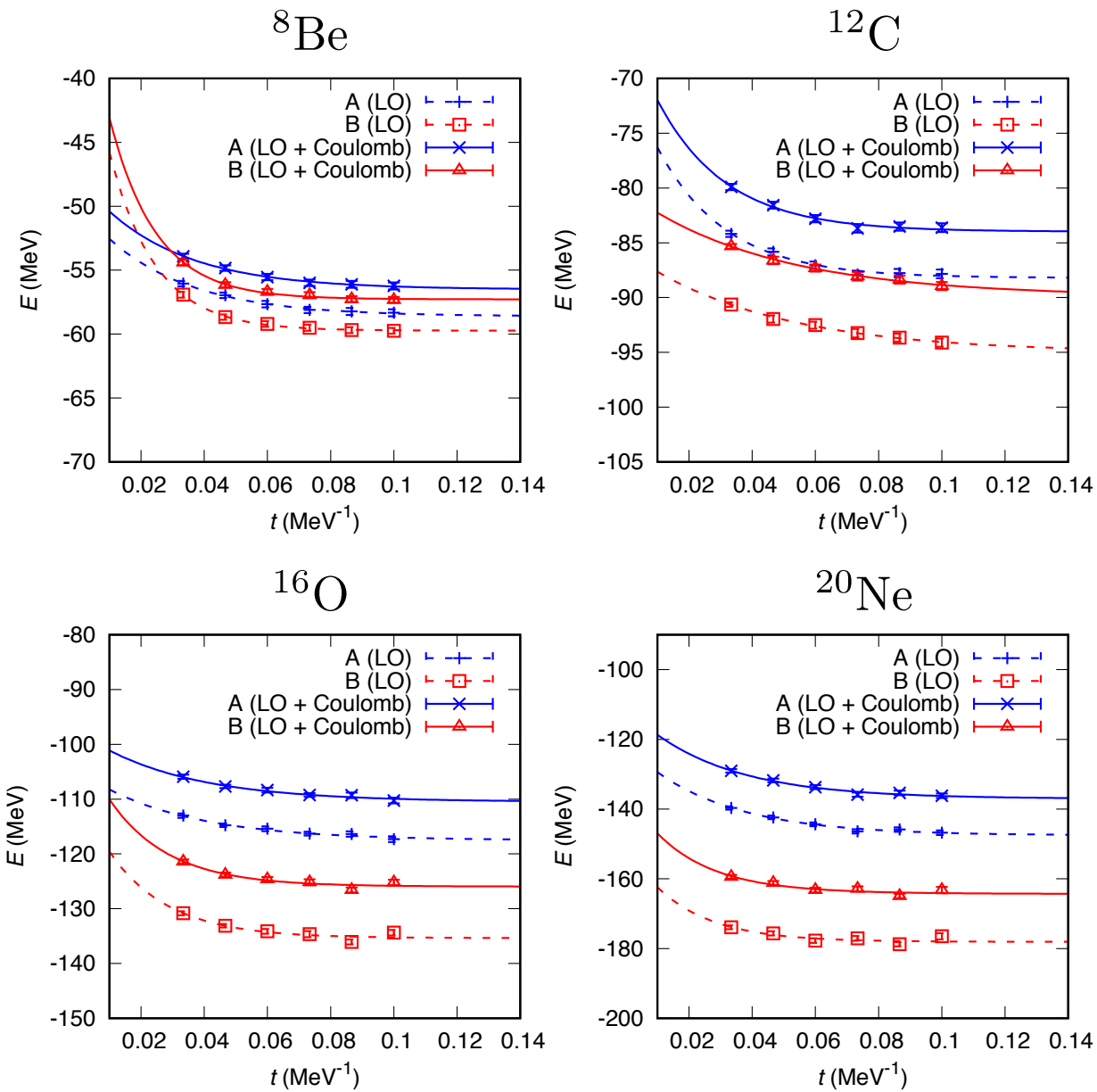

$^1S_0$
$^3S_1$
$^1P_1$
$^3P_0$
$^3P_1$
$^3P_2$
$^1D_2$
$^3D_1$
$^3D_2$
$^3D_3$
ε_1
ε_2
Nijmegen PWA
Continuum LO
Lattice LO-A
Lattice LO-B
δ or ε (deg)
p_{cms} (MeV)

Ground state energies



Both interactions significantly reduce the Monte Carlo sign oscillation problem, the original motivation for studying the different interactions.

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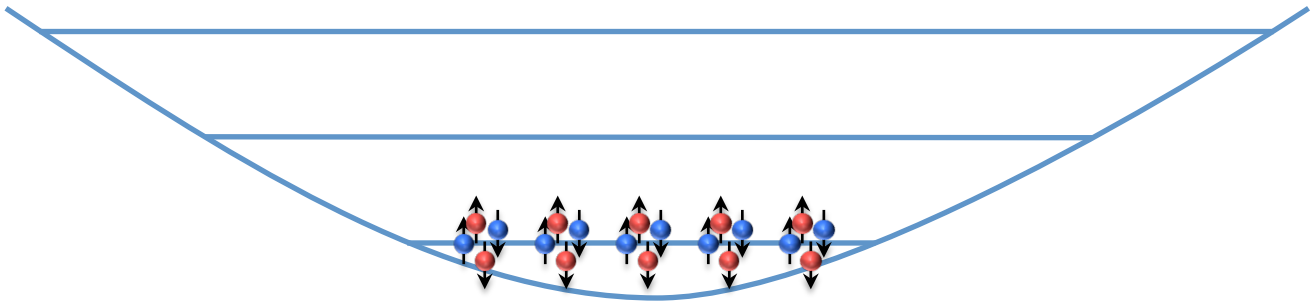
$$\frac{E_{^{8}\mathrm{Be}}}{E_{^{4}\mathrm{He}}} = 1.997(6)$$

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

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

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

Bose condensate of alpha particles!



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^{20}Ne	−148(1)	−178(1)	−137(1)	−164(1)	−160.645

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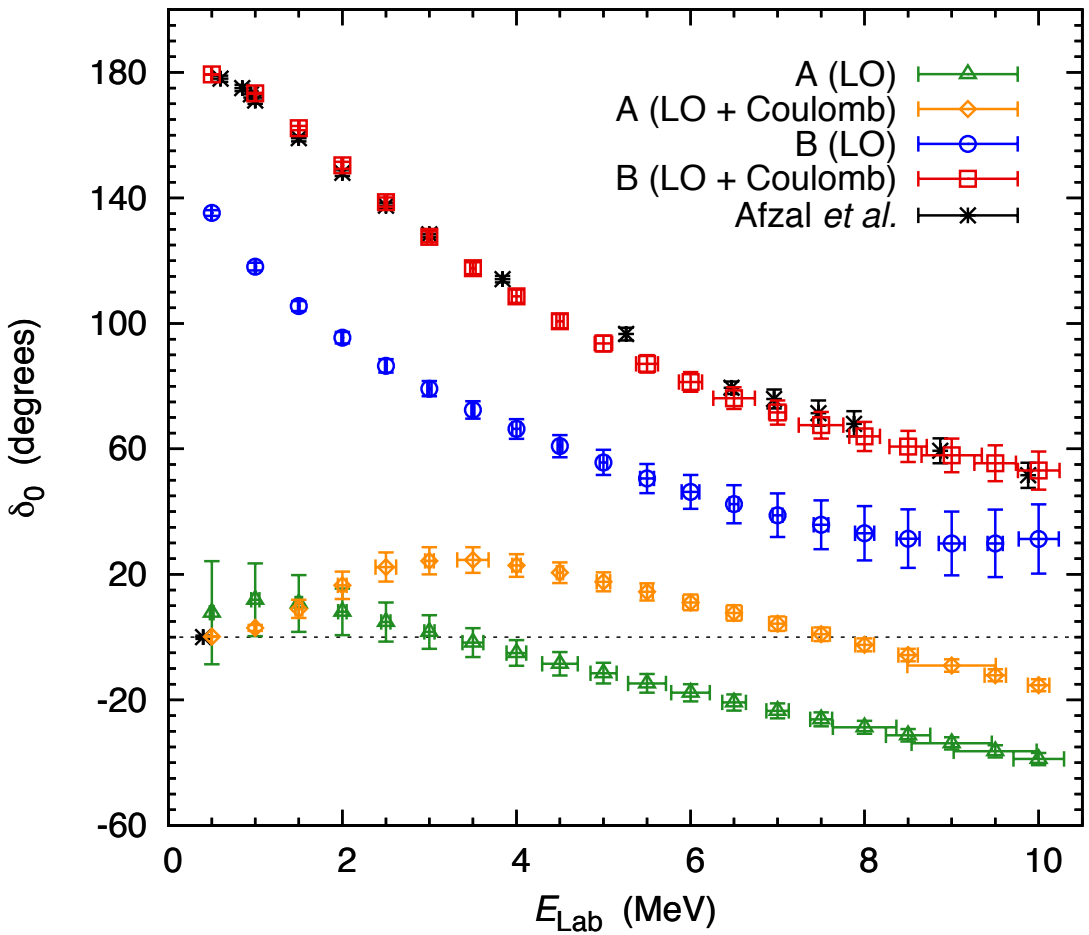
alpha-alpha S-wave scattering



Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, arXiv:1602.04539, Phys. Rev. Lett. in press

Interaction B was tuned to the nucleon-nucleon phase shifts, deuteron energy, and alpha-alpha phase shifts.

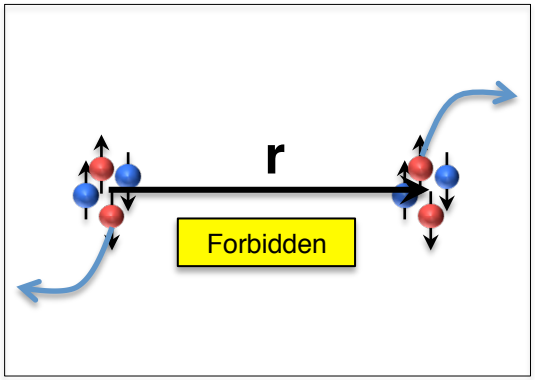
Interaction A was set by starting from interaction B, shutting off all local short-range interactions, and then adjusting the coefficients of the nonlocal short-range interactions to the nucleon-nucleon phase shifts and deuteron energy.

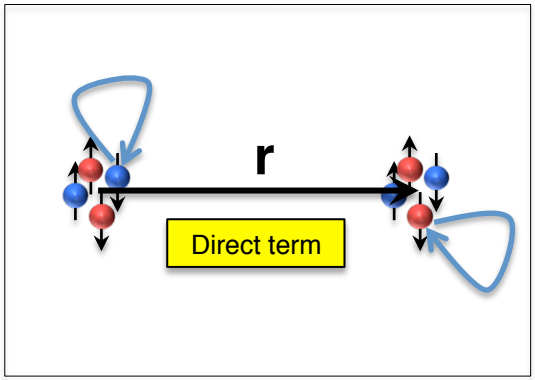
The alpha-alpha interaction is sensitive to the degree of locality of the interaction.

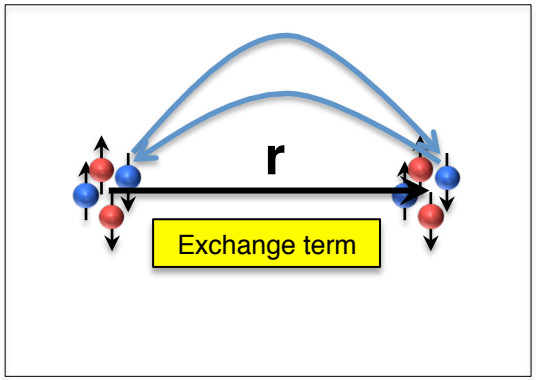
Why is the alpha-alpha interaction sensitive to the degree of locality of the interaction?

Tight-binding approximation

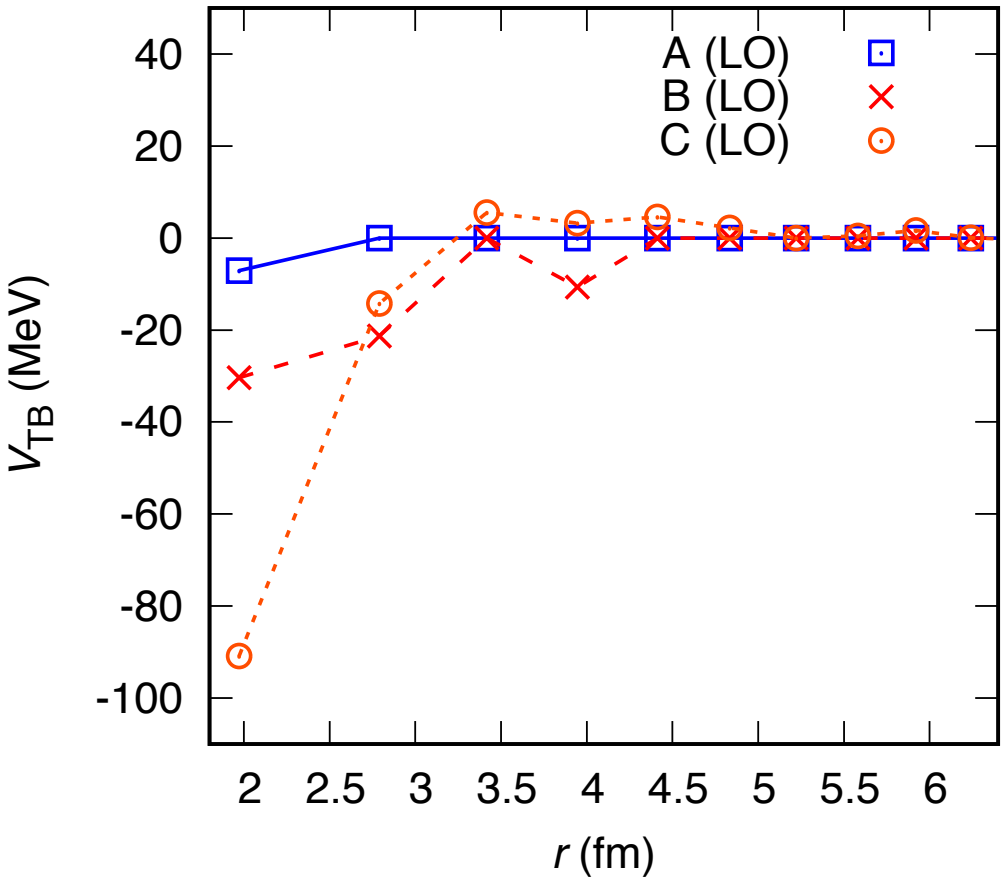
Qualitative picture: Treat the alpha particle radius as a small but nonzero parameter. Consider contributions of the nucleon-nucleon interaction to the effective low-energy alpha-alpha interaction.







Tight-binding potential



Interaction C is the interaction from the first half of this talk

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

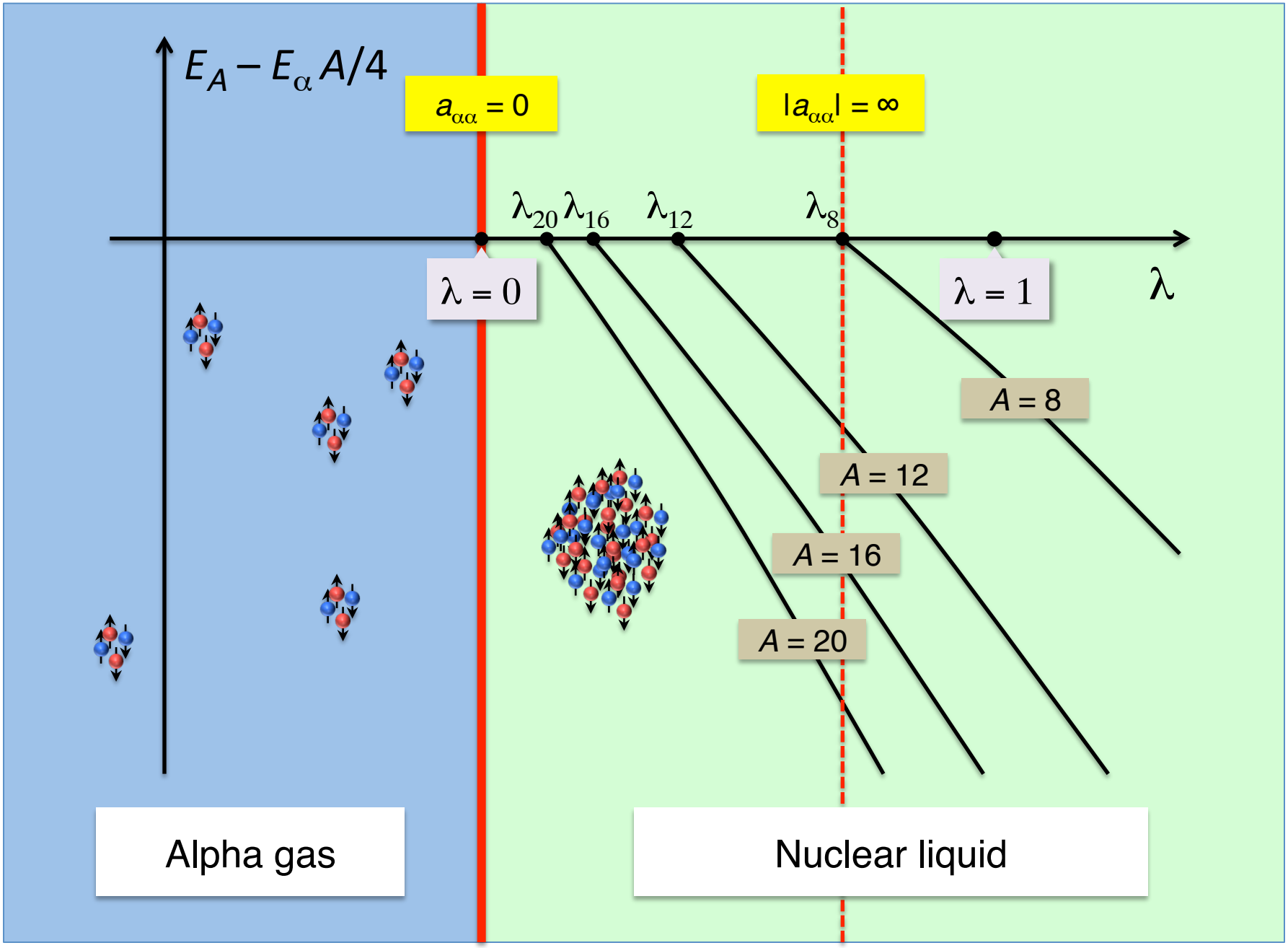
$$V_\lambda = (1-\lambda)V_{\mathrm{A}} + \lambda V_{\mathrm{B}}$$

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.

Stoof, PRA 49, 3824 (1994)

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

Applications

Ab initio chiral effective field theory is an excellent theoretical framework, however there is no guarantee it will continue to work well for nuclei with increasing numbers of nucleons. Cutoff dependence, higher-order corrections, and higher-body forces can become large, rendering calculations unreliable.

There are an infinite number of different ways to write *ab initio* chiral effective field theory interactions at any given order. While they may look equivalent for the low-energy nucleon-nucleon phase shifts, one can use light nucleus-nucleus scattering data to identify a more likely-to-succeed set of interactions where cutoff dependence, higher-order corrections, and higher-body forces appear to be small. Could be useful for *ab initio* nuclear structure and reaction calculations.

The road forward

More sharing of algorithms between lattice QCD and lattice EFT. Can one reduce the signal to noise in lattice QCD multi-nucleon observables by better importance sampling? Can the adiabatic projection method be adapted to lattice QCD? Can lattice EFT use better parallelization and GPUs to improve the speed and size of the simulations? Try to do lattice EFT simulations at nonzero temperature.

As already discussed by Francesco at this KITP program, one can use lattice QCD inputs in nuclear structure and reactions calculations. Many very interesting questions already at the three-nucleon level, and one can even look at two-nucleon properties in a strong external field (e.g., baryon number or gravitational trap). Straightforward to do direct matching between lattice EFT and lattice QCD at finite volume.

We are working to understand the detailed connection between nuclear forces and nuclear structure in nuclei. Current focus now is on neutron-rich nuclei. Which forces are really responsible for the binding of these extra neutrons? The answer to these and similar questions may help guide which questions are most interesting for lattice QCD to probe.

We are working to develop a new algorithm to do simulations with partial sign/phase quenching. Similar methods have been used in AFDMC and other auxiliary field simulations by Shiwei Zhang's group for strongly correlated electronic structure. This may lead to an improvement of the description of nuclear forces on the lattice by allowing a larger class of nonperturbative lattice interactions suitable for Monte Carlo simulations.

And many other things in progress. Busy and exciting times!