Nuclear binding near a quantum phase transition

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Progress in *Ab Initio* Techniques in Nuclear Physics
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Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak,
arXiv:1602.04539

Outline

Lattice effective field theory

How to do nonlocal interactions?

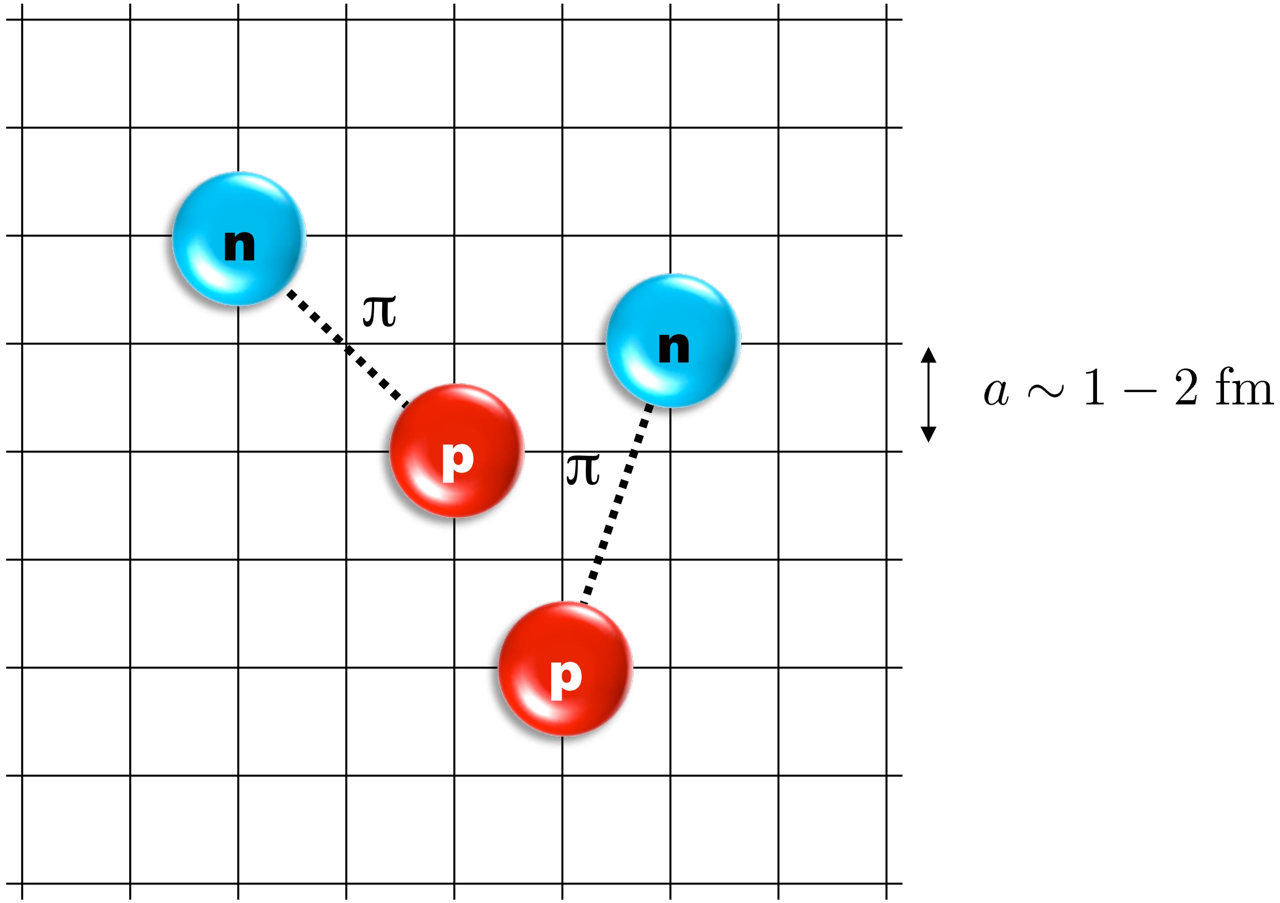
A surprise

Adiabatic projection method

Applications

Summary and outlook

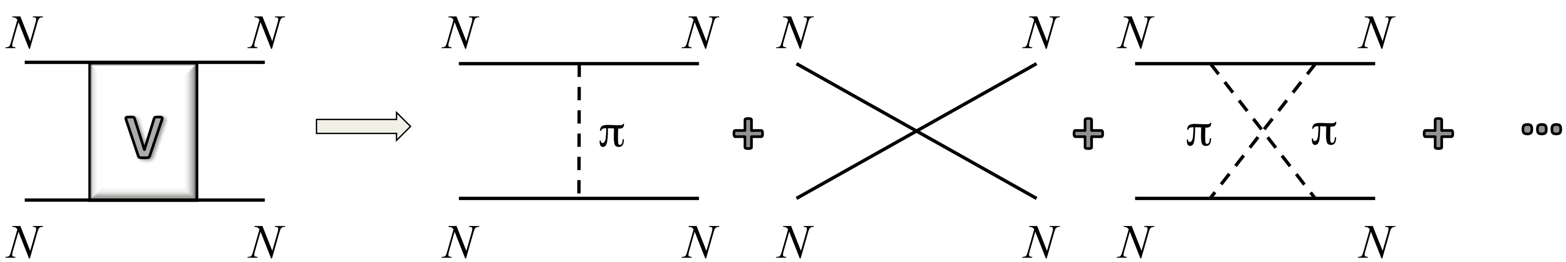
Lattice chiral effective field theory



Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

Chiral effective field theory

Construct the effective potential order by order



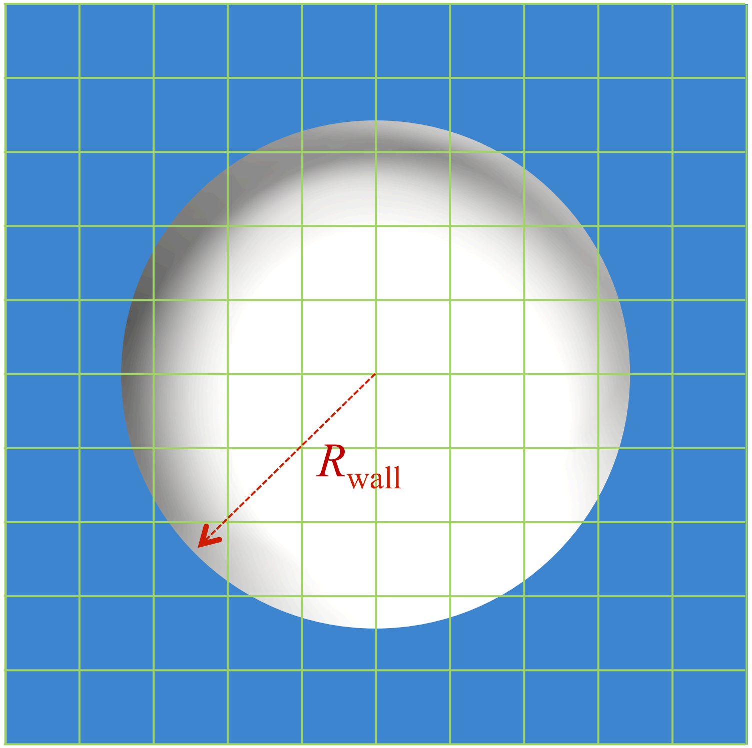
V^{OPEP} Contact interactions V^{TPEP}

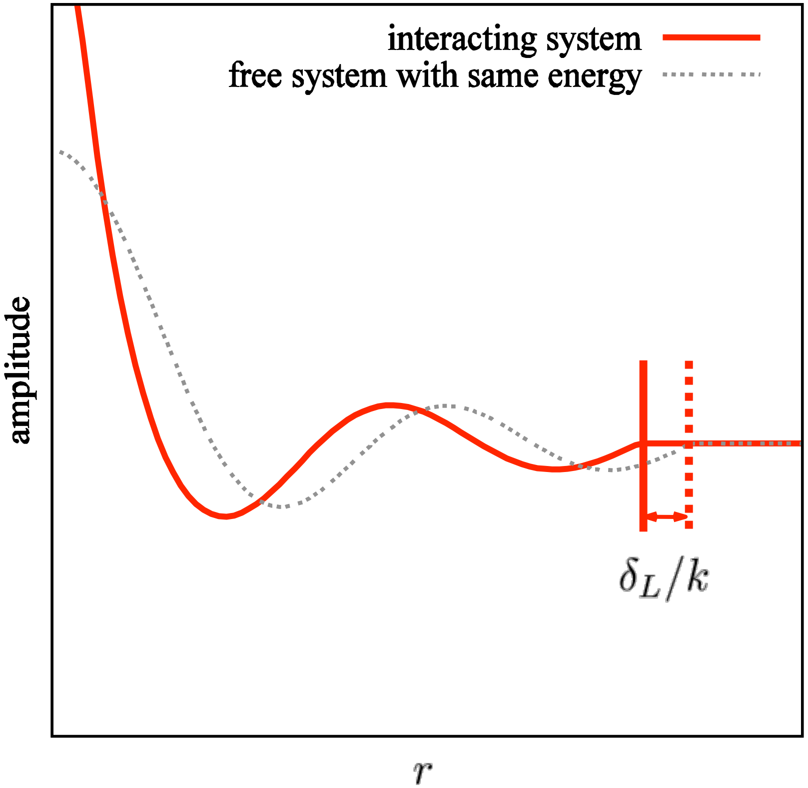
Leading order (LO) Next-to-leading order (NLO)

Spherical wall method

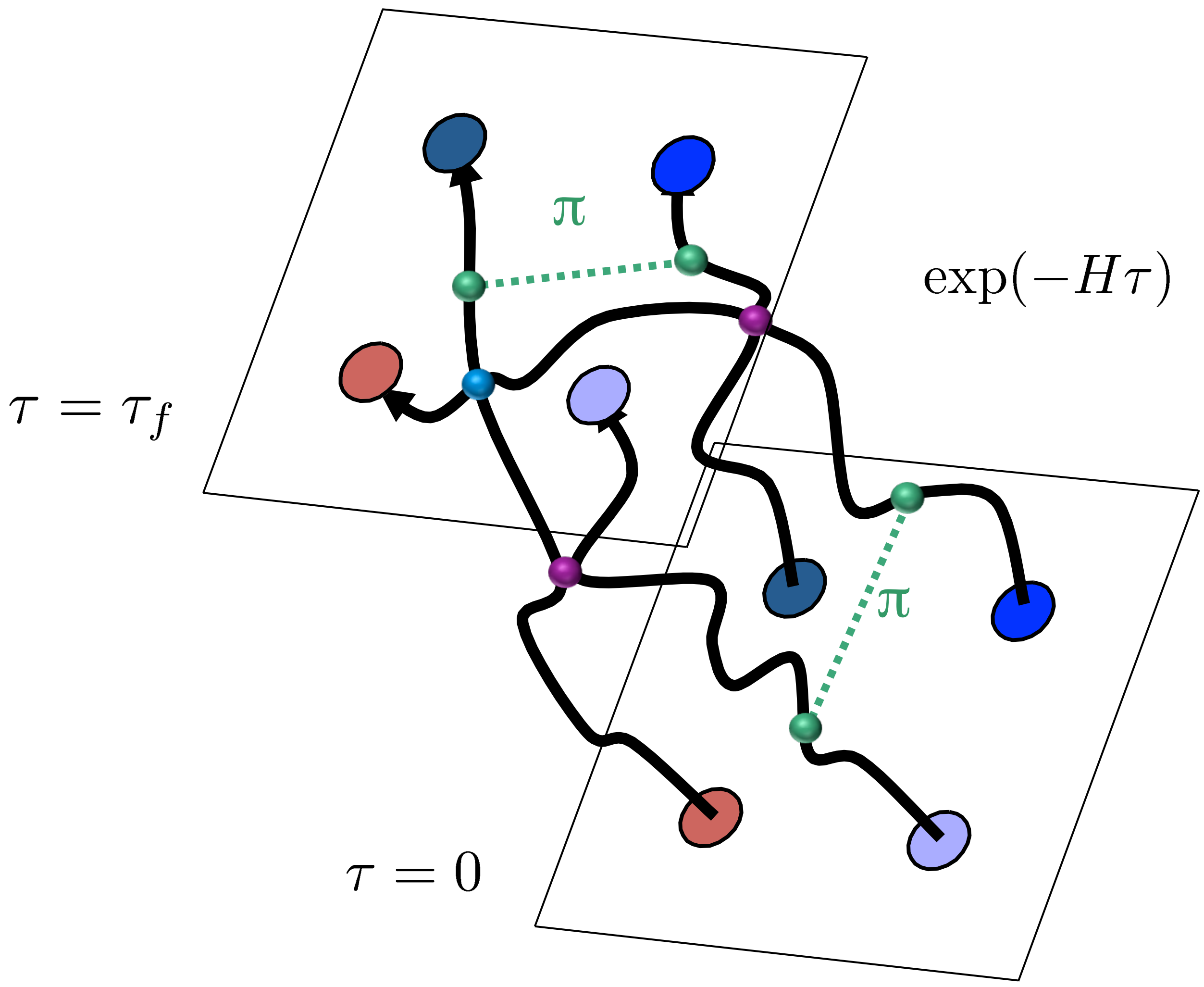
Spherical wall imposed in the center of mass frame

Borasoy, Epelbaum, Krebs, D.L., Meißner EPJA 34 (2007) 185
Carlson, Pandharipande, Wiringa, NPA 424 (1984) 47





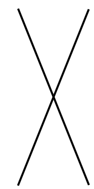
Euclidean time projection



Auxiliary field method

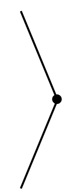
We can write exponentials of the interaction using a Gaussian integral identity

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



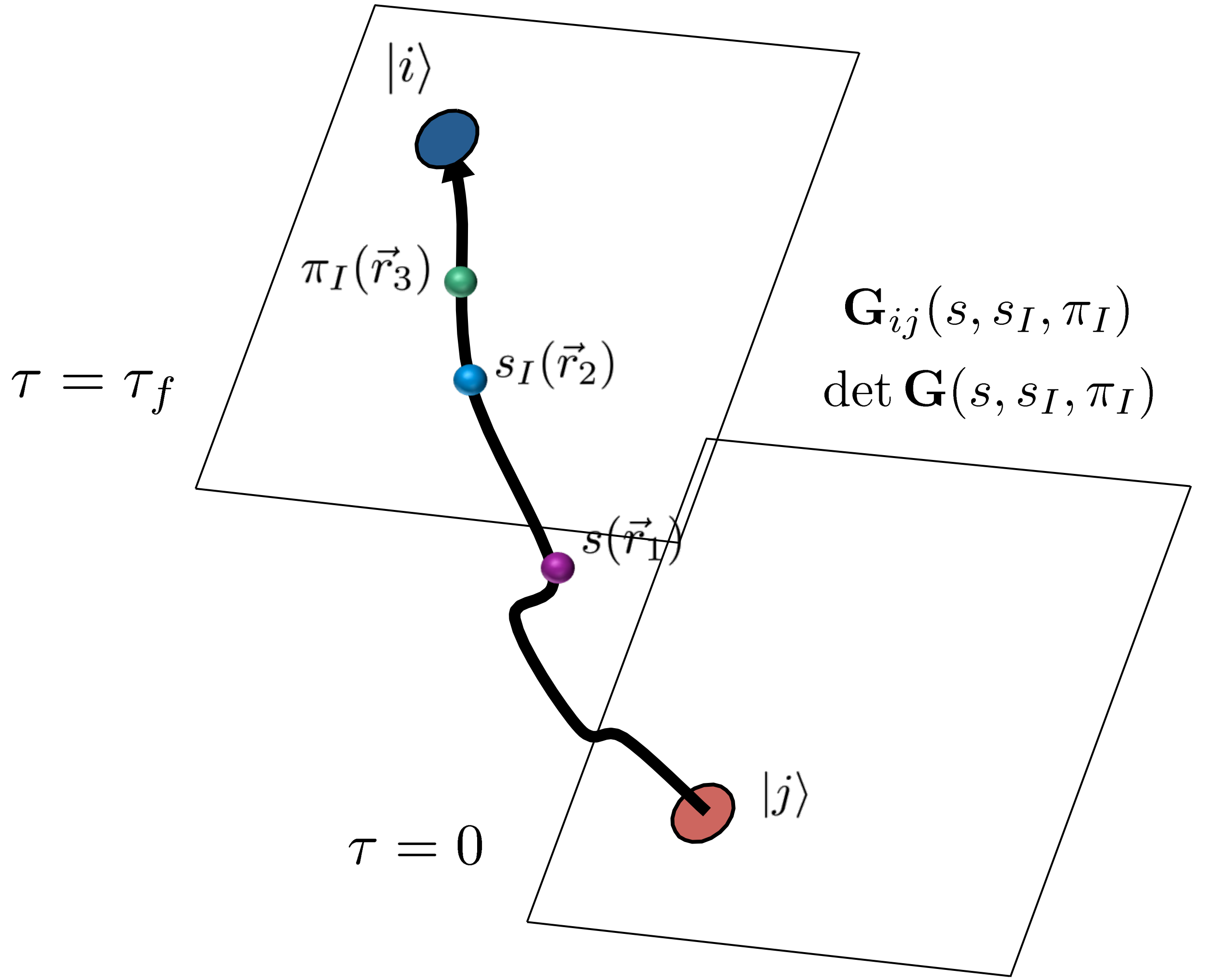
$(N^\dagger N)^2$

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



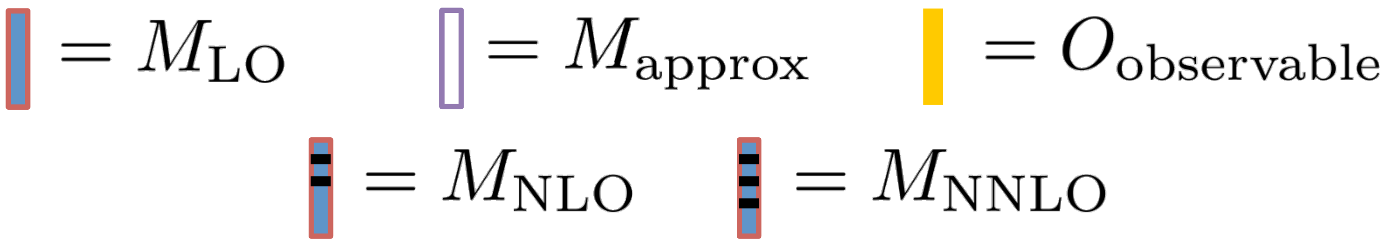
$sN^\dagger N$

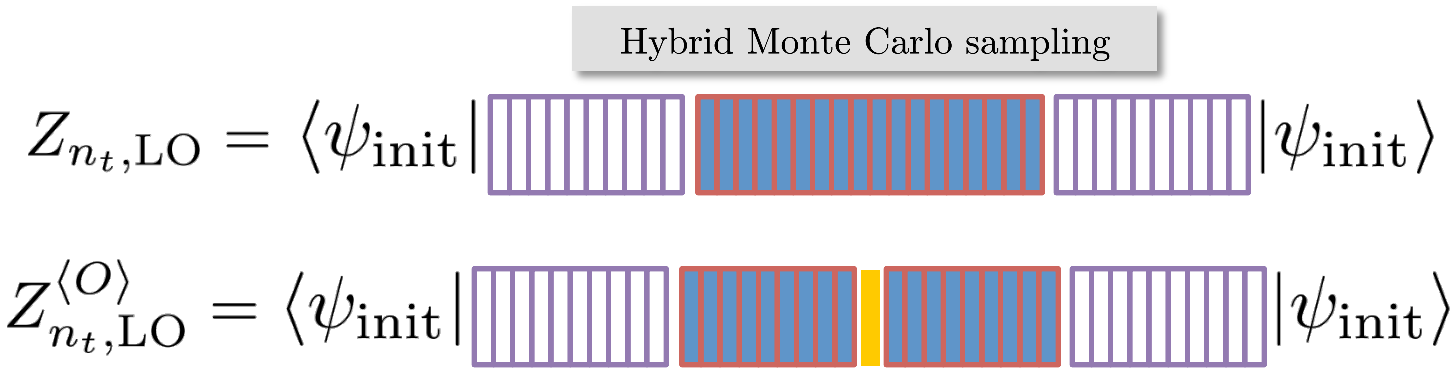
We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.



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

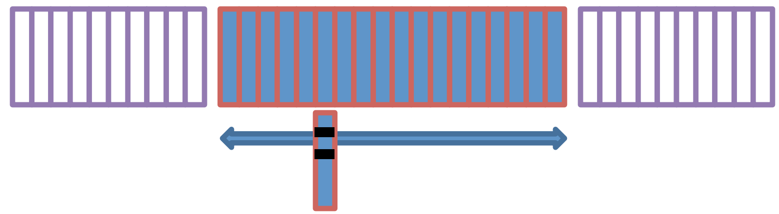
Schematic of lattice Monte Carlo calculation

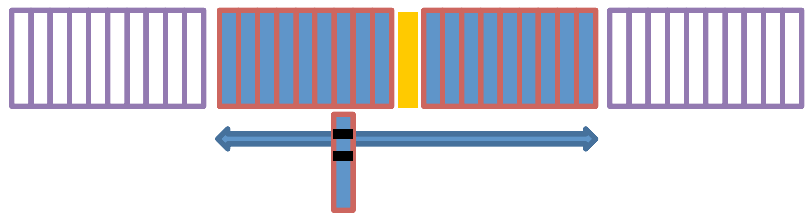




$$e^{-E_{0,{\rm LO}} a_t} = \lim_{n_t \to \infty} Z_{n_t+1,{\rm LO}} / Z_{n_t,{\rm LO}}$$

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

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

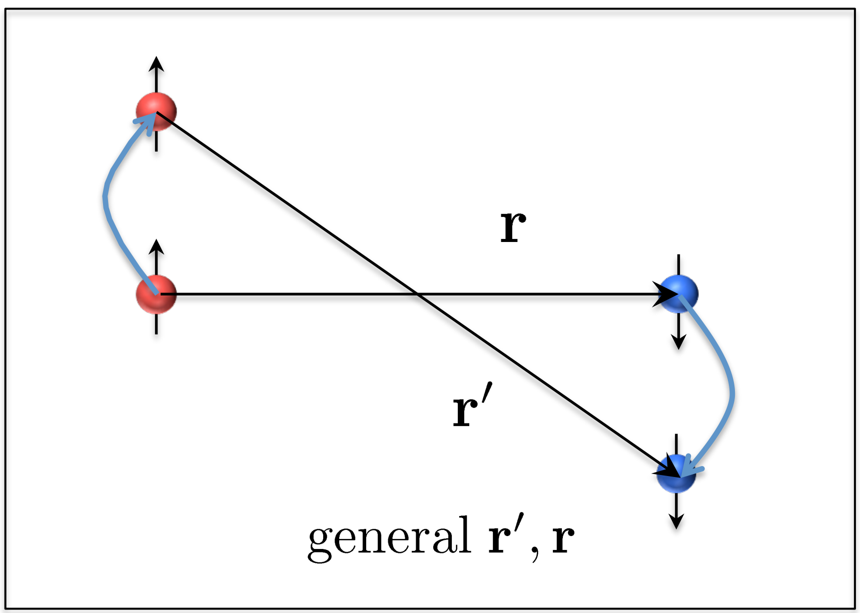
$Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$  $| \psi_{\mathrm{init}} \rangle$

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

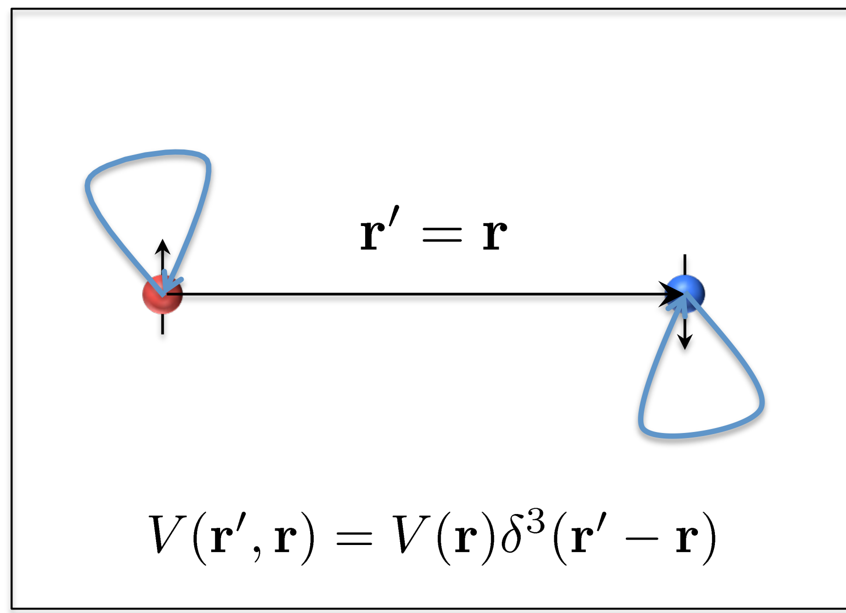
How to do nonlocal interactions?

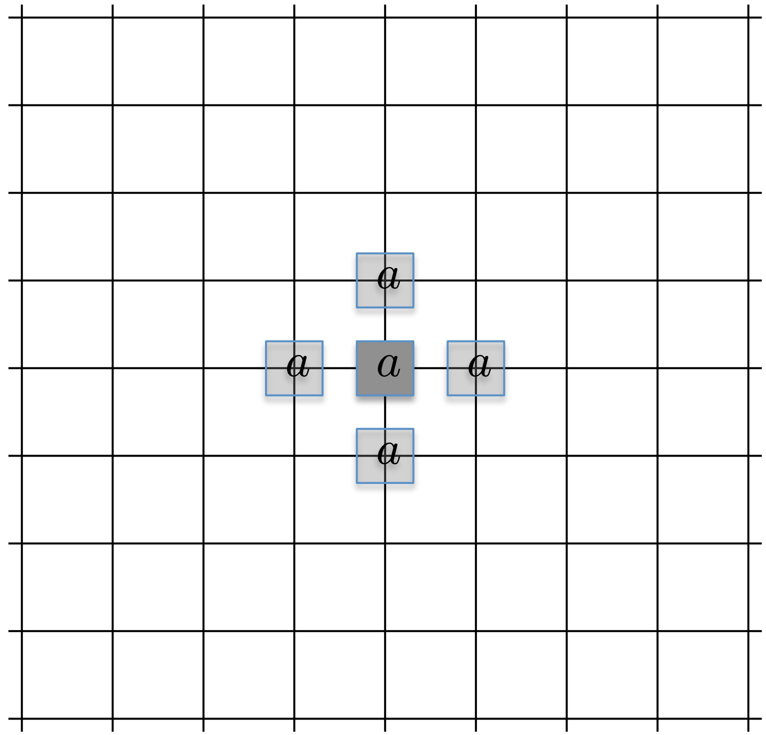
$$V(\mathbf{r}', \mathbf{r})$$

Nonlocal interaction



Local interaction





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

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

Nonlocal density operators

$$\rho_{\mathrm{NL}}(\mathbf{n}) = a^{\dagger}_{\mathrm{NL}}(\mathbf{n}) a_{\mathrm{NL}}(\mathbf{n})$$
$$\rho_{I,\mathrm{NL}}(\mathbf{n}) = a^{\dagger}_{\mathrm{NL}}(\mathbf{n}) [\tau_I] a_{\mathrm{NL}}(\mathbf{n})$$

Nonlocal S-wave interactions

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

We can simulate using auxiliary fields

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

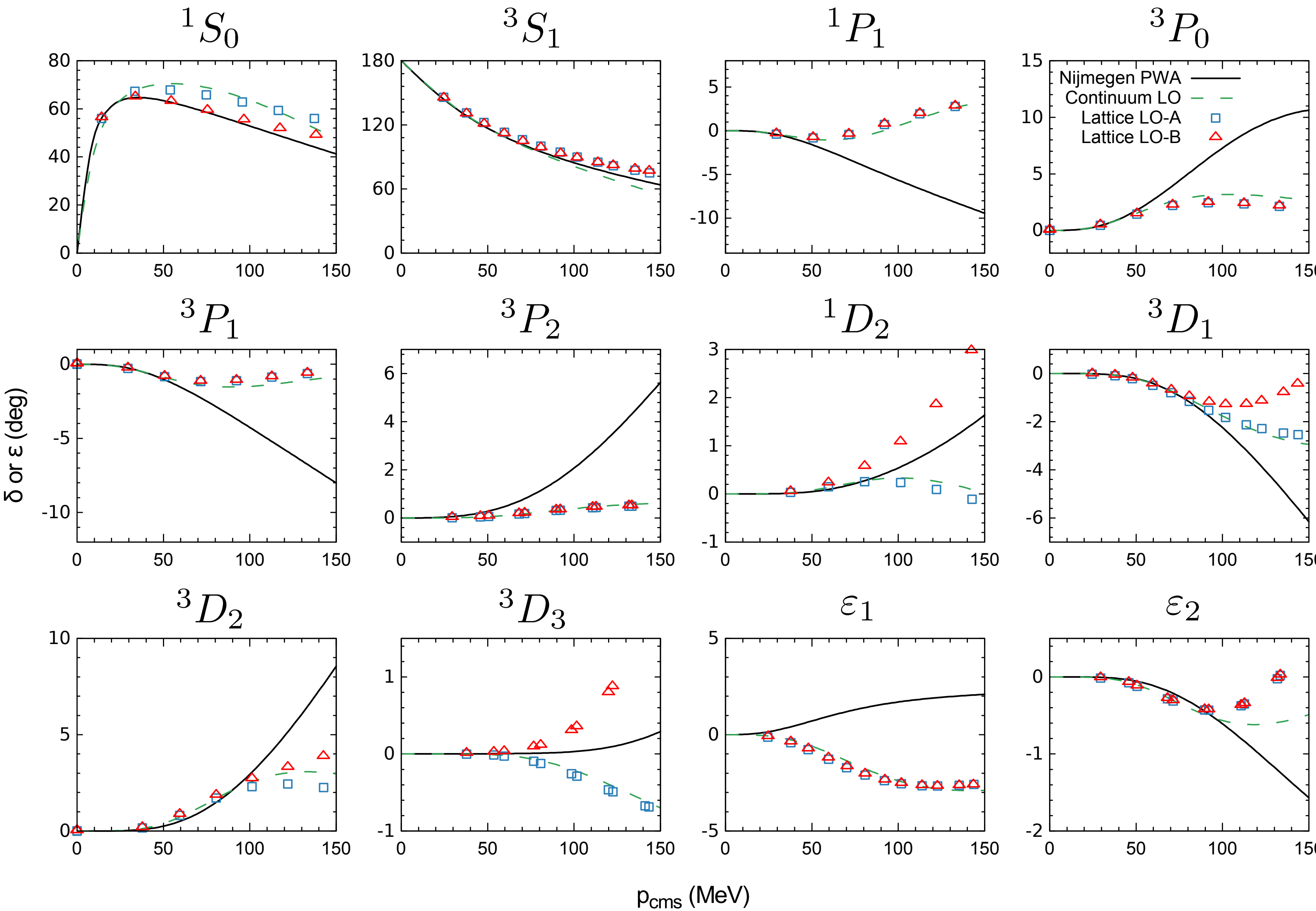
Interaction A at LO (LO + Coulomb)

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)

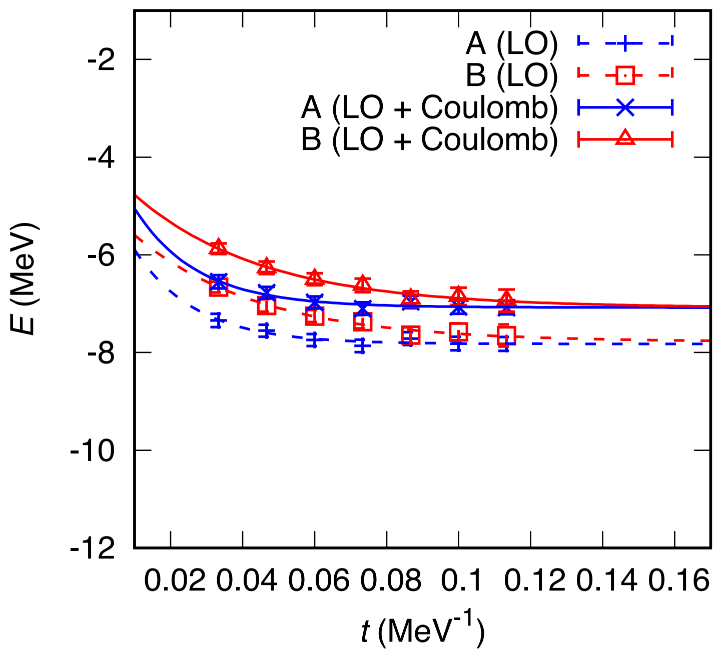
To keep the story more entertaining, we provide the full details of how the interactions are fitted later in the discussion.



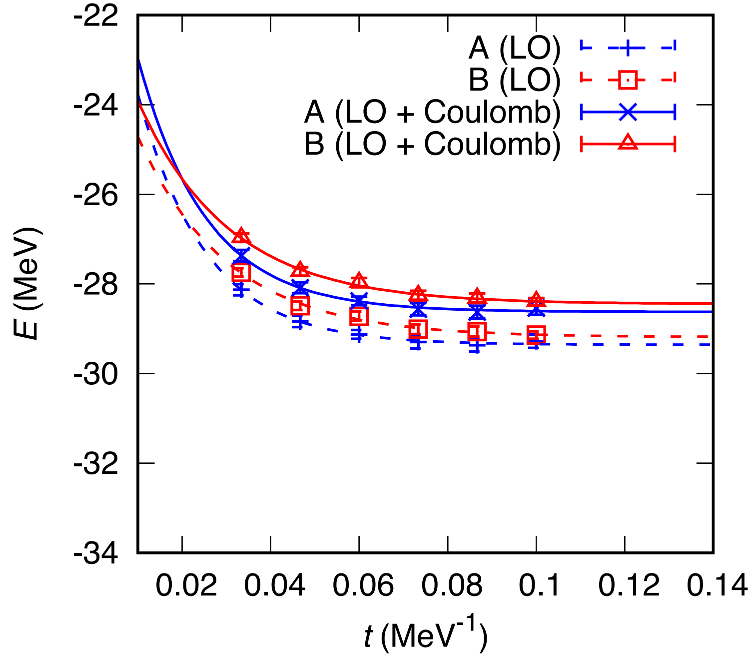
$^1S_0$
$^3S_1$
$^1P_1$
$^3P_0$
$^3P_1$
$^3P_2$
$^1D_2$
$^3D_1$
$^3D_2$
$^3D_3$
ε_1
ε_2
Nijmegen PWA
Continuum LO
Lattice LO-A
Lattice LO-B
δ or ε (deg)
p_{cms} (MeV)

Ground state energies

^{3}He

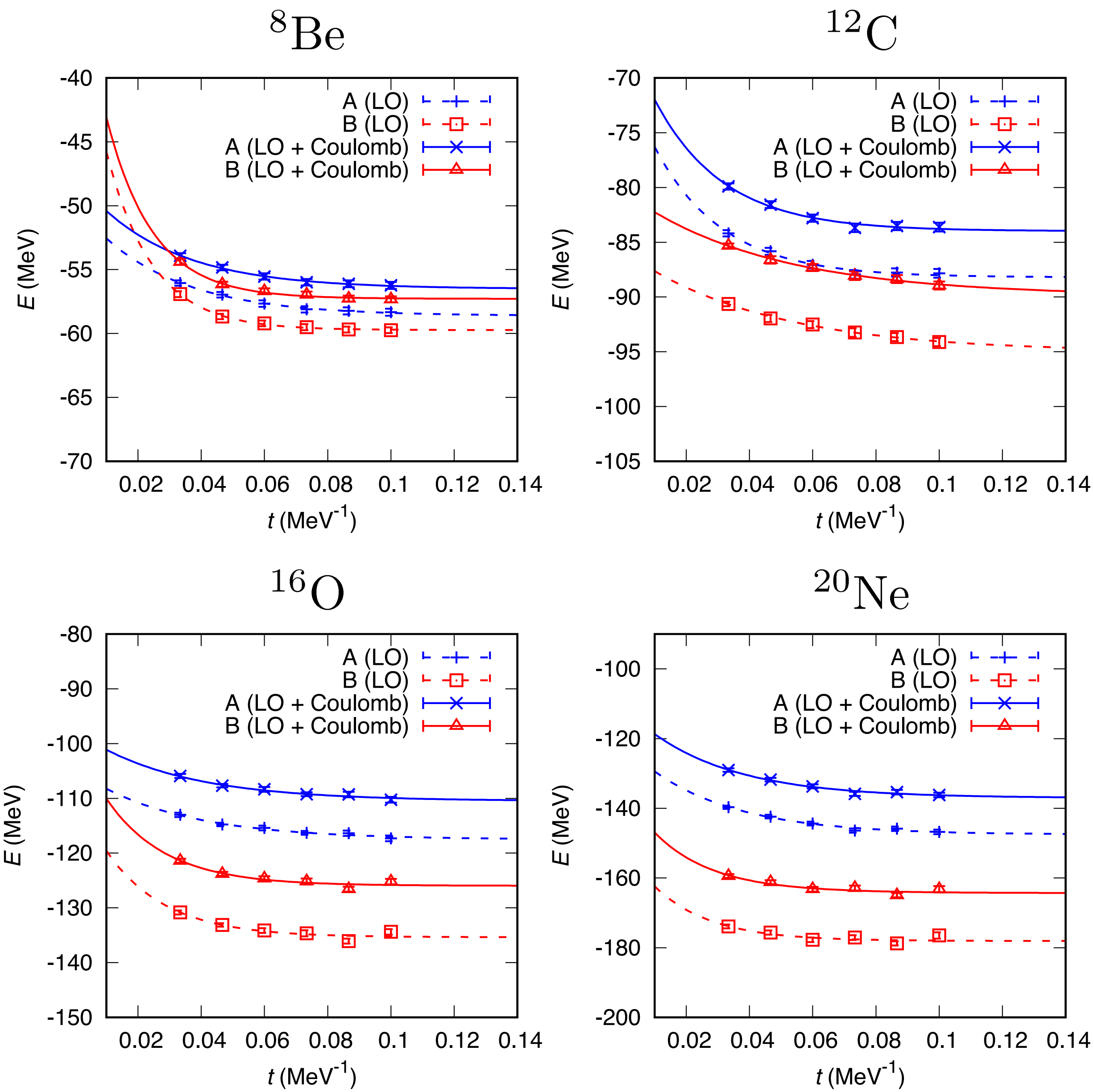


^{4}He



Both interactions significantly reduce the Monte Carlo sign oscillation problem, the original motivation for studying the new 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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$$\frac{E_{^{8}\mathrm{Be}}}{E_{^{4}\mathrm{He}}} = 1.997(6)$$

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

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

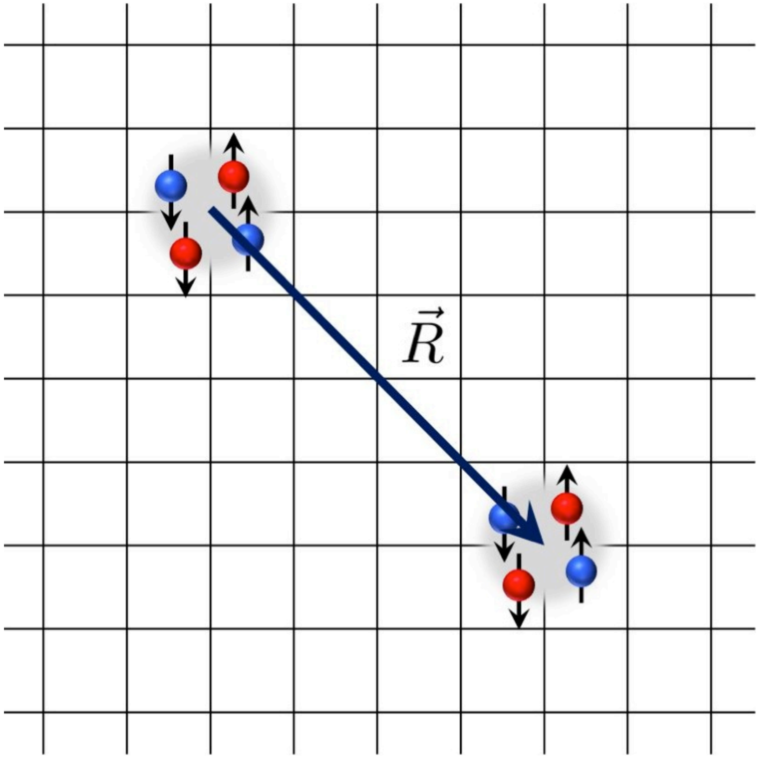
$$\frac{E_{^{20}\mathrm{Ne}}}{E_{^{4}\mathrm{He}}} = 5.03(3)$$

Bose condensate of alpha particles!

Adiabatic projection method

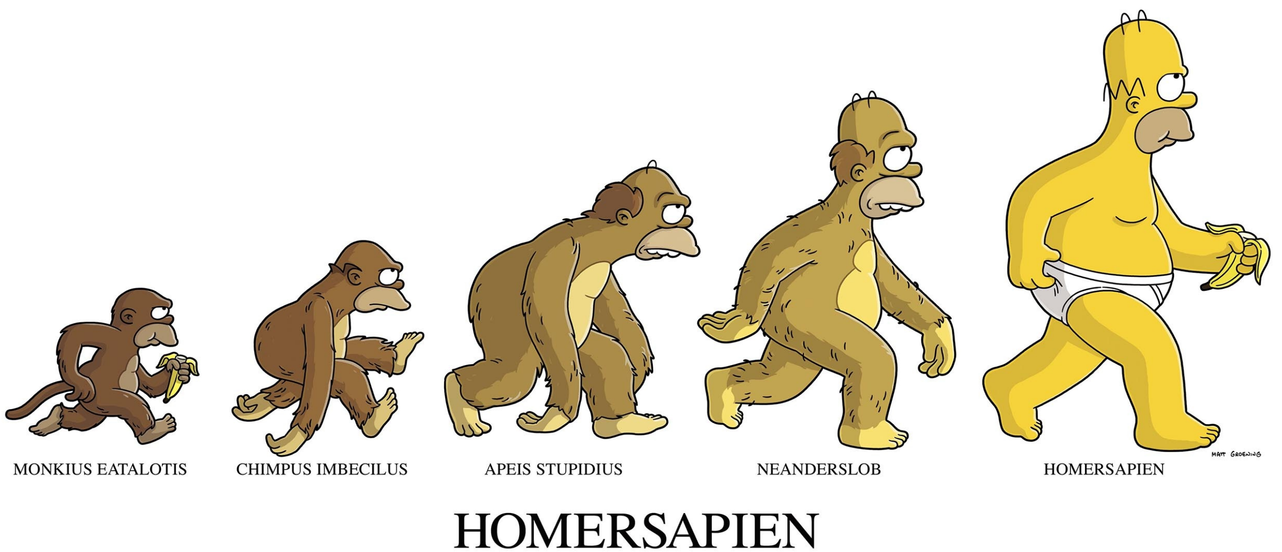
Start with localized cluster states for all possible separation vectors $\vec{R}$

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



Cluster evolution with Euclidean time

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$



M. Groening

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.

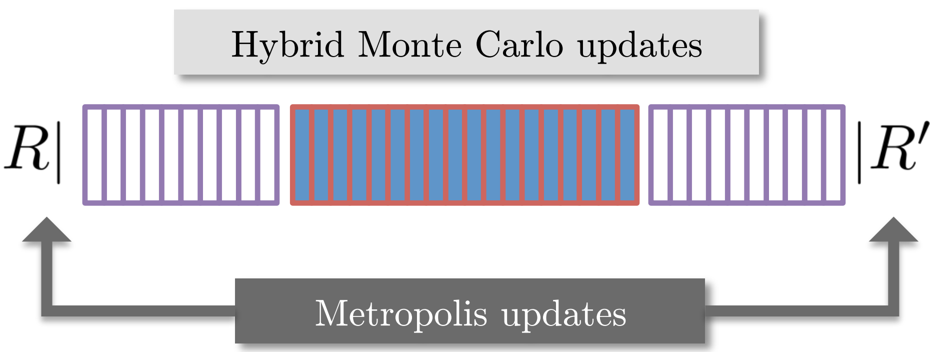
Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, PRC 106, 054612, 2015
Elhatisari, D.L., PRC 90, 064001, 2014

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

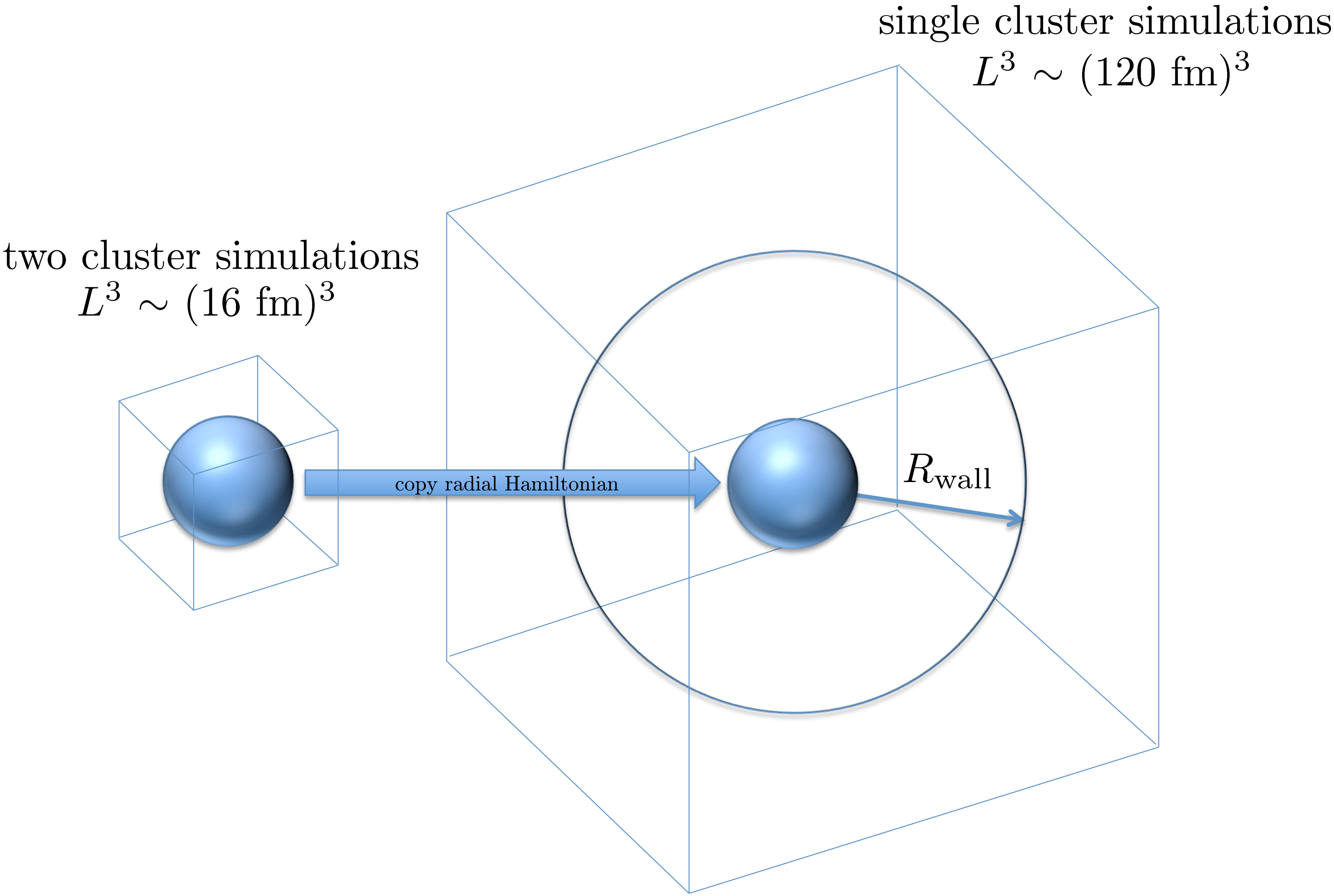
$$|R\rangle^{L,L_z} = \sum_{\vec{R}'} Y_{L,L_z}(\hat{R}')\delta_{R,|\vec{R}'|}|\vec{R}'\rangle$$

Monte Carlo updates of the auxiliary field updates and initial/final states

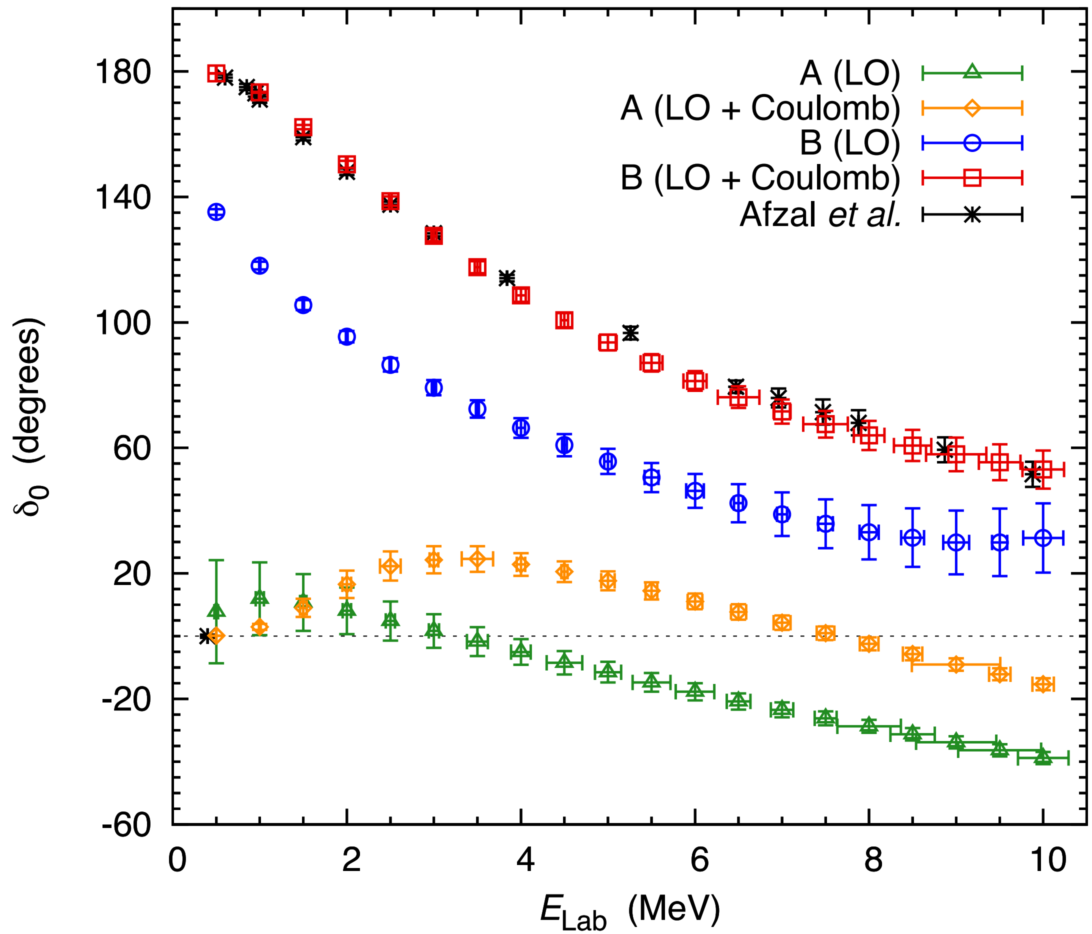
$$[Z_{n_t,\mathrm{LO}}]^{L,L_z}_{R,R'} = {}^{L,L_z}\langle R| \cdots |R'\rangle^{L,L_z}$$



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


single cluster simulations
$L^3 \sim (120\ \text{fm})^3$
two cluster simulations
$L^3 \sim (16\ \text{fm})^3$
copy radial Hamiltonian
R_{wall}

alpha-alpha S-wave scattering



Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, arXiv:1602.04539

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

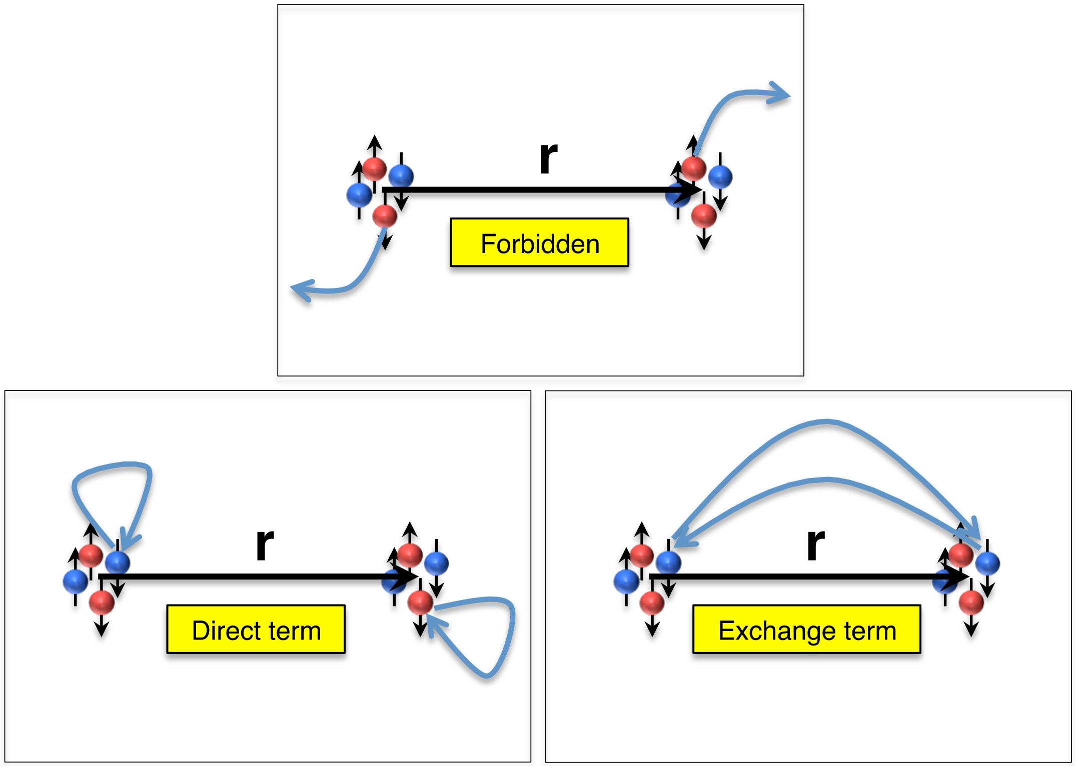
Interaction A was set by starting from interaction B, shutting off all local short-range interactions, and then adjusting the coefficients of the nonlocal short-range interactions to the nucleon-nucleon phase shifts and deuteron energy.

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

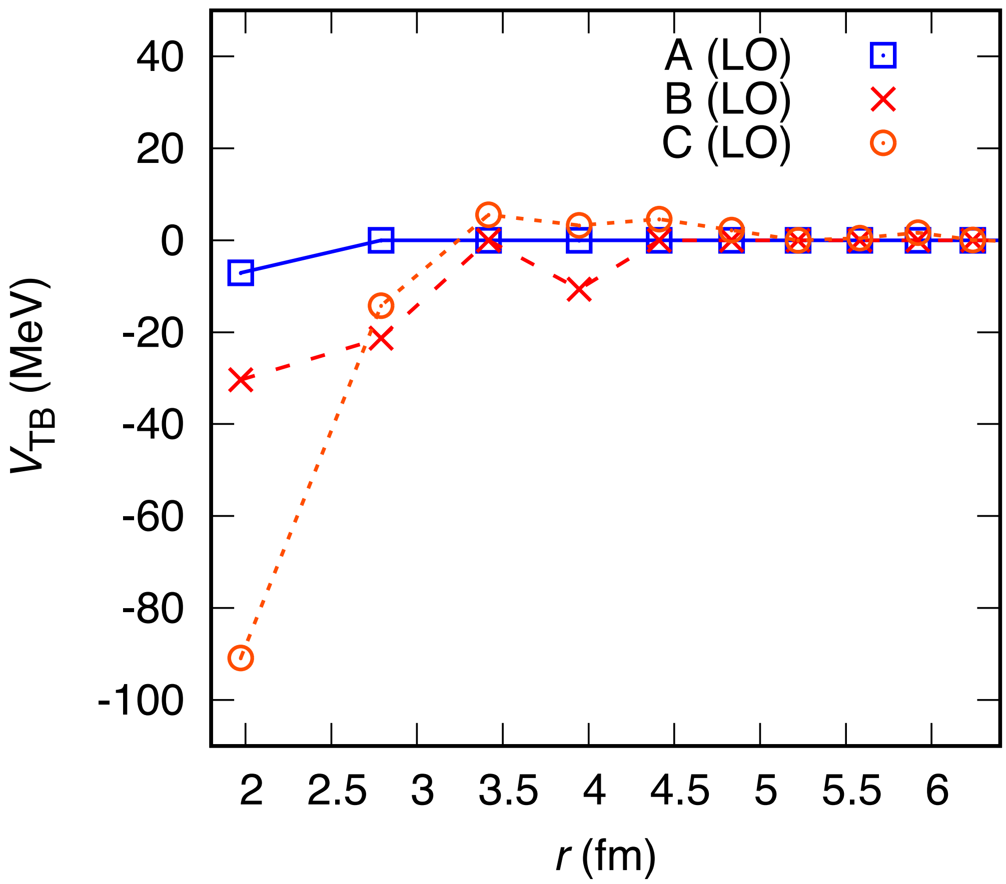
Why is the alpha-alpha interaction sensitive to the degree of locality of the interaction?

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

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

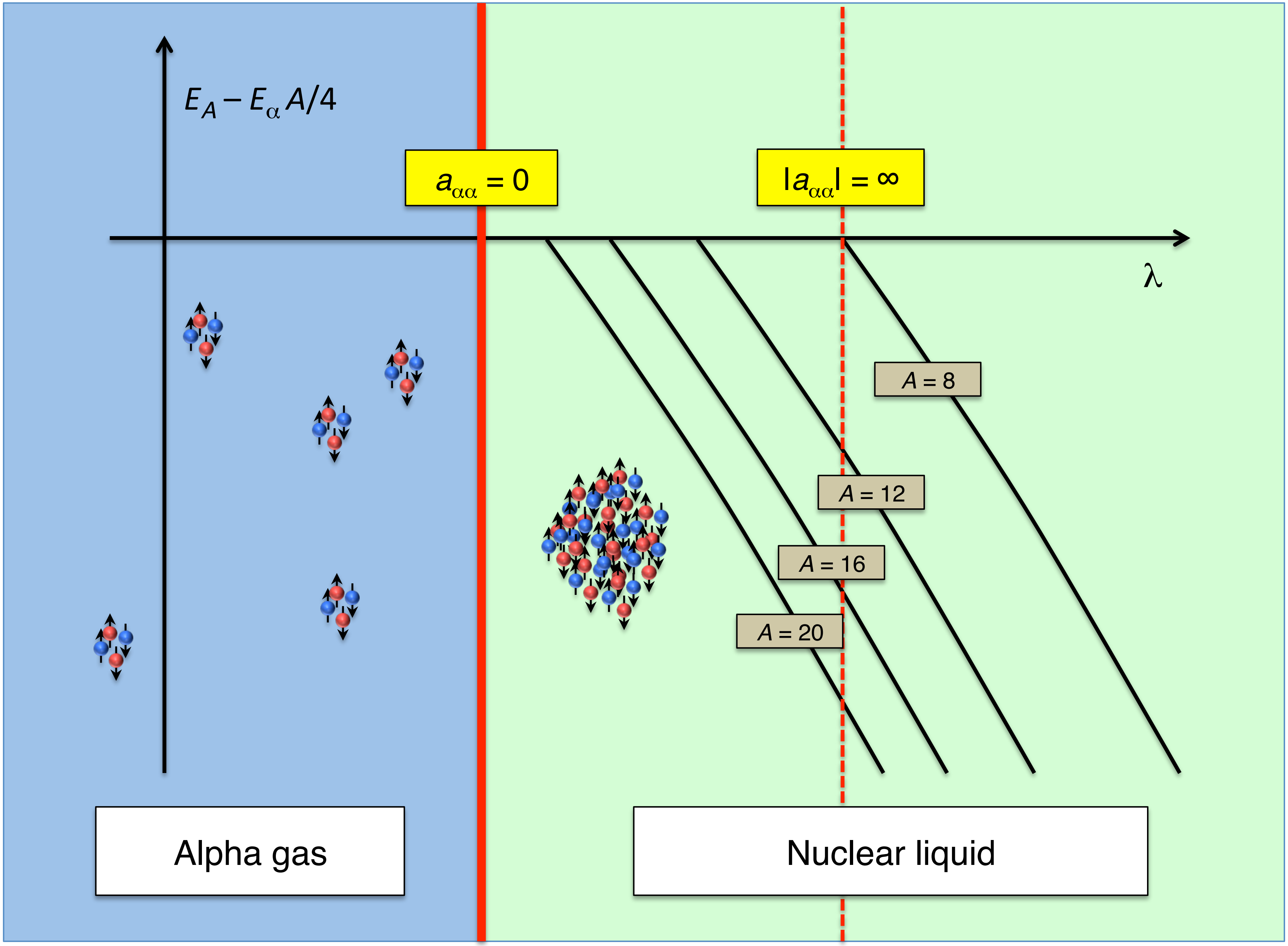
$$V_\lambda = (1-\lambda)V_{\rm A} + \lambda V_{\rm B}$$

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
$A = 8$
$A = 12$
$A = 16$
$A = 20$
Alpha gas
Nuclear liquid

Applications I

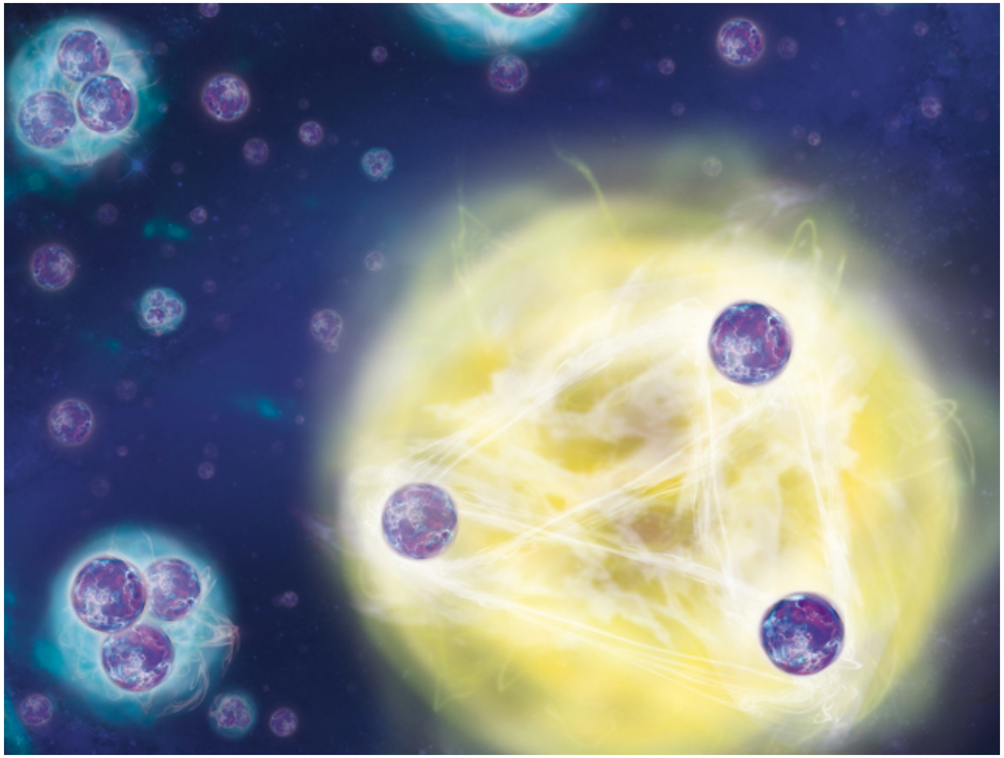
Ab initio chiral effective field theory is an excellent theoretical framework, however there is no guarantee it will work well for nuclei with increasing numbers of nucleons. Cutoff dependence, higher-order corrections, and higher-body forces can become large, rendering the calculation inefficient.

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. Should be useful for *ab initio* nuclear structure and reaction calculations.

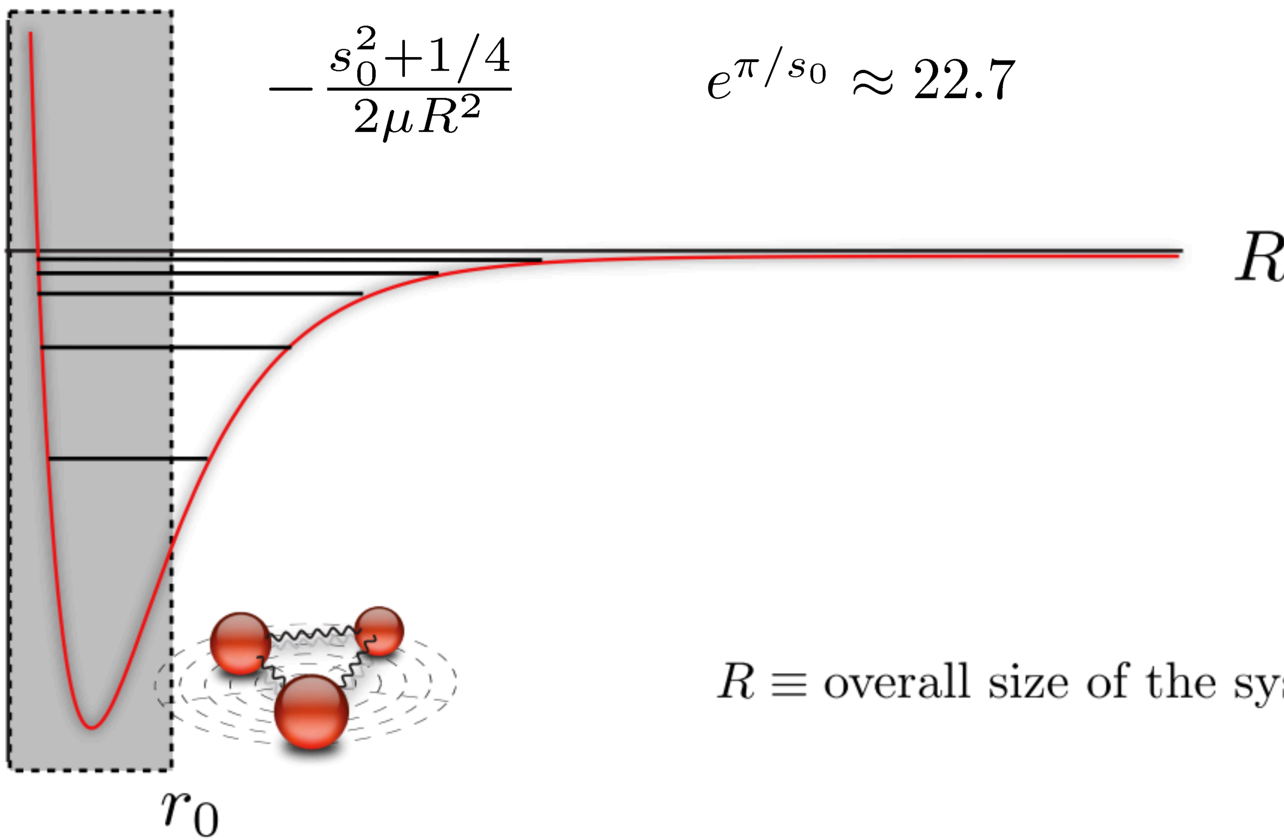
<u>Efimov effect</u>

Efimov, Sov. J. Nucl. Phys. 589 (1971); PRC 47, 1876 (1993)

Universality in three boson system at large scattering length

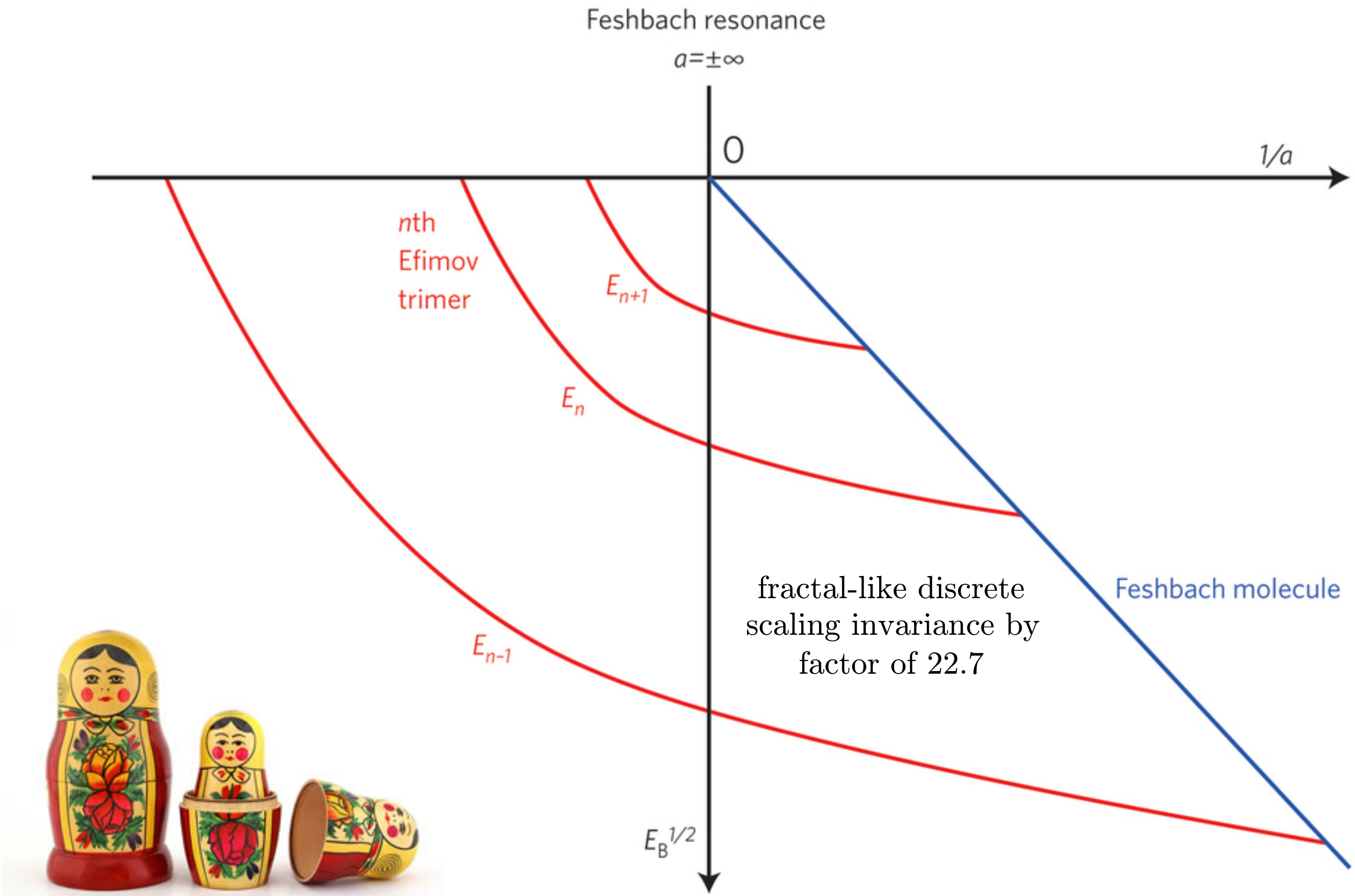


Credit: Quanta Magazine, Walchover, May 2014



$R \equiv$ overall size of the system

Credit: Jose D'Incao



Chin, Wang, Nat. Phys. 11 449 (2015)

Applications II

By adjusting the parameter λ in *ab initio* calculations, one can move the energy of any alpha cluster state up and down relative to alpha separation thresholds. This can be used as a new window to view the structure of these exotic nuclear states.

In particular, one can tune the alpha-alpha scattering length to infinity. In the absence of the Coulomb interaction, the Hoyle state of ^{12}C can be continuously deformed into a universal Efimov trimer.

Hoyle state of ^{12}C $\xrightarrow{\lambda}$ Universal Efimov trimer

Similarly, in the absence of the Coulomb interaction, the second 0^+ state of ^{16}O can be continuously deformed into a universal Efimov tetramer.

Second 0^+ of ^{16}O $\xrightarrow{\lambda}$ Universal Efimov tetramer

Summary and outlook

We have presented numerical evidence from *ab initio* lattice simulations showing that nature is near a quantum phase transition.

It is a first-order transition from a Bose-condensed gas of alpha particles to a nuclear liquid. Whether one has an alpha-particle gas or nuclear liquid is determined by the strength of the alpha-alpha interactions, and the alpha-alpha interactions depend on the strength and degree of locality of the nucleon-nucleon interactions.

Several potentially exciting applications include practical methods to improve *ab initio* nuclear structure and reaction calculations, a new theoretical window on alpha cluster states, and a connection to the universal physics of Efimov states.