Lattice improvement of nuclear shape calculations using unitary transformations

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Introduction

- Chiral lattice EFT (cf. plenary talk by Bing-Nan Lu today at 01:40) allows for simulations e.g. of ^{3}H, ^{4}He, ^{12}C, ^{16}O, ^{28}Si and nuclear matter.

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- It is based on an effective nucleus-nucleus Hamiltonian determined by Monte Carlo simulations using the adiabatic projection method.

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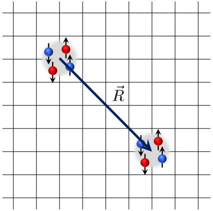

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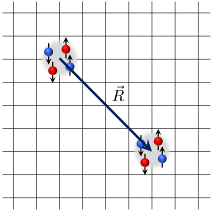

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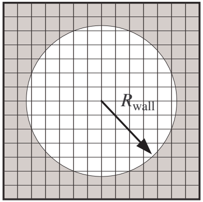
- From this adiabatic Hamiltonian, one can extract phase shifts by applying spherical wall boundary conditions & projection onto partial waves.

  (Lüscher's method is not accurate enough here because the error of the Monte-Carlo energy levels is larger than the separation between these levels.)

  Phys. Lett. B 760, 309 (2016); Phys. Rev. C 98, 044002 (2018); Phys. Rev. C 100, 064001 (2019)



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  (This property is also used for similarity renormalization group (SRG) transformations.)
- The contribution $\langle\psi|\left(U^\dagger r^2 U - r^2\right)|\psi\rangle$ induced by the unitary transformation is interpreted to be missing in the original lattice calculation.

Benchmark toy-model Hamiltonian

consider N spinless particles of mass $m = m_{\mathrm{nucl}} = 938.92\ \mathrm{MeV}$ in 1D,
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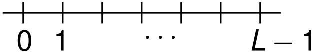
$x_i = 0, \ldots, L-1 \quad \forall\, i = 1, \ldots, N$ (use lattice units with $a = 1$)



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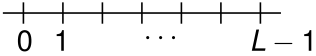

discretize H using $O(a^4)$-improved dispersion relation (Eur. Phys. J. A 34, 185 (2007)):

$$H = \frac{49}{12m} \sum_x a^\dagger(x) a(x) - \frac{3}{4m} \sum_x a^\dagger(x)\big(a(x+1) + a(x-1)\big)$$
$$+ \frac{3}{40m} \sum_x a^\dagger(x)\big(a(x+2) + a(x-2)\big)$$
$$- \frac{1}{180m} \sum_x a^\dagger(x)\big(a(x+3) + a(x-3)\big) + \frac{C}{2} \sum_x a^\dagger(x) a^\dagger(x) a(x) a(x)$$

Unitary transformation for two particles

solve Schrödinger equation $H\,|\psi\rangle = E\,|\psi\rangle$ using Lanczos algorithm
to determine ground state $\psi_A(x_1, x_2)$ as eigenvector of H

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modify wave function up to range R: (to tune $\langle r^n \rangle$ order by order)

$$\psi_B(c_{12}, d_{12}) = \psi_A(c_{12}, d_{12}) + \Delta\psi(c_{12}, d_{12}) \quad \text{for} \quad d_{12} = 0, 1, \ldots, R$$

with $\sum_{c_{12}} \Delta\psi(c_{12}, 0)$ fixed by conservation of wave function norm

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construct U as reflection transformation with $U|u\rangle = -|u\rangle$:

$$U = 1 - 2|u\rangle\langle u| \quad \text{for} \quad |u\rangle = |\Delta\psi\rangle / \sqrt{\langle\Delta\psi|\Delta\psi\rangle} \quad \text{or}$$

$$\langle x_1, x_2| U |x_1', x_2'\rangle = \delta_{x_1,x_1'}\delta_{x_2,x_2'} - 2\delta_{c_{12},c_{12}'} \frac{\Delta\psi(c_{12}, d_{12})\,\Delta\psi(c_{12}, d_{12}')}{\sum_{d_{12}''} |\Delta\psi(c_{12}, d_{12}'')|^2}$$

Unitary transformation for three particles

generalization for three particles (with $(i, j, k) = (1, 2, 3), (1, 3, 2), (2, 3, 1)$):

$$\langle x_1, x_2, x_3 | U_{3\mathrm{p}} | x_1', x_2', x_3' \rangle = \delta_{x_1, x_1'} \delta_{x_2, x_2'} \delta_{x_3, x_3'} - 2 \sum_{(i,j,k)} \delta_{c_{ij}, c_{ij}'} \frac{\Delta\psi(c_{ij}, d_{ij}) \, \Delta\psi(c_{ij}, d_{ij}')}{\sum_{d_{ij}''} |\Delta\psi(c_{ij}, d_{ij}'')|^2} \delta_{x_k, x_k'}$$

not unitary (since additional terms do not cancel in $U_{3\mathrm{p}} U_{3\mathrm{p}}^\dagger$ as for 2 particles)

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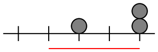

$\Rightarrow$ switch off operator U if spectator particle k comes too close to c_{ij}

(This makes the transformation “locally unitary” for the particles i and j.)

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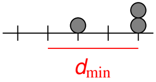

$\Rightarrow$ switch off operator U if spectator particle k comes too close to c_{ij}

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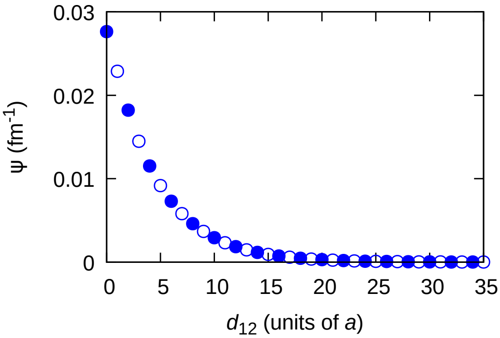
calculate $\langle \psi_{3\text{p}} | U_{3\text{p}}^\dagger r^2 U_{3\text{p}} | \psi_{3\text{p}} \rangle$ with $\psi_{3\text{p}}(x_1, x_2, x_3)$ as eigenvector of H

Results for two particles

plot wave function vs. d_{12} for each c_{12}:

(ψ obtained at even/odd distances separately)



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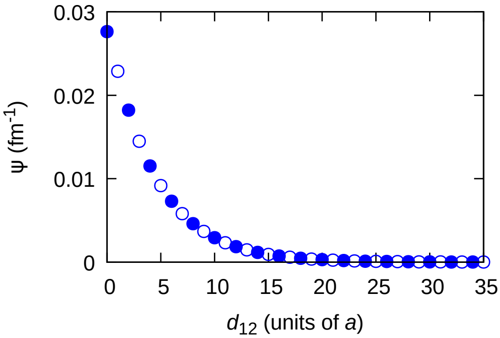
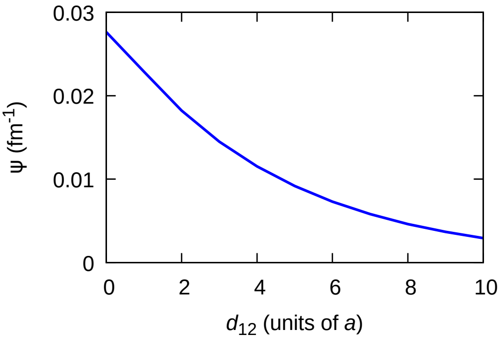


vary e.g. $\Delta\psi(c_{12}, 2a)$ in possible domain:



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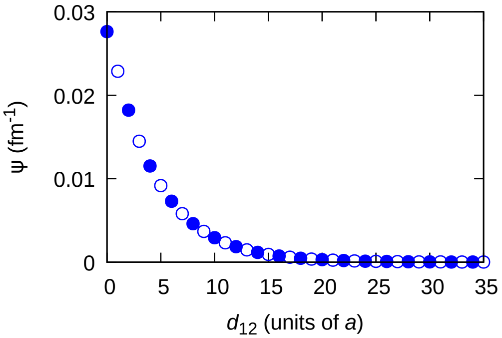

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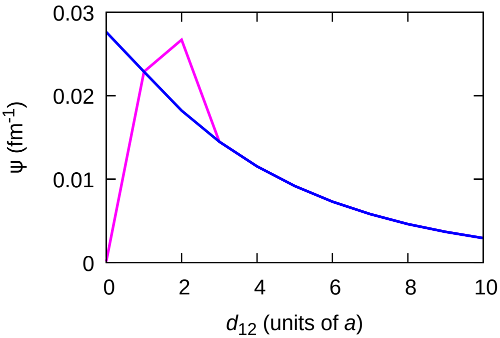

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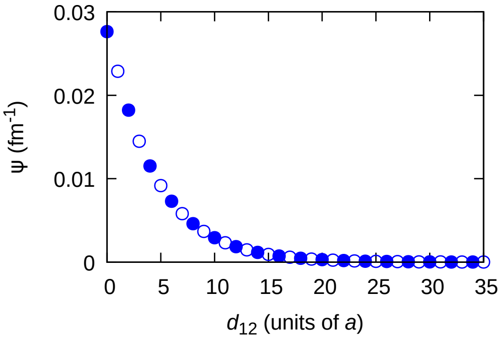

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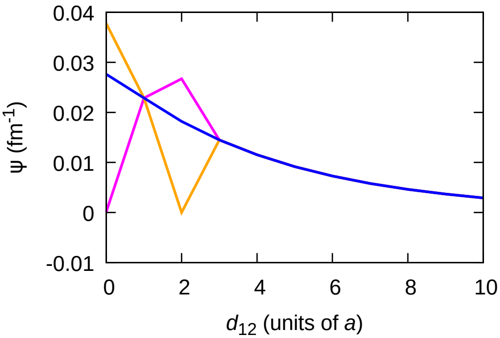

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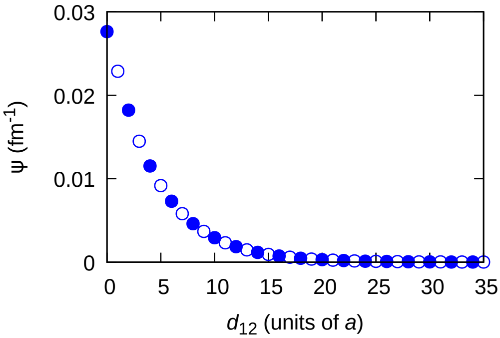

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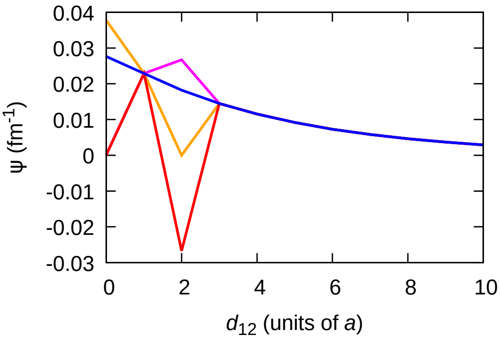

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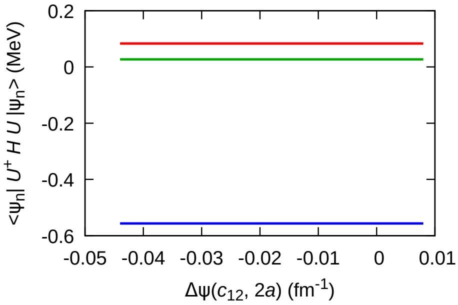

(ψ_n is n-th lowest eigenstate of Hamiltonian with zero total momentum;
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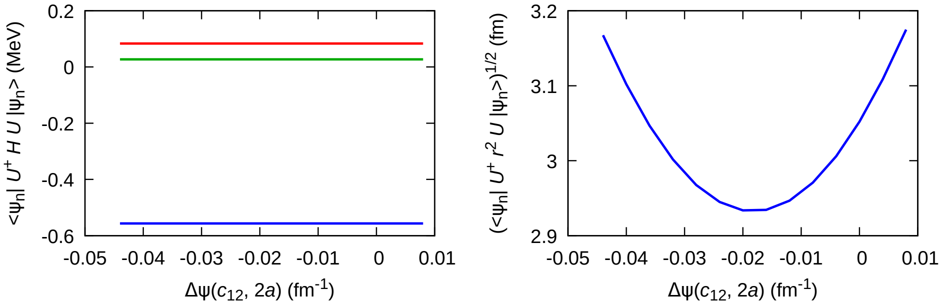
- significant dependence of RMS radius on $\Delta\psi(c_{12}, 2a)$



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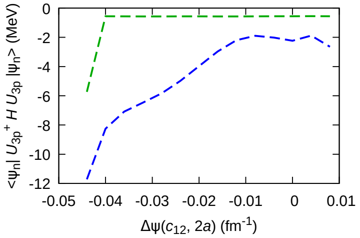

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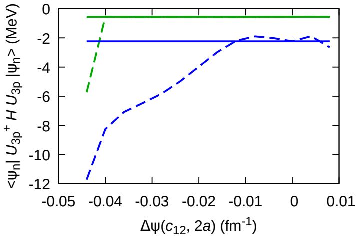

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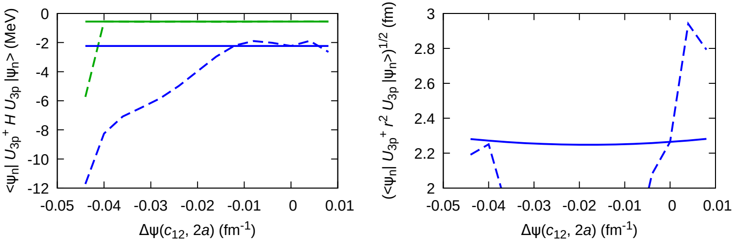

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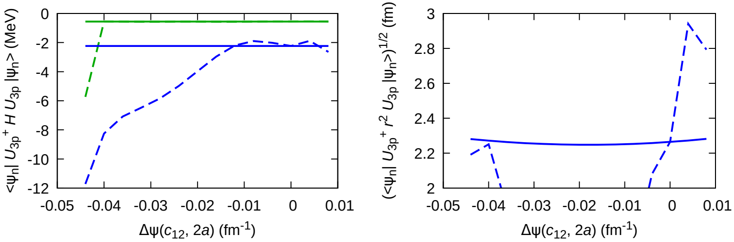

- prediction for $N > 3$ may be improved by additional three-body term in U:

$$\langle x_1, x_2, x_3 | \, (U'_{3\rm p} - U_{3\rm p}) \, | x'_1, x'_2, x'_3 \rangle = \delta_{c_{123}, c'_{123}} f(\{c_{ij}\}, \{c'_{ij}\}, d_{12}, d_{13}, d'_{12}, d'_{13})$$

with $c_{123} = (x_1 + x_2 + x_3)/3$

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- for $N \geq 4$: let unitary transformation act on all pairs of particles simultaneously (system extensivity)
- choose smaller L for three particles than for two particles

Thank you for your attention!

Backup slides

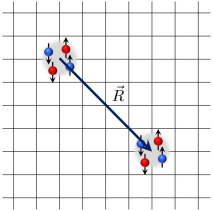
Adiabatic projection method

define two-cluster states (here in 1D):

$$|d\rangle = \sum_{x=0}^{L-1} |x+d\rangle_{\text{cluster 1}} \otimes |x\rangle_{\text{cluster 2}}$$

evolve them in Euclidean time to obtain dressed cluster states $|d\rangle_\tau = e^{-H\tau}|d\rangle$

calculate matrix elements ${}_\tau\langle d| H |d'\rangle_\tau$ of adiabatic Hamiltonian using Monte Carlo simulation



Phys. Rev. C 92, 054612 (2015); Nature 528, 111 (2015)

Modification of H vs. modification of ψ

There are two different points of view on applying the unitary transformation:

- apply U to wave function:

$$(\langle\psi| U^\dagger)H(U|\psi\rangle), \qquad (\langle\psi| U^\dagger)r^2(U|\psi\rangle)$$

- apply U to operators:

$$\langle\psi|(U^\dagger H U)|\psi\rangle, \qquad \langle\psi|(U^\dagger r^2 U)|\psi\rangle$$

Notice that combining these two possibilities would cause no effect:

$$\cancel{\langle\psi| U^\dagger U H U^\dagger U|\psi\rangle = \langle\psi| H|\psi\rangle}, \qquad \cancel{\langle\psi| U^\dagger U r^2 U^\dagger U|\psi\rangle = \langle\psi| r^2|\psi\rangle}$$

Similarity renormalization group (SRG) transformations

make Hamiltonian $H(0)$ more diagonal using a unitary transformation:

$$H(s) = U(s)H(s=0)U^\dagger(s)$$

where the Hamiltonian can be split as

$$H(s) = H_{\text{diag}}(s) + H_{\text{off-diag}}(s) \quad \text{with} \quad H(s) \xrightarrow{s\to\infty} H_{\text{diag}}(s), \quad H_{\text{off-diag}}(s) \xrightarrow{s\to\infty} 0$$

solve SRG flow equation to obtain $H(s)$:

$$\frac{\mathrm{d}H(s)}{\mathrm{d}s} = \left[\frac{\mathrm{d}U(s)}{\mathrm{d}s}U^\dagger(s), H(s)\right]$$

Lect. Notes Phys. 936, 477 (2017)

Operators & states

annihilation/creation operators for distinguishable particles: ((anti)symmetrize later)

$$a^{(\dagger)}(x) = a_1^{(\dagger)}(x) + \cdots + a_N^{(\dagger)}(x), \quad \langle x_1, \ldots, x_N | y_1, \ldots, y_N \rangle = \delta_{x_1,y_1} \ldots \delta_{x_N,y_N},$$

$$a_i(x) \, |x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_N\rangle = \delta_{x,x_i} \, |x_1, \ldots, x_{i-1}, \mathrm{vac}, x_{i+1}, \ldots, x_N\rangle \,,$$

$$a_i(x) \, |x_1, \ldots, x_{i-1}, \mathrm{vac}, x_{i+1}, \ldots, x_N\rangle = a_i^\dagger(x) \, |x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_N\rangle = 0,$$

$$a_i^\dagger(x) \, |x_1, \ldots, x_{i-1}, \mathrm{vac}, x_{i+1}, \ldots, x_N\rangle = |x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_N\rangle$$

r^2-operator in second quantization:

$$r^2 = \frac{1}{N} \sum_{x=0}^{L-1} a^\dagger(x) a(x) \left(x - \frac{1}{N} \sum_{x'=0}^{L-1} a^\dagger(x') a(x') x' \right)^2$$

states with zero total momentum:

$$|d_1, \ldots, d_{N-1}\rangle_{P_{\mathrm{tot}}=0} = \sum_{x=0}^{L-1} |x + d_1, \ldots, x + d_{N-1}, x\rangle$$

Center of mass & distance

The periodic boundary conditions must be taken into account in the definition of the center of mass c and the distance d:

$$c_{ij} = \begin{cases} (x_i + x_j)/2 & \text{if } |x_i - x_j| < L - |x_i - x_j| \\ (x_i + x_j - L)/2 \mod L & \text{if } |x_i - x_j| \geq L - |x_i - x_j| \end{cases},$$

$$d(x, y) = \min(|x - y|, L - |x - y|)$$