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Lattice improvement of nuclear shape calculations using unitary transformations

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We present a method to improve the lattice effective field theory description of the shape of atomic nuclei by applying unitary transformations to the eigenvectors of the Hamiltonian. The employed unitary operator U is constructed as a reflection transformation from the original and the desired wave functions. Similarly to a derivative expansion, it can be improved systematically so that one can tune the $\langle r^n \rangle$ expectation values order by order for the two-particle system. Moreover, the effects of U in the three-particle system have been investigated. The method might be helpful to reduce lattice artifacts in radii and electromagnetic moments of nuclei.

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1. Introduction

Since lattice QCD is still restricted to systems of few quarks, it cannot be used to simulate heavier atomic nuclei yet. Therefore, a lattice version of chiral effective field theory (EFT) has been developed instead (see Refs. [1, 2] for recent reviews). It was applied successfully to calculate the ground state and excited Hoyle state of several light and medium-mass nuclei [3–7] as well as properties of nuclear matter [8].

Moreover, lattice chiral EFT also allows one to analyze nucleus-nucleus scattering (e.g. $\alpha - \alpha$ scattering) using the adiabatic projection method [9, 10]. This method yields an "adiabatic" effective Hamiltonian for two nuclear clusters determined by Monte Carlo simulations. Afterwards, scattering phase shifts can be extracted from the adiabatic Hamiltonian using spherical wall boundary conditions and projection onto partial waves [11–14]. (Lüscher's finite-volume formula [15–17] is not precise enough for nuclear scattering simulations because the statistical uncertainty of the Monte-Carlo energy levels for such systems is larger than the separation between these levels.)

Although the phase shifts obtained from nuclear lattice simulations are meanwhile in good agreement with experimental data, this does not necessarily hold for other observables like radii, that typically come out too small. While such deviations are generally expected to be cured by the inclusion of exchange current operators that can be derived systematically in chiral EFT [18], using coarse lattices may potentially amplify the issue by introducing large artifacts. In this context, one may try to reduce the amount of lattice artifacts by systematically exploiting the unitary ambiguity in the Hamiltonian, i.e. the appearance of infinitely many lattice interactions that produce the same on-shell part of the S-matrix.

Therefore, our aim is to modify the lattice wave function such that the nuclear radii are described correctly without introducing many-body correction terms to the r^2 operator (as it has been done in Ref. [19]). This shall be achieved by applying a unitary transformation U to the wave function ψ and calculating the expectation value of the *untransformed* r^2-operator for $U|\psi\rangle$. Then, the radius of the ground state wave function will be changed but the expectation values of the Hamiltonian H (and thus the phase shifts) will remain invariant. (Such a property of a unitary operator is also used for similarity renormalization group (SRG) transformations (see e.g. Ref. [20])). The contribution $\langle\psi| (U^\dagger r^2 U - r^2) |\psi\rangle$ to the r^2 expectation value induced by U can be interpreted to be missing in the original lattice calculation.

Our paper presents a method to find such a unitary transformation for a one-dimensional benchmark system. In Sections 2 and 3, the toy-model Hamiltonian and the construction of the unitary transformation will be described. Afterwards, we will show the corresponding numerical data in Section 4 and summarize our results in Section 5.

2. Toy-model Hamiltonian

In order to demonstrate our method for a simple example, we consider the one-dimensional system of N spinless bosons which all have the nucleon mass $m = m_{\text{nucl}} = 938.92$ MeV. On a periodic lattice with spacing a and length L, the particle coordinates are restricted to the lattice sites as

$$x_i = 0, \ldots, (L-1)a = 0, \ldots, (L-1) \text{ l.u.} \tag{1}$$

for each particle index $i = 1, \ldots, N$. The abbreviation "l.u." (which will be omitted in the following) means "lattice units", i.e. all quantities are dimensionless and must be multiplied by an appropriate power of a to obtain their physical values.

Following Ref. [11], the free term in the Hamiltonian is discretized using the $O(a^4)$-improved lattice dispersion relation:

$$\begin{aligned} H_{\text{free}} = \frac{49}{36m} \sum_x a^\dagger(x)a(x) - \frac{3}{4m} \sum_x a^\dagger(x)(a(x+1) + a(x-1)) \\ + \frac{3}{40m} \sum_x a^\dagger(x)(a(x+2) + a(x-2)) - \frac{1}{180m} \sum_x a^\dagger(x)(a(x+3) + a(x-3)), \end{aligned} \tag{2}$$

where $a^\dagger(x)$ and $a(x)$ denote creation and annihilation operators at the lattice site x, respectively. The "nuclear force" is described by a two-particle contact interaction with the negative coefficient $C = -10$ MeV fm:

$$H = H_{\text{free}} + V \quad \text{with} \quad V = \frac{C}{4} \sum_x a^\dagger(x)a^\dagger(x)a(x)a(x). \tag{3}$$

This choice for the coefficient C produces a bound state with a reasonable binding energy both in the two-particle and the three-particle case.

3. Construction of unitary transformation

3.1 Modification of the wave function

As mentioned in the introduction, the unitary transformation shall be constructed from a modification of the ground state wave function. This wave function can be obtained in the two-particle case from the Schrödinger equation

$$\sum_{x_1'} \sum_{x_2'} \langle x_1, x_2 | H | x_1', x_2' \rangle \underbrace{\langle x_1', x_2' | \psi \rangle}_{=\psi(x_1', x_2')} = E \underbrace{\langle x_1, x_2 | \psi \rangle}_{=\psi(x_1, x_2)}. \tag{4}$$

Generally, the N-particle states in coordinate space are normalized as

$$\langle x_1, \ldots, x_N | y_1, \ldots, y_N \rangle = \delta_{x_1, y_1} \ldots \delta_{x_N, y_N} \tag{5}$$

and the creation and annihilation operators $a^{(\dagger)}(x) = a_1^{(\dagger)}(x) + \cdots + a_N^{(\dagger)}(x)$ act on them like

$$a_i(x) \, | x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_N \rangle = \delta_{x, x_i} \, | x_1, \ldots, x_{i-1}, \text{vac}, x_{i+1}, \ldots, x_N \rangle, \tag{6}$$

$$a_i^\dagger(x) \, | x_1, \ldots, x_{i-1}, \text{vac}, x_{i+1}, \ldots, x_N \rangle = | x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_N \rangle, \tag{7}$$

$$a_i(x) \, | x_1, \ldots, x_{i-1}, \text{vac}, x_{i+1}, \ldots, x_N \rangle = a_i^\dagger(x) \, | x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_N \rangle = 0. \tag{8}$$

(Notice that the particles are still distinguishable here because the (anti)symmetrization can be performed later by projecting the Hamiltonian onto partial waves. Then, one would find that the ground state wave function is symmetric with respect to the interchange of the coordinates x_1 and x_2, which corresponds to the one-dimensional S-wave.)

After calculating the matrix elements of the Hamiltonian in Eq. (4), the Schrödinger equation can be solved using the Lanczos algorithm in order to determine the ground state (S-channel) wave function $\psi_{\mathrm{A},1}$ as an eigenvector of H. The wave function can then be modified up to a range R via

$$\psi_{\mathrm{B},1}(c_{12}, d_{12}) = \psi_{\mathrm{A},1}(c_{12}, d_{12}) + \Delta\psi(c_{12}, d_{12}) \quad \text{for} \quad d_{12} = 0, 1, \ldots, R \tag{9}$$

where we introduced relative coordinates (centers of mass and distances) defined as

$$c_{ij} = \begin{cases} (x_i + x_j)/2 & \text{if } |x_i - x_j| < L - |x_i - x_j| \\ (x_i + x_j - L)/2 \mod L & \text{if } |x_i - x_j| \geq L - |x_i - x_j| \end{cases}, \tag{10}$$

$$d_{ij} = d(x_i, x_j) = \min(|x_i - x_j|, L - |x_i - x_j|) \tag{11}$$

taking into account the periodic boundary conditions. The modification $\Delta\psi(c, d)$ is constrained by the requirement to preserve the wave function normalization, $\sum_d |\psi_{\mathrm{B},1}(c, d)|^2 = \sum_d |\psi_{\mathrm{A},1}(c, d)|^2$. For a modification range $R = 1, 2, 3, \ldots$, it should be possible to tune the expectation values $\langle r^2 \rangle, \ldots, \langle r^{2R} \rangle$ order by order. (The corresponding operators are defined as

$$r^n = \frac{1}{N} \sum_x a^\dagger(x) a(x) \left(x - \frac{1}{N} \sum_{x'} a^\dagger(x') a(x') x' \right)^n \tag{12}$$

in the N-particle system.) In the $R = 0$ case, there would be no modification of ψ at all because $\Delta\psi(c_{12}, 0)$ is fixed by the conservation of the wave function norm.

3.2 Two-particle case

For our purpose, we define the unitary operator, inspired by Ref. [21], as

$$U = 1 - \frac{1}{2} \sum_x \sum_{d_1} \sum_{d_2} u(x, d_1) u(x, d_2)\ a^\dagger\left(x - \frac{d_2}{2}\right) a^\dagger\left(x + \frac{d_2}{2}\right) a\left(x - \frac{d_1}{2}\right) a\left(x + \frac{d_1}{2}\right) = U^\dagger \tag{13}$$

with the normalized wave function difference

$$u(x, d) = \frac{\Delta\psi(x, d)}{\sqrt{\sum_{d'} |\Delta\psi(x, d')|^2}} \tag{14}$$

that is real and symmetric in one-dimensional S-wave, i.e. $u(x, d) = u^*(x, d) = u(x, -d)$. This choice of U corresponds to a simple reflection transformation because

$$\langle x_1, x_2 | U | x_1', x_2' \rangle = \delta_{x_1, x_1'} \delta_{x_2, x_2'} - 2\delta_{c_{12}, c_{12}'} u(c_{12}, d_{12}) u(c_{12}, d_{12}') \tag{15}$$

$$\Rightarrow \sum_{x_1'} \sum_{x_2'} \langle x_1, x_2 | U | x_1', x_2' \rangle \underbrace{\langle x_1', x_2' | u \rangle}_{= u(c_{12}', d_{12}')} = - \underbrace{\langle x_1, x_2 | u \rangle}_{= u(c_{12}, d_{12})} \tag{16}$$

since the function u is normalized correctly according to Eq. (14):

$$\sum_{d_{12}} (u(c_{12}, d_{12}))^2 = 1. \tag{17}$$

It is easy to see that the employed unitary transformation maps the corresponding wave functions: $|\psi_{\mathrm{B},1}\rangle = U\,|\psi_{\mathrm{A},1}\rangle$. Moreover, it should be mentioned that the operator U in Eq. (13) is Galilean invariant, which can be seen by projecting it onto the states

$$|d_1,\ldots,d_{N-1}\rangle_P = \frac{1}{\sqrt{L}}\sum_x \exp\left(iP\left(\frac{d_1}{2}+\cdots+\frac{d_{N-1}}{2}+x\right)\right)|x+d_1,\ldots,x+d_{N-1},x\rangle \tag{18}$$

with a specific total momentum P: Obviously,

$${}_P\langle d|\,U\,|d'\rangle_P = \delta_{d,d'} - \frac{2}{L}\sum_x u\left(\frac{d}{2}+x,d\right)u\left(\frac{d}{2}+x,d'\right) \tag{19}$$

is independent of P.

3.3 Three-particle case

Naively, one could attempt to generalize the two-particle unitary transformation for three particles as

$$H_{\mathrm{naive}} = H + \sum_{(i,j,k)}(U_{ijk}H_{ijk}U_{ijk} - H_{ijk}), \tag{20}$$

where the sum runs over the index combinations $(i,j,k) = (1,2,3)$, $(1,3,2)$, $(2,3,1)$ and H_{ijk}, U_{ijk} are defined via the matrix elements

$$\begin{aligned}\langle x_1,x_2,x_3|\,H_{ijk}\,|x_1',x_2',x_3'\rangle &= \langle x_i|\,H_{\mathrm{free}}\,|x_i'\rangle\,\delta_{x_j,x_j'}\delta_{x_k,x_k'} + \delta_{x_i,x_i'}\,\langle x_j|\,H_{\mathrm{free}}\,|x_j'\rangle\,\delta_{x_k,x_k'}\\ &\quad + \langle x_i,x_j|\,V\,|x_i',x_j'\rangle\,\delta_{x_k,x_k'},\end{aligned} \tag{21}$$

$$\langle x_1,x_2,x_3|\,U_{ijk}\,|x_1',x_2',x_3'\rangle = \langle x_i,x_j|\,U\,|x_i',x_j'\rangle\,\delta_{x_k,x_k'}. \tag{22}$$

This transformation has the disadvantage that it cannot be written in the form $UHU^\dagger$ and thus cannot be applied easily to the wave function as $U\,|\psi\rangle$. Therefore, we consider the full matrix element

$$\langle x_1,x_2,x_3|\,U\,|x_1',x_2',x_3'\rangle = \delta_{x_1,x_1'}\delta_{x_2,x_2'}\delta_{x_3,x_3'} - 2\sum_{(i,j,k)}\delta_{c_{ij},c_{ij}'}u(c_{ij},d_{ij})u(c_{ij},d_{ij}')\delta_{x_k,x_k'} \tag{23}$$

of U from Eq. (13) instead. However, the operator U is not unitary in the three-particle case because the sum over (i,j,k) introduces additional terms that do not cancel in $\langle x_1,x_2,x_3|\,UU^\dagger\,|x_1',x_2',x_3'\rangle$ as for two particles. Fortunately, this problem can be cured by "switching off" the transformation if the spectator particle k comes too close to the center of mass c_{ij} of the particles on which U acts:

$$\begin{aligned}\langle x_1,x_2,x_3|\,U_{3\mathrm{p}}\,|x_1',x_2',x_3'\rangle &= \delta_{x_1,x_1'}\delta_{x_2,x_2'}\delta_{x_3,x_3'} - 2\sum_{(i,j,k)}\delta_{c_{ij},c_{ij}'}u(c_{ij},d_{ij})u(c_{ij},d_{ij}')\delta_{x_k,x_k'}\\ &\quad\times\theta\big(d(c_{ij},x_k)\geq d_{\min}\big)\end{aligned} \tag{24}$$

with the Heaviside function

$$\theta(x\geq x_0) = \begin{cases}1 & \text{if } x\geq x_0\\ 0 & \text{otherwise}\end{cases}. \tag{25}$$

If the distance $d_{\min}$ is chosen large enough as compared with the range of U, more precisely $d_{\min} > 3R/2$, the transformation reduces to an effective unitary two-body operator for the particles i and j (cf. the numerical results shown below). Like the operator U in the two-particle case, $U_{3\mathrm{p}}$ is Hermitian as well.

4. Computational results

4.1 Two-particle case

For a benchmark calculation, we use the lattice spacing $a = (100\ \text{MeV})^{-1} = 1.9733$ fm and choose the lattice length $L = 71a$ such that the wave function approximately vanishes at the boundary of the lattice. (Notice that we switched back to physical units in order to simplify the interpretation of the numerical results.) The left plot in Fig. 1 shows the original wave function $|\psi_{\text{A},1}\rangle$ and several modified wave functions $|\psi_{\text{B},1}\rangle = U\,|\psi_{\text{A},1}\rangle$ for different choices of $\Delta\psi(c_{12}, 2a)$ whereas $\Delta\psi(c_{12}, a) = 0$ and $\Delta\psi(c_{12}, d_{12} > 2a) = 0$.

In the following, we consider the Hamiltonian projected onto states with zero total momentum via ${}_{P=0}\langle d|\,H\,|d'\rangle_{P=0}$ and denote its n-th lowest eigenstate by $|\psi_{\text{A},n}\rangle$. While the expectation values $\langle\psi_{\text{A},n}|\,H\,|\psi_{\text{A},n}\rangle$ and $\langle\psi_{\text{B},n}|\,UHU\,|\psi_{\text{B},n}\rangle = \langle\psi_{\text{A},n}|\,U^2HU^2\,|\psi_{\text{A},n}\rangle$ of the Hamiltonian are the same because U is unitary, the transformed RMS radius depends significantly on the wave function. The latter can be seen from the right part of Fig. 1 where $\sqrt{\langle\psi_{\text{A},1}|\,Ur^2U\,|\psi_{\text{A},1}\rangle}$ is plotted as a function of $\Delta\psi(c_{12}, 2a)$. It should be emphasized that $\sqrt{\langle\psi_{\text{A},1}|\,U^2r^2U^2\,|\psi_{\text{A},1}\rangle}$ does not depend on the wave function modification and therefore is not suitable to produce the effect desired here.

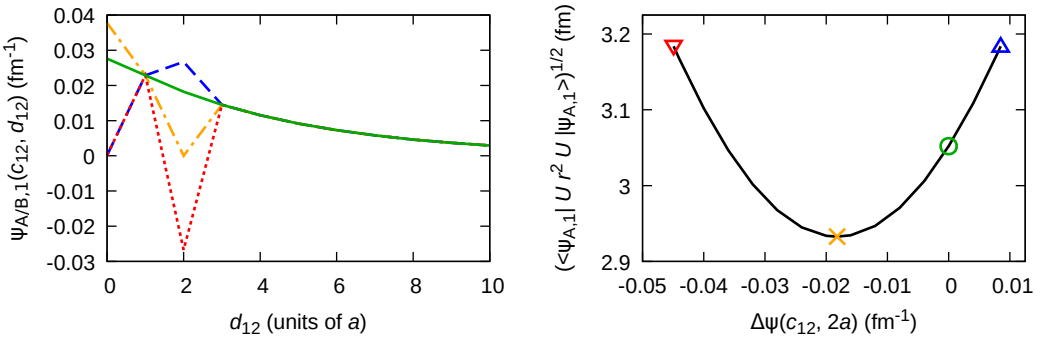

Figure 1: Left plot: examples of the modification of the original two-particle wave function $\psi_{\text{A},1}$ (solid green line) at $d_{12} = 2a$ in the possible range allowed by the conservation of the norm. For the values $(\Delta\psi(c_{12}, 2a))_{\text{min}} = -0.0449205\ \text{fm}^{-1}$ (dotted red line) and $(\Delta\psi(c_{12}, 2a))_{\text{max}} = 0.0084945\ \text{fm}^{-1}$ (dashed blue line), the modified wave function $\psi_{\text{B},1}$ approximately vanishes at the origin. The dot-dashed orange line corresponds to the case $\psi_{\text{B},1}(c_{12}, 2a) \approx 0$ that appears for $((\Delta\psi(c_{12}, 2a))_{\text{min}} + (\Delta\psi(c_{12}, 2a))_{\text{max}})/2$.
Right plot: Transformed two-particle RMS radius as a function of the wave function modification at $d_{12} = 2a$. The red lower triangle, orange cross, green circle and blue upper triangle correspond to the wave functions of the same colors in the left plot.

4.2 Three-particle case

In the three-particle system, we again restrict ourselves to states with zero total momentum and denote the n-th lowest eigenstate of ${}_{P=0}\langle d_1, d_2|\,H\,|d_1', d_2'\rangle_{P=0}$ and ${}_{P=0}\langle d_1, d_2|\,H_{\text{naive}}\,|d_1', d_2'\rangle_{P=0}$ by $|\psi_{\text{3p},n}\rangle$ and $|\psi_{\text{3p,naive},n}\rangle$, respectively. As already mentioned in Section 3.3, the energy expectation values $E_{\text{3p,naive},n} = \langle\psi_{\text{3p,naive},n}|\,H_{\text{naive}}\,|\psi_{\text{3p,naive},n}\rangle$ are distorted by the naive application of the operator U (cf. the left plot in Fig. 2).

In contrast to this, switching off the transformation at particle-dimer distances smaller than $d_{\text{min}} = 4a$ leads to an effective unitary operator U_{3p} that leaves the energy expectation values

$E_{3\mathrm{p},n} = \langle\psi_{3\mathrm{p},n}|\, U_{3\mathrm{p}}^2 H U_{3\mathrm{p}}^2\, |\psi_{3\mathrm{p},n}\rangle$ invariant. ($d_{\min} = 4a$ is the minimal possible value that restores the unitarity of U at the three-body level.) As expected, one observes that one can affect the three-body radius by means of the employed unitary transformation (cf. the right plot in Fig. 2).

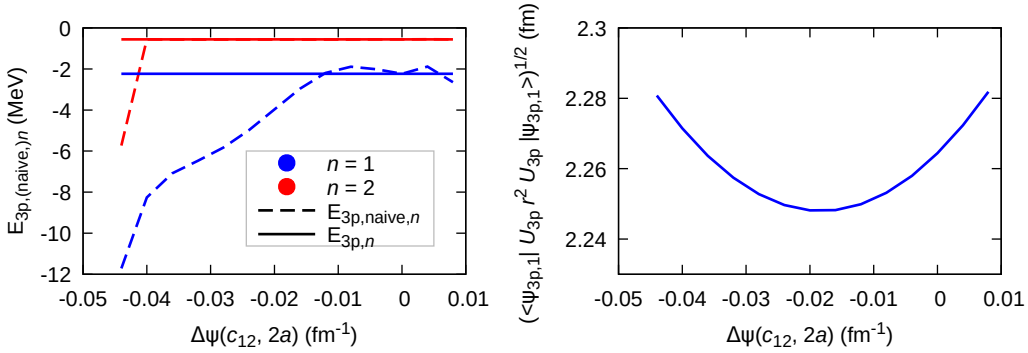

Figure 2: Expectation values of the three-particle Hamiltonian (left plot) and transformed three-particle RMS radius (right plot) as functions of the wave function difference at $d_{12} = 2a$ without (dashed lines) and with (solid lines) switching off the unitary transformation at short particle-dimer distances. The energy for $n = 2$ corresponds to a scattering state whose r^2 expectation value does not converge in the limit $L \to \infty$ and is thus not shown here.

5. Summary and outlook

In this paper, we have developed a method to tune the lattice result for the $\langle r^2 \rangle$ expectation value to experimental data. It has been shown that the two-particle and three-particle RMS radius can be changed without affecting the phase shifts by applying a unitary transformation U to the wave function. We have tested our method for a one-dimensional toy-model system.

The generalization of the procedure to arbitrary $\langle r^n \rangle$ expectation values or electromagnetic moments should be straightforward by using a unitary transformation with a larger range and thus more parameters. (This approach is similar to tuning the coefficients of the derivative expansion of the potential.) However, we expect our method to yield good results after correcting the first few $\langle r^n \rangle$ expectation values in practice.

A naive extension of the considered two-particle transformation to $N > 2$-particle systems violates unitarity. A simple way to restore unitarity of the operator U for the three-particle system is provided by "switching off" the transformation at short particle-dimer distances that are smaller than a threshold $d_{\min}$ related to the range of U. Using this method allowed us to study the effect of the two-body charge density operators, induced by the considered unitary transformation, on the three-particle RMS radius. To extend these results to $N \geq 4$-particle systems, the unitary transformation should additionally possess system extensivity, i.e. it should act on all pairs of particles simultaneously.

Finally, our method should be straightforwardly extendable to three spatial dimensions, non-zero spin and isospin as well as a realistic nuclear interaction. Work along these lines is in progress.

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