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Phase shifts in $I = 2$ $\pi\pi$-scattering from two lattice approaches

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We compare two approaches used for computing scattering phase shifts and other low-energy observables in lattice QCD: the finite size method invented by Lüscher as well as the recently introduced HAL QCD method which is based on the extraction of multi body potentials from Nambu-Bethe-Salpeter wave functions. We perform quenched QCD simulations featuring lattices with spatial extents of 1.8 fm to 5.5 fm, a lattice spacing of 0.115 fm and a pion mass of 940 MeV. We compute phase shifts and scattering length of $\pi\pi$ scattering in the I=2 channel for either method and compare the results.

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[†]A footnote may follow.

1. Introduction

Recent developments in lattice QCD, algorithmic techniques and computer technology allow us to perform ab-initio calculations of multi-hadron scattering observables. This helps us getting deeper insights and a better understanding of the nuclear force.
The most common approach to these kind of problems is the finite volume method invented by Lüscher [1, 2]. It is based on the idea that information on scattering phase shifts of two-particles can be extracted by computing energy differences between the interacting and the non-interacting system contained in a box. Recently, HAL QCD proposed another method which employs the Nambu-Bethe-Salpeter wave function in order to extract interaction kernels (potentials) in a lattice simulation [3, 4]. From these kernels, low-energy observables such as scattering phase shifts and lengths can be obtained by solving the corresponding Schrödinger equation.
In this paper, we compare these two approaches by applying them to the I=2 two-pion scattering problem, which can be evaluated very precisely in present day lattice calculations. In principle, both methods should give the same results but are affected by different systematic uncertainties which we carefully address in this paper.

2. Potential method

As an input for both methods, we need to compute the single-pion as well as the double pion correlation functions defined by $C_\pi(t,t_0) \equiv \sum_{\mathbf{x}} \left\langle \pi^+(t,\mathbf{x}) J_{\pi^-}(t_0) \right\rangle / V$ and $C_{\pi\pi}(t,t_0,\mathbf{r}) \equiv \sum_{\mathbf{x}} \left\langle \pi^+(t,\mathbf{x}+\mathbf{r})\pi^+(t,\mathbf{x}) J_{\pi^-}(t_0) J_{\pi^-}(t_0) \right\rangle / V$. Here, V is the spatial volume of the lattice and J_{π^-} a pseudo-scalar interpolating operator. In this paper, we employ plain wall sources[1]. In order to suppress potential statistical and systematic effects, we consider the ratio $R(t,t_0,\mathbf{r}) \equiv C_{\pi\pi}(t,t_0,\mathbf{r}) / C_\pi^2(t,t_0)$. Note that the summed ratio $R(t,t_0) \equiv \sum_{\mathbf{r}} R(t,t_0,\mathbf{r})$ drops off exponentially fast with the energy difference $\Delta E = 2\sqrt{k^2+m_\pi^2} - 2m_\pi$ for $|t-t_0| \to \infty$. Therefore, one can compute the asymptotic momentum k^2 from the effective mass plateau of $R(t,t_0)$ and the pion mass m_π. In a second step, the obtained k^2 is plugged into the energy-eigenvalue equation of two particles in a box which is then solved for the scattering phase shift $\delta(k)$. This is Lüscher's famous finite volume approach and all relevant information can be found in [1].
The HAL QCD potential method instead makes use of the spatial information contained in $R(t,t_0,\mathbf{r})$: one can show [6] that $R(t,t_0,\mathbf{r})$ obeys the time-dependent Schrödinger-like equation

$$\left(-\frac{\partial}{\partial t} + \frac{1}{4m_\pi}\frac{\partial^2}{\partial t^2} + \frac{\nabla_{\mathbf{r}}^2}{m_\pi} \right) R(t,t_0,\mathbf{r}) = \int \mathrm{d}^3 r' \, U(\mathbf{r},\mathbf{r}') R(t,t_0,\mathbf{r}'), \tag{2.1}$$

where U is a non-local kernel function. We expand it in terms of derivatives, where we only keep the (ultra-local) LO term $V_C(r)$. Substituting this expansion into (2.1) and solving for $V_C(r)$ yields

$$V_C(r) = \frac{1}{m_\pi} \frac{\nabla_{\mathbf{r}}^2 R(t,t_0,\mathbf{r})}{R(t,t_0,\mathbf{r})} - \frac{\frac{\partial}{\partial t} R(t,t_0,\mathbf{r})}{R(t,t_0,\mathbf{r})} + \frac{1}{4m_\pi} \frac{\frac{\partial^2}{\partial t^2} R(t,t_0,\mathbf{r})}{R(t,t_0,\mathbf{r})}. \tag{2.2}$$

Expression (2.2) allows us to compute $V_C(r)$ on the lattice. Subsequently, we insert this potential into the Schrödinger equation

$$\left(k^2 + \nabla_{\mathbf{r}}^2\right) \psi_{\mathbf{k}}(\mathbf{r}) = m_\pi V_C(r) \psi_{\mathbf{k}}(\mathbf{r}) \tag{2.3}$$

[1] A study which also includes Gaussian sources can be found in [5]

which can then be solved for arbitrary k^2 in the continuum and infinite volume limit.[2] For that purpose, the potential is interpolated using a barycentric rational interpolation and set to zero for $r>r_{\max}$, where $r_{\max}$ is the largest observed distance. [3] By matching the resulting wave function $\psi_{\mathbf{k}}$ for large $|\mathbf{r}|$ to the asymptotic form predicted by scattering theory

$$\psi_{\mathbf{k}}(r) \overset{r\to\infty}{\longrightarrow} e^{i\delta(k)}\big(\cos\delta(k)\, j_0(kr) - \sin\delta(k)\, n_0(kr)\big), \tag{2.4}$$

we are able to extract the scattering phase shift $\delta\equiv\delta(k)$.
Once the scattering phase shifts δ for different asymptotic momenta k are extracted, we can fit the data to the effective range expansion

$$\frac{k\cot\delta(k)}{m_\pi} = \frac{1}{m_\pi a_{\pi\pi}^{I=2}} + \frac{1}{2} m_\pi r_{\mathrm{e}} \left(\frac{k^2}{m_\pi^2}\right) + P\,(m_\pi r_e)^3 \left(\frac{k^2}{m_\pi^2}\right)^2 + \mathscr{O}\left(\left(\frac{k^2}{m_\pi^2}\right)^3\right) \tag{2.5}$$

in order to obtain the scattering length $a_{\pi\pi}^{I=2}$.

3. Setup and error treatment

We generate approximately 400 statistically independent quenched configurations using the Wilson plaquette action at β=5.8726, corresponding to $a\sim$0.115 fm. We use volumes with spatial extents of L_s/a=16, 24, 32 and 48 with a fixed temporal extent of L_t/a=128. In the valence sector, we use 2 HEX smeared, tree-level clover improved Wilson quarks [7 – 10], which exhibit small cutoff effects on spectral quantities [11, 9]. The pion mass was tuned to $m_\pi\sim$940 MeV and we use Dirichlet boundary conditions in temporal direction. A more detailed study involving smaller pion masses and anti-periodic boundary conditions can be found in [5]. In order to improve statistics, we use four sources per config with a relative shift of 32 time-slices.
The statistical error is computed by repeating the analysis on 2000 bootstrap samples. We estimate the systematic uncertainty with the histogram method [8 – 10, 12 – 14]. The following possible sources of systematic uncertainty were considered:

- Contributions from excited states: we vary the lower bound of the fitting range for extracting m_π (potential and Lüscher's method), ΔE (Lüscher's method) and $V_C(r)$ (potential method). We consistently used the time intervals R_1=[15, 48], R_2=[24, 48], R_3=[33, 48].

- Violation of rotational invariance: finite volume and discretization effects break rotational invariance. Whereas this source of systematic uncertainty is hard to estimate in Lüscher's method, it can be well assessed in the potential method. This is done by extracting the potential along three extreme lattice directions, i.e. on-axis, along a plane-diagonal and along the cubic-diagonal.

- Asymptotic regime: in the potential method, the phase shift is extracted from the wave function in the asymptotic regime. In order to make sure that we reached that regime, we use five disjoint regions in r from which we extract δ and propagate the differences among these regions into the final systematic error.

[2] Note that the energy of the two-particle system has to be below the threshold of inelastic scattering.

[3] We also applied phenomenologically motivated fits which smoothly approach zero in the large distance limit but found no significant difference in the final results from the interpolation approach.

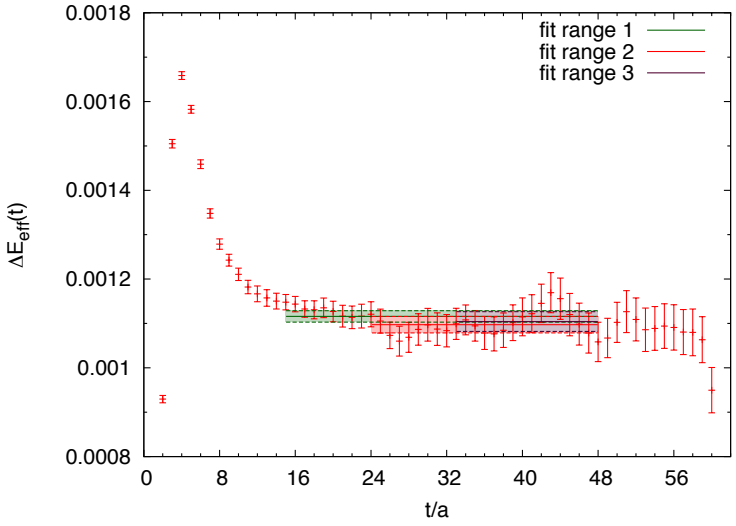

Figure 1: Constant fits to effective mass plateau of $R(t,t_0)$. Bands indicate the corresponding errors from the fits. Note that the systematic uncertainty attributed to the choice of the fitting range (R_1, R_2, R_3) is small (L_s=3.7 fm).

- Higher orders in effective range expansion: we fit $\delta(k)$ to the effective range expansion (2.5) where we either include only terms up to NLO or up to NNLO.

This amounts to 3·3·5·2=90 analyses for the potential method and 3·2=6 different analyses for Lüscher's method. The results obtained from the different analyses are collected in a histogram. In case of the scattering phase $\delta(k)$ we assign a weight of one to each analysis. In case of the scattering length, the results were weighted with the quality-of-fit obtained from the fit to the effective range expansion (we have checked that choosing a unit weight instead yields compatible results, i.e. the central value changes by less than 0.1σ and the systematic error increases by less than 1%). In all cases, the median of the resulting distribution yields our central value and the central 68% the systematic error.

4. Results

$a_{\pi\pi}^{I=2}$[fm]	value	stat.	sys. total	exc. states	rot.-inv.	asympt.	ERE
Potential	-0.1568	0.0005	0.0063	0.0002	0.0062	0.0	0.0006
Lüscher	-0.1615	0.0020	0.0020 + ?	0.0017	?	–	0.0008

Table 1: Results for scattering lengths $a_{\pi\pi}^{I=2}$ obtained from either method at m_π∼940 MeV, including a full error budget. The breakups include the effect of excited states (column 5), the violation of rotational invariance (column 6, not estimated for Lüscher's method, see text), the asymptotic behavior of the wave-function (column 7, applicable only for the potential method) and different orders in the effective range expansion (column 8). Due to correlations, the errors do not sum up to 100% when added in square.

Figure 1 displays the effective mass plateau of $R(t,t_0)$ with different fits for all three ranges R_i. It demonstrates that effects of excited states are small in the considered fit regions. The analogous

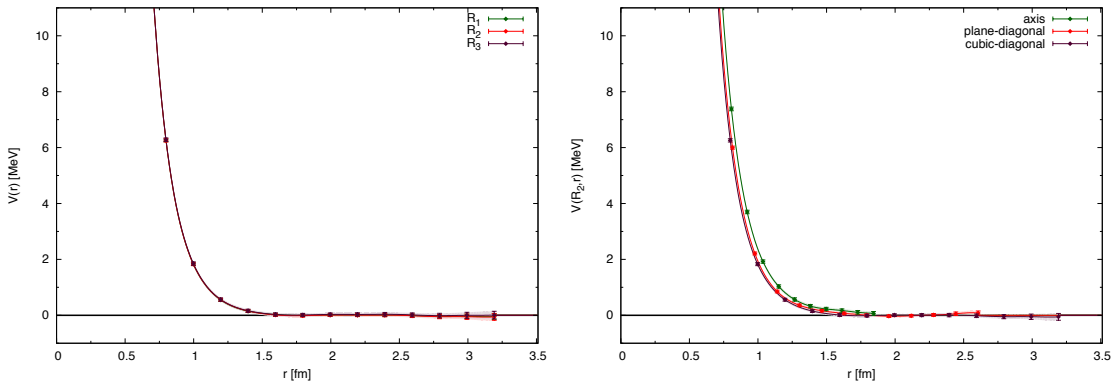

Figure 2: Left: two-pion potential on different ranges R_i computed on the cubic diagonal (points). Right: two-pion potential for R_2 but evaluated on axis (green squares), along plane-diagonals (red circles) or cubic-diagonal (purple diamonds). In both cases, the bands indicate the result for the interpolation (L_s=3.7 fm).

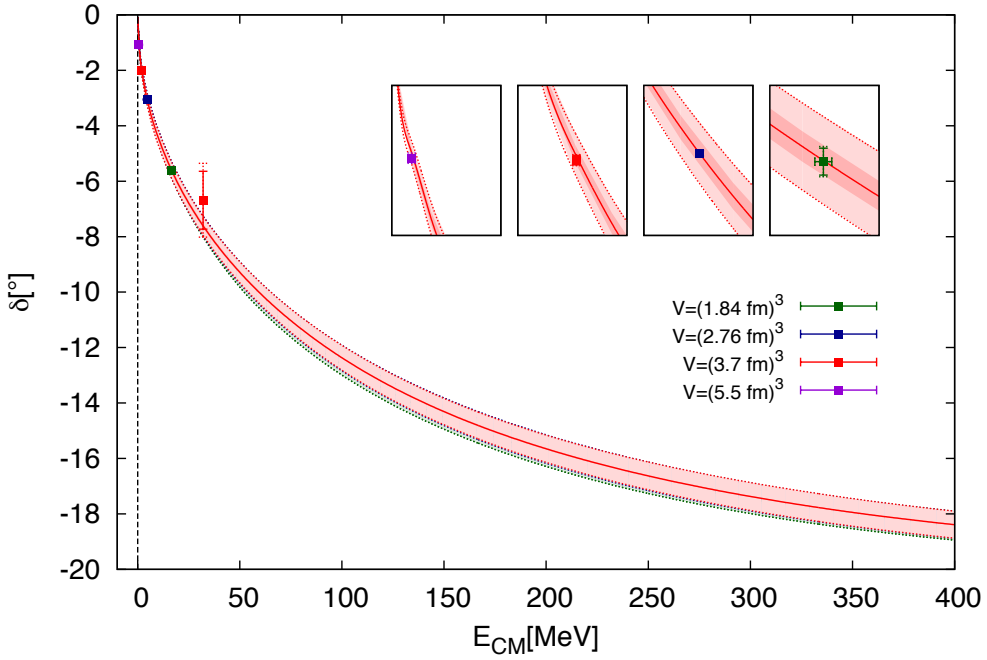

Figure 3: Scattering phase shifts obtained from the potential and Lüscher's method. The red band is obtained by the HAL QCD method using the potential obtained from L_s=3.7 fm. The green band is obtained from L_s=1.8 fm, and almost overlaps with one from L_s=3.7 fm. The point data are obtained by Lüscher's method with the center-of-mass frame on each volumes, except for the red point around $E_{\rm cm} \sim 30$ MeV, which is obtained on the L_s=3.7 fm volume by applying Lüscher's method to boosted system with center-of-mass momentum $P_{\rm cm}=2\pi/L_s$.

plot for the potential method is shown in the left panel of Figure 2. It depicts the r dependence of the potentials, extracted from the lattice cubic-diagonal and different time slices R_i. The good agreement among the curves suggests that higher orders in the derivative expansion are small. This is different for the effect of rotational invariance breaking, as can be seen from the right panel of Figure 2. It displays the potentials obtained on the same temporal range R_2 but from different lattice directions. Here we observe deviation between the on-axis data and the other two. This uncertainty induced by rotational invariance violation is the major contribution to the overall systematic error of the potential method.

The fitted potential can be inserted into the Schrödinger equation (2.3) which can then be solved for arbitrary k^2 in order to obtain the two-pion wave functions $\psi_{\mathbf{k}}$ in infinite volume. From these we compute the scattering phase shifts $\delta(k)$. The computed curve can be compared to the phase shifts obtained from Lüscher's method. This is done in Figure 3, where the bands correspond to the results obtained from the potential method and the points correspond to those obtained from Lüscher's method. We observe that the results of both methods agree very well. In the potential method, the red band corresponds to the results obtained from L_s=3.7 fm. The same curve is drawn for L_s=1.84 fm in green and highly agrees with the results obtained at L_s=3.7 fm, since only a tiny fraction of it can be seen at the lower edge of the red band. Comparing the potential on different volumes, we find that the finite volume artifact in the potential is negligible; all potentials agree within errors. As a result, the phase shifts obtained from potentials computed on $L_s=(1.8-5.5)$ fm agree very well within errors. In Lüscher's method, the phase shifts at different energies are mostly obtained in the center-of-mass frame by changing the lattice spatial volume. We also study the non-rest frame extension of Lüscher's method for L_s=3.7 fm, which corresponds to the data point at $E_{\mathrm{CM}}\sim$30 MeV. The error bar is rather large since it is extracted in a boosted system with boost momentum $\mathbf{P}_{\mathrm{cm}}=(1,0,0)$.

Finally, we want to compare the scattering lengths $a_{\pi\pi}^{I=2}$ obtained from either method. Since finite volume effects are small in the potential method, we extract the scattering length from our reference lattice with L_s=3.7 fm in that case. For Lüscher's method we have to take into account all four different volumes in order to perform the $k\to 0$ extrapolation. Table 1 displays the results of these extrapolations along with an error budget. It exhibits that the dominant source of systematic uncertainty is the violation of rotational invariance. This uncertainty is hard to estimate in Lüscher's approach since the spatial information on the two-particle correlation functions is lost: the systematic error for that method is thus underestimated. Furthermore, the contributions from excited states is more relevant for this method than for the potential method. Therefore, the potential method is well suited for analyzing multi-baryon systems in which the signal degrades exponentially fast with time.

5. Summary

We have performed an I=2 $\pi\pi$ scattering study in quenched QCD with heavy pions of $m_\pi \sim$ 940 MeV. In the determination of scattering phase shifts on the lattice, two different approaches have been employed with a particular emphasis on the examination of systematic uncertainties in each method: Lüscher's finite volume approach and the HAL QCD potential method. The results of the phase shift and the scattering length have been found to agree well between the two methods.

We have observed that the largest systematic uncertainty in the potential method stems from the violation of rotational invariance, while such a systematic uncertainty is difficult to estimate in Lüscher's method and thus has been neglected in this study. While Lüscher's method is sensitive to excited state contaminations, the time-dependent potential method can compensate a gross of these effects. This is especially important when multi-baryon systems are considered. Furthermore, the potential approach allows for extracting the scattering phase at arbitrary momenta, as long as the energy of the system is below the inelastic threshold.

References

[1] M. Luscher. *Volume Dependence of the Energy Spectrum in Massive Quantum Field Theories. 2. Scattering States*. *Commun.Math.Phys.*, **105**:153–188, 1986.

[2] Martin Luscher. *Two particle states on a torus and their relation to the scattering matrix*. *Nucl.Phys.*, **B354**:531–578, 1991.

[3] N. Ishii, S. Aoki, and T. Hatsuda. *The Nuclear Force from Lattice QCD*. *Phys.Rev.Lett.*, **99**:022001, 2007.

[4] Sinya Aoki, Tetsuo Hatsuda, and Noriyoshi Ishii. *Theoretical Foundation of the Nuclear Force in QCD and its applications to Central and Tensor Forces in Quenched Lattice QCD Simulations*. *Prog.Theor.Phys.*, **123**:89–128, 2010.

[5] T. Kurth, N. Ishii, T. Doi, S. Aoki, and T. Hatsuda. *Phase shifts in I=2 $\pi\pi$-scattering from two lattice approaches*. *JHEP*, **1312**:015, 2013.

[6] Noriyoshi Ishii et al. *Hadron-Hadron Interactions from Imaginary-time Nambu-Bethe-Salpeter Wave Function on the Lattice*. *Phys.Lett.*, **B712**:437–441, 2012.

[7] Stefano Capitani, Stephan Durr, and Christian Hoelbling. *Rationale for UV-filtered clover fermions*. *JHEP*, **0611**:028, 2006.

[8] S. Durr, Z. Fodor, C. Hoelbling, S.D. Katz, S. Krieg, et al. *Lattice QCD at the physical point: light quark masses*. *Phys.Lett.*, **B701**:265–268, 2011.

[9] S. Durr, Z. Fodor, C. Hoelbling, S.D. Katz, S. Krieg, et al. *Lattice QCD at the physical point: Simulation and analysis details*. *JHEP*, **1108**:148, 2011.

[10] S. Durr, Z. Fodor, C. Hoelbling, S.D. Katz, S. Krieg, et al. *Precision computation of the kaon bag parameter*. *Phys.Lett.*, **B705**:477–481, 2011.

[11] S. Durr, Z. Fodor, C. Hoelbling, R. Hoffmann, S.D. Katz, et al. *Scaling study of dynamical smeared-link clover fermions*. *Phys.Rev.*, **D79**:014501, 2009.

[12] Szabolcs Borsanyi, Stephan Durr, Zoltan Fodor, Christian Hoelbling, Sandor D. Katz, et al. *High-precision scale setting in lattice QCD*. *JHEP*, **1209**:010, 2012.

[13] S. Durr, Z. Fodor, J. Frison, C. Hoelbling, R. Hoffmann, et al. *Ab-Initio Determination of Light Hadron Masses*. *Science*, **322**:1224–1227, 2008.

[14] S. Durr, Z. Fodor, T. Hemmert, C. Hoelbling, J. Frison, et al. *Sigma term and strangeness content of octet baryons*. *Phys.Rev.*, **D85**:014509, 2012.