physics760 Computational Physics

Analysis of π-π lattice QCD scattering data

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Correlation functions of pions that were computed with lattice QCD methods are analyzed. The effective masses of single pions and two interacting pions are extracted. Using a finite size formula by Lüscher, the S-wave scattering length is computed.

Contents

1 Data generation

Monte Carlo methods can be used to simulate quantum systems. Key pieces are Feynman's path integral formalism and Euclidean spacetime. In the latter, the metric tensor η has signature ± 4 and the weight factor in the path integral is $\exp(-S_{\mathrm{cl}})$ instead of $\exp(\mathrm{i}S_{\mathrm{cl}})$; S_{cl} is the classical action (Creutz and Freedman 1980, Section 2). A Monte Carlo algorithm like the Metropolis algorithm can then be used to generate configurations which are already distributed by the weight of the classical action. Therefore, expectational values of observables are simply calculated and averaged over all available configurations (ibid., (3.7)).

The group of Andreas Kell, Martin Efferz and Simon Blanke have used this for the harmonic oscillator in their Computational Physics project this year. I also did this in my bachelor's thesis last year (Ueding 2014).

For quantum chromodynamics (QCD), the theory of the strong force, this methodology can be used as well. The action of QCD is used with a hybrid Monte Carlo algorithm to generate configurations of gauge fields on a four dimensional lattice. This process is done for several ensembles which differ in parameters like the quark mass. Ensemble generation takes a lot of computing time, so the results are made available to download.

As with the harmonic oscillator on the lattice, expectation values of observables can be computed for each configuration of the ensembles and then averaged (without weight) over all ensembles yielding an estimate for the observable. Since this uses a field theory, particles of interest can be created at the beginning of time and annihilated laster on. This way, specific particle configurations (like π–π scattering) can be examined without needing to generate new configurations.

Using the correct operators, it is possible to construct correlation functions which contain information about the energies/masses of the involved particles, analogously to (Creutz and Freedman 1980, (4.14)) for the harmonic oscillator. I was given those correlation functions to analyze.

2 Analysis methods

Figure 1 shows the data flow in the analysis. This section will go through the whole analysis in the order of the flow chart. The methods used will be explained along the way when they are needed.

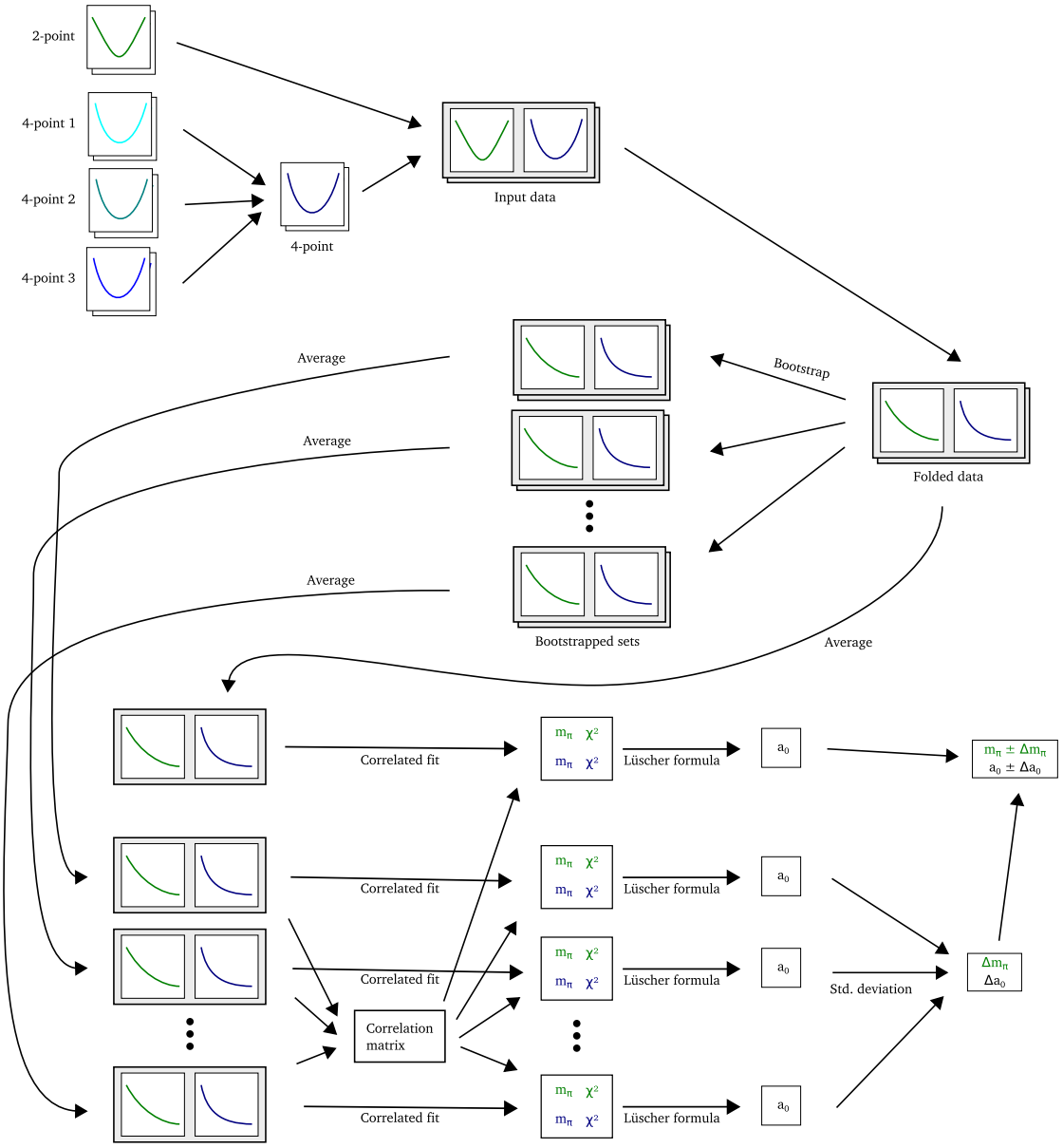

Figure 1: Data flow in the analysis. The first step is the import of the data, which is covered in Section 2.1. The two and four point functions are combined into pairs for each configuration. The data is then folded in half. The bootstrap step is covered in Section 2.2. Then a correlated fit is performed, see Section 2.3 for details. The second to last step is the application of Lüscher's formula, see Section 2.4. The results are shown in Section 3.

2.1 Import data

The data that I was given is organized in different ensembles (like A30.32, A100.24) as mentioned in the introduction. For each ensemble, multiple configurations were simulated. The output of each configuration is one two-point correlation function $C_\pi(t)$ and three four-point correlation functions $C^{(i)}_{\pi\pi}(t)$. Those three different contractions are combined into a single $\pi\pi$-correlation function:

$$C_{\pi\pi}(t) = C^{(1)}_{\pi\pi}(t) + C^{(2)}_{\pi\pi}(t) - 2C^{(3)}_{\pi\pi}(t). \tag{1}$$

Some of the ensembles had multiple versions of the data in it. I analyzed all of them sorted by file name. In the tables, you will find the ensembles multiple times, those are the different versions.

The number of configurations in each ensemble is called N.

In both space and time, the lattice used in the computation has periodic boundary conditions. The spatial lattice extent is called L, the temporal one T. This leads to a symmetry where the time slices t and $T-t$ closely related. The correlation functions $C(t)$ with $t = |t_1 - t_2|$ are symmetric in t_1 and t_2, such that only the data in the interval $[0, T/2]$ carries independent information. Before starting any other calculations with the data, it is folded in half and averaged. The data then looks like in Figure 3 which appears laster on.

2.2 Bootstrap

All error estimation is done with the bootstrap method. One other known method to compute errors is the Gaussian error propagation. This method involves computing derivatives of the functions applied to the data, which can be either numerically unstable or just not really applicable: How does the variance of the mean change when you change the input data?

In order to get rid of all those problems at the same time one does a meta analysis of the data itself. To get back to the example of the mean, let X be the set of N data points ($x_i \in \mathbb{R}$). Then the estimator of the mean $\bar{\mu}$ can be computed directly from X. Now R bootstrap samples X^r (upper index, no power) are computed from the set by randomly selecting N elements from X and putting them into X^r. Since X is sampled from the original distribution, it resembles the original distribution as good as it can with only N elements. X^r therefore is sampled from an approximation of the original distribution. Then the estimators for the means $\bar{\mu}^r$ are computed from the bootstrapped sets. The mean of all the $\bar{\mu}^r$ should give $\bar{\mu}$, which was computed from the original data. The error estimate is then the standard deviation of all the $\bar{\mu}^r$. (*Physics 509: Bootstrap and Robust Parameter Estimation*, Slide 5)

The number of bootstrap samples R was set to $R = 3N$ for each ensemble.

2.3 Correlated fit

The pion masses are contained in the correlation functions in the form of an exponential decay constant. Since time is periodic in this simulation, the correlation function is also periodic with the temporal lattice extent T. Therefore, the expectation is not a simple exponential decay, $\exp(-\lambda t)$, but a cosh-like function. The four-point functions also have a constant contribution due to the finite lattice extent. For both two and four point functions, the functions that I fitted to the folded data with parameters $\boldsymbol{\lambda}$ are:

$$m_\pi(t, \lambda) = \lambda_1 \left[\exp(-\lambda_2 t) + \exp(-\lambda_2 [T - t])\right] \tag{2}$$

and

$$m_{\pi\pi}(t, \lambda) = \lambda_1 \left[\exp(-\lambda_2 t) + \exp(-\lambda_2 [T - t])\right] + \lambda_3. \tag{3}$$

The parameter λ_3 is a lattice artifact that will vanish for $L \to \infty$.

In order to determine the fit range, I have used the effective mass as shown in Figure 2. The plateau starts at $t/a = 13$, so those are the points I have used. The folded correlation functions with the fit functions are shown in Figure 3.

The correlation functions themselves are highly correlated with respect to time. Therefore, a regular least squared fit would give a χ^2 that would be way too low for the assumed degrees of freedom. The p-values usually end up around 1, which does not imply a perfect fit but rather that the data fits the model *too well*. This, in turn, means that errors and residuals are over-estimated with the given model. A different model is called for: the correlated fit.

For the correlated fit, a new likelihood function is needed. I chose to keep the falling exponential likelihood function but incorporate the correlation into the χ^2. First, a correlation matrix $\boldsymbol{C}$ is needed, which is computed from the R bootstrap samples: (Michael and McKerrell 1995, Section 2)

$$C_{ij} := \frac{1}{R[R-1]} \sum_{r=1}^{R} [x_{ir} - \bar{x}_{iR}][x_{jr} - \bar{x}_{jR}], \quad \bar{x}_{iR} := \frac{1}{R} \sum_{r=1}^{R} x_{ir}. \tag{4}$$

Using this correlation matrix, a new χ^2 can be defined which incorporates the inverse

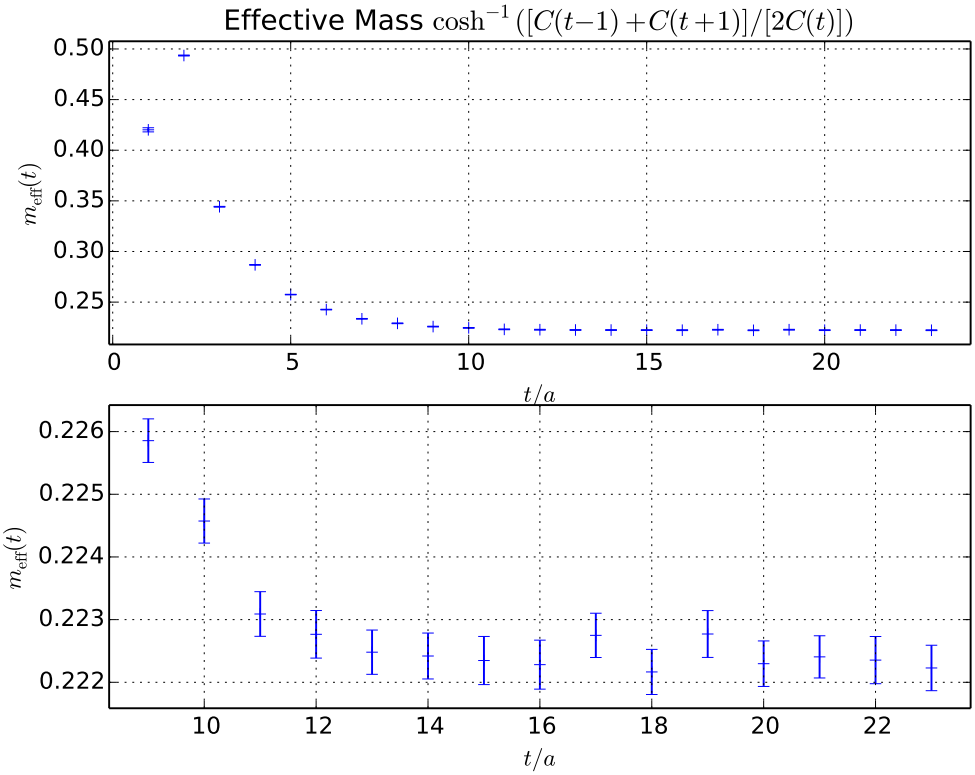

Figure 2: Effective mass of A100.24 ensemble.

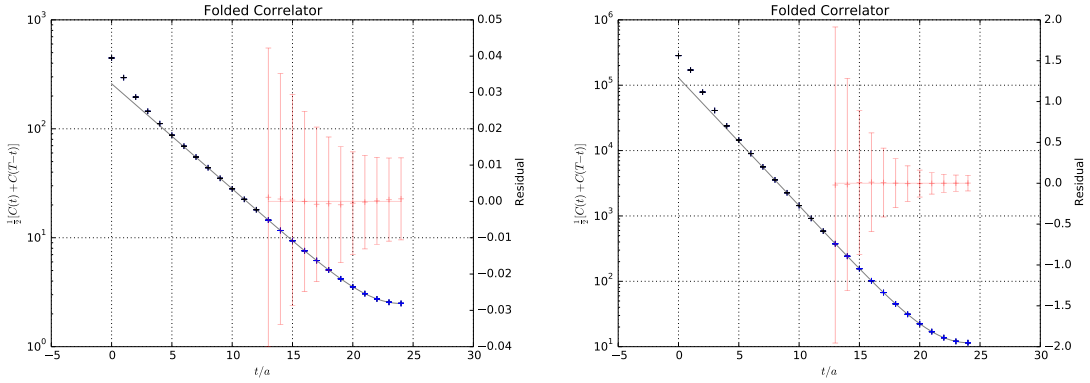

Figure 3: Folded correlation functions with cosh-like fit function. On the left side, the two point function is shown using a logarithmic ordinate scale. The four point function is shown on the right. Only the blue data points were used for fitting. The right ordinate shows the residuals in great magnification (red). One can see that the errors seem way too large compared to the residuals. This is a result of the autocorrelation of the data points. Ensemble is A100.24.

correlation matrix:

$$\chi^2_{\text{corr}} := \sum_{i,j}^{T} \left[\bar{x}_{iR} - f(t_i, \lambda)\right] C^{-1}_{ij} \left[\bar{x}_{jR} - f(t_j, \lambda)\right]. \tag{5}$$

The regular χ^2 has $\boldsymbol{C}^{-1} = \boldsymbol{1}$ and is just the sum of the squared residuals.

In the curve fitting process, a function like `scipy.optimize.curve_fit` tries to find the parameters $\boldsymbol{\lambda}$ such that χ^2 becomes minimal. In my implementation, I used the function `scipy.optimize.leastsq` which tries to minimize the squared norm of a vector valued function. With a Cholesky decomposition, this can be done like so: Define the square bracket in Equation (5) to be the residual vector $\boldsymbol{r}(\boldsymbol{\lambda})$. Then the matrix multiplication can be written as

$$\chi^2 = \boldsymbol{r}^{\mathrm{T}} \boldsymbol{C}^{-1} \boldsymbol{r}. \tag{6}$$

The Cholesky decomposition gives me $\boldsymbol{C}^{-1} = \boldsymbol{U}^{\dagger}\boldsymbol{U}$, where $\boldsymbol{U}$ is a upper triangle matrix. Then I can write

$$\chi^2 = [\boldsymbol{U}\boldsymbol{r}]^{\dagger}[\boldsymbol{U}\boldsymbol{r}] = \|\boldsymbol{U}\boldsymbol{r}\|^2 \tag{7}$$

where $\boldsymbol{U}\boldsymbol{r}$ is a vector that can be fed into `scipy.optimize.leastsq`.

As shown in Figure 1, the correlation matrix computed from the bootstrap samples is also used to fit the original data. Each fit yields a value for m_π and $m_{\pi\pi}$. The computed masses are shown in Table 1.

2.4 Scattering length

There is a relation between mass difference to scattering length (Lüscher 1986, (1.3)):

$$m_{\pi\pi} = 2m_\pi - \frac{4\pi a_0}{m_\pi L^3}\left[1 + c_1\frac{a_0}{L} + c_2\frac{a_0^2}{L^2}\right], \quad c_1 = -2{,}837\,297, \quad c_2 = 6{,}375\,183 \tag{8}$$

Using the computed m_π and $m_{\pi\pi}$ with Lüscher's formula, I can numerically solve for the scattering length a_0. In my program, I use `scipy.optimize.brentq` that is based on the algorithm by Brent (1973). The computed scattering lengths are shown in Table 1.

Equation (8) can be motivated like so: Let $\hat{H} = \hat{H}_0 + \hat{V}$ be the Hamiltonian for two identical particles where $\hat{H}_0$ is the free Hamiltonian and $\hat{V}$ a spherically symmetric potential with a limited range (or faster than $1/\sqrt{r}$ decay). Then the probability that the two particles are in interaction range scales like L^{-3} as this is the inverse volume which the two particles occupy. The most prominent finite size effect scales to the third power, all other effects can only have higher powers of L^{-1}.

In the first order of the potential V, the ground state (all momenta are zero) will have an energy shift proportional to L^{-3} (ibid., (2.24)):

$$\Delta E = \frac{1}{2L^3}\hat{V}(\mathbf{0},\mathbf{0}) + \mathcal{O}(V^2).$$

The scattering amplitude T as well as the S-wave scattering length a_0 can be expanded in powers of $\hat{V}$ (Born series). Using first order term from (ibid., (2.18)), above equation can be rewritten with the scattering length (ibid., (2.25)):

$$\Delta E = -\frac{4\pi a_0}{mL^3} + \mathcal{O}(V^2).$$

To first order on the potential V, the leading term scales with L^{-3}, like in Equation (8). To obtain more terms, a complete perturbation expansion needs to be written out. That expansion will be both in terms of L^{-1} and V. Lüscher then was able to group those terms in powers of L^{-1} and obtain Equation (8).

ensemble	m_π	$m_{\pi\pi}$	a_0
A100.24	0,222 38(23)	0,451 25(52)	−1,346(29)
A100.24	0,222 33(40)	0,450 83(95)	−1,287(132)
A100.24	0,222 39(24)	0,451 11(53)	−1,316(39)
A30.32	0,124 16(55)	0,251 35(144)	−0,904(273)
A40.20	0,147 79(78)	0,314 29(162)	−1,426(52)
A40.24	0,144 47(52)	0,298 15(109)	−1,255(51)
A40.24	0,144 53(31)	0,298 42(71)	−1,272(51)
A40.32	0,141 26(22)	0,286 26(55)	−1,228(92)
A60.24	0,172 75(52)	0,352 78(126)	−1,194(112)
A60.24	0,172 79(48)	0,354 04(99)	−1,361(91)
A80.24	0,199 30(24)	0,405 11(57)	−1,228(43)
B55.32	0,155 53(22)	0,315 89(55)	−1,676(117)
D45.32	0,120 47(46)	0,250 57(137)	−2,416(205)

Table 1: Computed masses from correlation functions. The last column shows the scattering length a_0 which is computed using Lüscher's formula, Equation (8).

3 Results

My analysis of the correlation functions gives me values for the masses of a single pion (m_π) and a pair of them ($m_{\pi\pi}$). Using Equation (8), I was able to compute the S-wave scattering length a_0 from the energy difference. Those values are listed in Table 1.

The different ensembles assume different masses for the quarks. The first number behind the letter gives the assumed quark mass. In most cases, a lower quark mass also yields a lower pion mass m_π. Those pion masses are not directly the physical ones, one needs to extrapolate to the physical point. The masses and scattering lengths are given in lattice units and depends on the lattice spacing. The product of mass and scattering length, $a_0 m_\pi$, is independent of the lattice spacing and a good measure for extrapolation. Table 2 shows this product, as well as the decay constant.

The results from Table 2 are shown in Figure 4. My data points have no marker, the reference values have a diamond marker. The solid black line is the expectation, not a fit.

As can be seen with the comparison to the reference data, that my values are a lot less accurate than the reference ones. For most points, my errors are a lot larger. The statistical uncertainty on my values is high enough for them to be compatible with the reference and expectation.

The range of fitting was set manually by looking at the plateau of the effective masses (see

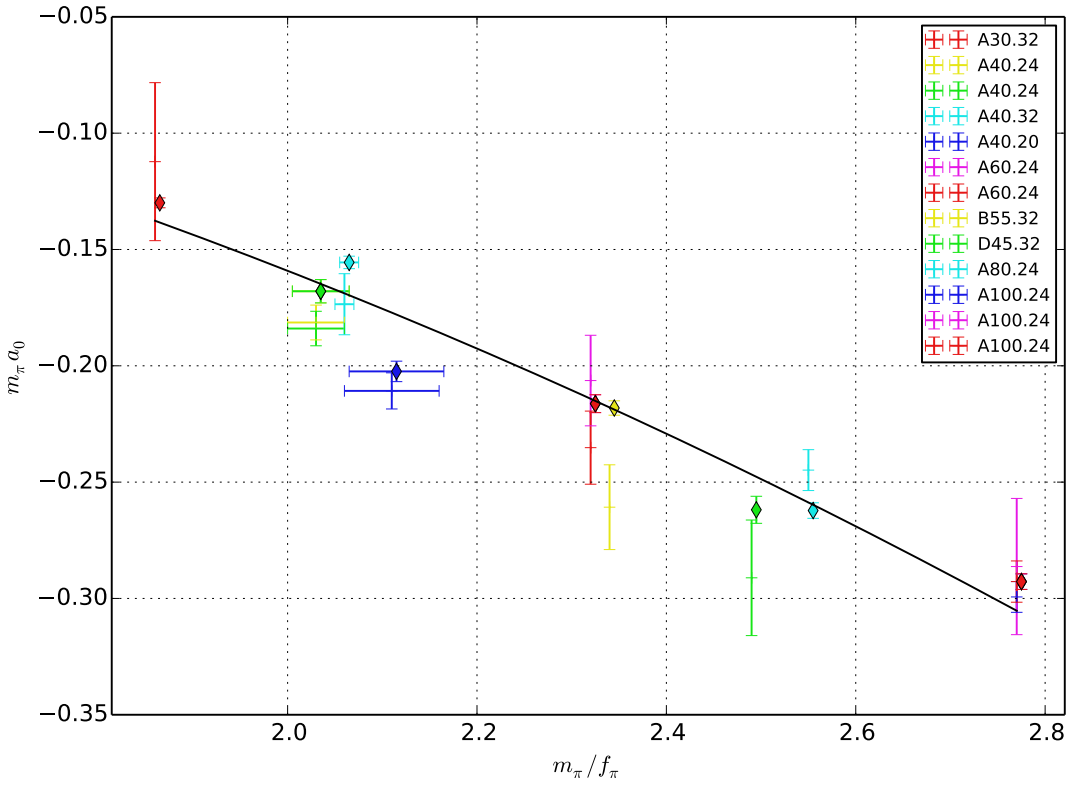

Figure 4: $m_\pi a_0$ as a function of m_π / f_π as shown in Table 2. Diamond data points are taken from draft paper from Carsten Urbach's workgroup. Some ensembles had multiple versions of the correlation functions in them, this plot shows all of them in lexical order of the pathname.

ensemble	L	T	$a_0 m_\pi$	m_π / f_π
A100.24	24	48	−0,2993(66)	2,77
A100.24	24	48	−0,2862(292)	2,77
A100.24	24	48	−0,2927(88)	2,77
A30.32	32	64	−0,1122(339)	1,86
A40.20	20	48	−0,2107(77)	2,11
A40.24	24	48	−0,1813(74)	2,03
A40.24	24	48	−0,1839(74)	2,03
A40.32	32	64	−0,1735(131)	2,06
A60.24	24	48	−0,2063(194)	2,32
A60.24	24	48	−0,2351(157)	2,32
A80.24	24	48	−0,2448(87)	2,55
B55.32	32	64	−0,2607(182)	2,34
D45.32	32	64	−0,2911(248)	2,49

Table 2: Lattice size of the ensembles together with computed quantities. These data points are also shown in Figure 4. The pion decay constants are taken from (Helmes et al. 2014, table 1).

Figure 2). This introduces some statistical errors which cannot be quantified with the current machinery. A way to get beyond this limitation is to run the whole analysis with all possible fit ranges. The different result are then weighted by the p-values of the respective fit.

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