

S-wave $\pi\pi$ I=0 and I=2 scattering with physical pion mass

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The π - π scattering phase shifts for both the s-wave I=0 and I=2 channels are determined from a lattice calculation performed on 741 gauge configurations obeying G-parity boundary conditions with a physical pion mass and lattice size $32^3 \times 64$. The phase shifts are determined for both stationary and moving π - π systems, at four different center of mass momenta. We implement several interpolating operators including a sigma operator and $\pi\pi$ operator with the pions carrying relatively larger momentum. We use both correlated fitting and the generalized eigenvalue treatment and compare these two results with dispersive predictions. A detailed excited state contamination error analysis is included.

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1. Introduction

CP violation is one of the most important topics in particle physics, and a consistency check of the measure of the CP violation between its experimental value and theoretical prediction for various processes is one of the best approaches to find new physics beyond the standard model. Among these processes, the process of a kaon decaying to two pions is one of the most sensitive. The quantity, $\text{Re}(\epsilon'/\epsilon)$, which serves as a measure of CP violation, has been measured experimentally[1] with less than 10 percent error, while its standard model value remains hard to calculate, due to the non-perturbative nature of QCD.

Lattice calculation allows us to numerically calculate $\text{Re}(\epsilon'/\epsilon)$ from first principles. In 2015 we published our first result[2] for $\text{Re}(\epsilon'/\epsilon)$ based on 216 configurations, which is 2σ different from the experimental value. One important sub-problem in this calculation is $\pi\pi$ scattering, since the $\pi\pi$ interactions in the $k \rightarrow \pi\pi$ final states are important. Lots of groups have done $\pi\pi$ scattering calculation on the lattice before, but our calculation is the first to be performed with physical pion masses and including disconnected diagrams. Our 2015 calculated value, $23.8(4.9)^\circ$ at the kaon mass, is 3σ different from 37.6° , the value predicted by combining dispersive methods with experimental data. This was initially believed to be a pure statistical error issue. A more precise calculation with 1436 configurations measured results in a bigger discrepancy as large as 7σ .

One error which might lead to this discrepancy could be excited state contamination. This effect is hard to detect when we have only a single operator, since a fitting where the number of states larger than the number of operators is usually difficult. For that reason we began to introduce extra operators in our calculation. The first operator we added is the sigma operator(σ). As shown last year[4], the calculated phase shift for $\pi\pi_{I=0}$ scattering can be updated to $30.9(1.5)(3.0)^\circ$ (Here the second error is the excited state contamination, estimated using old method), which is around 2σ different from phenomenological value. In order to have better control over the size of excited state contamination error, we added another operator this year, which is generated by two pions with higher momenta, while keeping the total momentum zero. The details of this operator will be explained later. We performed our calculation with 741 configurations, and we find this extra operator does not offer a significant improvement over the two-operator result. Combining the new result with a new method of analyzing the excited state contamination error gives what we believe to be reliable results for $\pi\pi$ scattering in a stationary frame calculation.

We can also calculate $\pi\pi$ scattering phase shift with a moving frame, which gives phase shifts at lower center of mass energy and allows us to calculate Lellouch-Lüscher factor more precisely.

2. Computational methods

Many of the details of our calculation have been explained in our previous work[4] and will not be presented here. Notice for the stationary frame calculation we have two 4-quark $\pi\pi$ operators (which I will call them $\pi\pi$ operators for simplicity), and for moving frame calculations we have three $\pi\pi$ operators, and how we construct them will be explained later. For the stationary $\pi\pi_{I=0}$ calculation, in addition to the two $\pi\pi$ operators, we have the 2-quark operator (which will be labeled as σ operator). The structure of these operators are shown below:

$$\sigma(t, \vec{p} = \vec{s} - \vec{s} = 0) = \frac{1}{V} \sum_{\vec{k}} \bar{q}(\vec{k} - \vec{s}, t) q(\vec{k} - \vec{s}, t) \times h(\vec{k}) \quad (2.1)$$

$$\pi^i(t, \vec{p} = \vec{p}_1 + \vec{p}_2) = \frac{1}{V} \sum_{\vec{k}} \bar{q}(\vec{k} - \vec{p}_1, t) \tau^i \gamma^5 q(\vec{k} + \vec{p}_2, t) \times h(\vec{k}) \quad (2.2)$$

$$\pi^i \pi^j(t, t+4, \vec{p}_{tot} = \vec{p}_1 + \vec{p}_2) = \pi^i(t, \vec{p}_1) \pi^j(t+4, \vec{p}_2) \quad (2.3)$$

where q and \bar{q} are isodoublet quark fields and $h(\vec{p})$ is the Fourier transform of the smearing function.

How we treat the σ operator has been discussed last year[4]. Due to the G-parity boundary condition(GPBC), pion operators carry non-zero momentum. In this calculation we introduce two kinds of pion operator, $\pi(111)$, where the pion carries momentum $(\pm\pi/L, \pm\pi/L, \pm\pi/L)$, and $\pi(311)$, where one component of the pion momentum is replaced by $\pm 3\pi/L$. Using these single-pion operators we can construct two stationary $\pi\pi$ operators, one comprising two $\pi(111)$ operators and the other two $\pi(311)$, both with zero total momentum. Since we are interested in $\pi\pi$ scattering with a specific angular momentum, we need to project all different $\pi\pi$ operators onto the representation we are interested in. In this calculation we are only interested in the S-wave scattering phase shift, so we always project onto the naive representation. We label the projected $\pi\pi$ operators as $\pi\pi(111, 111)$ and $\pi\pi(311, 311)$. We can combine the two kinds of pion operators in different ways to construct moving $\pi\pi$ operators with three different total momenta, and for each total momentum we have three different $\pi\pi$ operators, constructed with 0, 1 and 2 instances of the $\pi(311)$ operator, with the $\pi(111)$ operator otherwise used. We label the S-wave projected operators as $\pi\pi(111, 111)$, $\pi\pi(111, 311)$, $\pi\pi(311, 311)$.

For each isospin and total momentum, we can calculate the correlator matrix between multiple operators by

$$C_{ij}^I(t_{src}, t_{snk}, p_{tot}) = \langle O_i^I(t_{src}, p_{tot}) O_j^I(t_{snk}, -p_{tot}) \rangle \quad (2.4)$$

Each element in this correlator matrix can be expanded by inserting a tower of states, each represented by a cosh function. There is another time-independent term which describes the so-called ‘‘around the world term’’ where one pion is propagating along the positive time direction while the other is propagating along the negative direction. For the $I=0$ channel, we have an additional vacuum term which dominates the error. Before fitting we perform a vacuum subtraction to remove it. These correlation functions are fitted by a procedure which will be written down explicitly in next section. A new technique for testing the goodness of fit has been adopted as an improvement on the usual χ^2 test, which takes into account the effects of autocorrelation and non-Gaussian underlying distribution[3]. After fitting we obtain the energies of those states we include in the expansion, and we can generalize Lüscher’s formula[5] to the case where we impose GPBC on a moving frame calculation and then convert those energies into scattering phase shifts. We can compare those phase shifts with dispersive predictions[6] as a crosscheck. We also performed a GEVP calculation of those energies, and calculate their corresponding phase shift as a crosscheck.

3. Finite volume energy

Depending on whether the total momentum is non-zero and which isospin channel we are calculating, we have four different cases to discuss. The first case is the $\pi\pi_{I=2}$ scattering in the stationary frame. In this case we have two operators: $\pi\pi(111, 111)$ and $\pi\pi(311, 311)$. We perform two correlated fits, one with a single operator and a single state, and the other with two operators

and two states. The fit function can be written down as follows:

$$C_{ij}(t) = \sum_{n=1}^{n_{state}} A_{in} \cdot A_{jn} \cdot (e^{-E_n t} + e^{-E_n(Lt-t)}) + C_{ij} \quad (3.1)$$

where n_{state} represents the number of states, A_{is} represents the overlap between the i -th operator and the s -th state, C_{ij} represents the around the world constant and E_n represents the energy of the n -th state. As for the fit range, we fix the t_{max} as 25 and tune the t_{min} . The fitted ground state energies as functions of t_{min} for both fitting setups are plotted in the left panel of Figure 1.

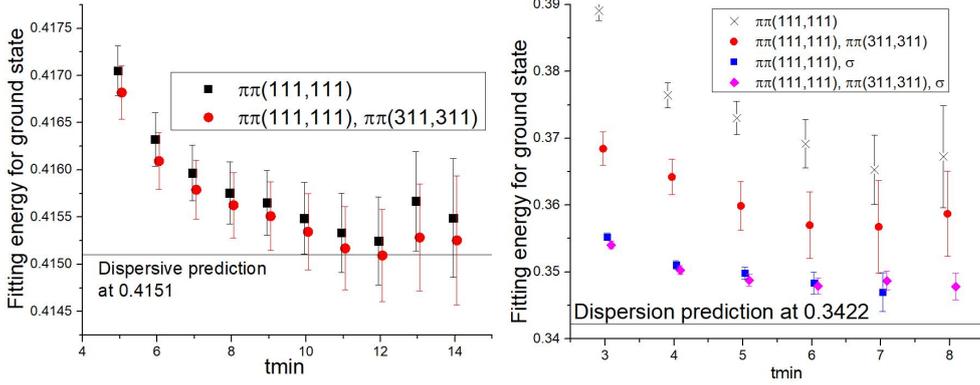


Figure 1: The ground state energies as functions of t_{min} for several different fitting setups in the stationary frame calculation. Left: $I=2$ $\pi\pi$ correlator; right: $I=0$ $\pi\pi$ correlator. The solid line in both plots represents the dispersive predictions.

Comparing these two fit results, the introduction of the second operator, $\pi\pi(311,311)$, only slightly lowers the ground state energy, which suggests it only has small effect in $\pi\pi_{I=2}$ calculation. Listed in table 1 is the normalized overlap matrix. The fact that this matrix is highly diagonal suggests that the extra operator can give us only a little information about the ground state, which is consistent with its small effect on ground state energy. It is also worth noting that the around the world constant is significantly resolved from 0, which suggests we need to include it in fitting.

$\pi\pi_{I=2}$	state ₀	state ₁	$\pi\pi_{I=0}$	state ₀	state ₁	state ₂
op ₀	1.0(0.0)	0.072(56)	$\pi\pi(111,111)$	1.0(0.0)	0.47(2)	0.31(7)
op ₁	-0.068(3)	1.0(0.0)	$\pi\pi(311,311)$	0.053(9)	-0.84(12)	1.0(0.0)
			σ	1.0(0.0)	-0.83(3)	-0.87(22)

Table 1: Normalized overlap between operators and states in the stationary frame calculation. For each row, the biggest overlap is normalized to 1. Left: $\pi\pi_{I=2}$; right: $\pi\pi_{I=0}$

The second case is $\pi\pi_{I=0}$ scattering in the stationary frame. In this case we have three operators: $\pi\pi(111,111)$, $\pi\pi(311,311)$ and σ . We perform four correlated fits, one with a single operator and a single state, two with two operators and two states, and another one with all three operators and three states when t_{min} is small than 6, and two states for other t_{min} 's since the fitting can't distinguish the third state when t_{min} exceeds 5. The fit function is almost the same as the one we use for stationary $\pi\pi_{I=2}$, with one difference that we drop the around the world term since the fitting which includes the around the world term shows it is consistent with 0 in this case. By dropping it we improve the statistical error by a factor of 1.5. We fix t_{max} as 15 rather than 25 since

data with higher t are extremely noisy due to the disconnected diagram. We then tune the t_{\min} . The fitted ground state energies as functions of t_{\min} for all four fitting setups are plotted in Figure 1.

Comparing these 4 fit results suggests that the σ operator substantially suppresses the excited state contamination. Without including the σ operator, introducing the $\pi\pi(311, 311)$ operator gives a lower energy compared with the single operator result, but after we include the σ operator, $\pi\pi(311, 311)$ operator gives us no improvement in ground state energy. The fact that the normalized overlap matrix in table 2 is highly off-diagonal also supports the argument that extra operators are helpful in controlling the excited state contamination error. The fact that $\pi\pi(111, 111)$ couples significantly to both the first and second excited states suggests that our old single operator is affected by excited state contamination.

The third case is $I=2$ scattering in a moving frame. In this case we have three operators: $\pi\pi(111, 111)$, $\pi\pi(311, 111)$ and $\pi\pi(311, 311)$. We perform four correlated fits as we did in stationary $\pi\pi_{I=0}$ fitting. The fit function is the same as the one we choose for stationary $\pi\pi_{I=2}$ fitting. We fix the t_{\max} as 25. Plotted in Figure 2 are the fitted ground state energies as functions of t_{\min} for all 4 fitting setups, with $p_{tot} = (2, 0, 0)\frac{\pi}{L}$. For the other two total momenta, $(2, 2, 0)\frac{\pi}{L}$ and $(2, 2, 2)\frac{\pi}{L}$, the plots and the corresponding energy results are similar and their phase shifts will be discussed in the next section. Comparing those fit results, we reach a similar conclusion as in the stationary $\pi\pi_{I=2}$ fitting: the introduction of the extra two operators has no observable effect on the ground state energy. We are led to the same conclusion by looking at the normalized overlap matrix listed in table 2. This matrix is also highly diagonal, and the overlap between the extra two operators and the ground state is smaller than 0.04, suggesting those two extra operators overlap little with the ground state, which means they can't improve the results of ground state energy obtained from single state fitting.

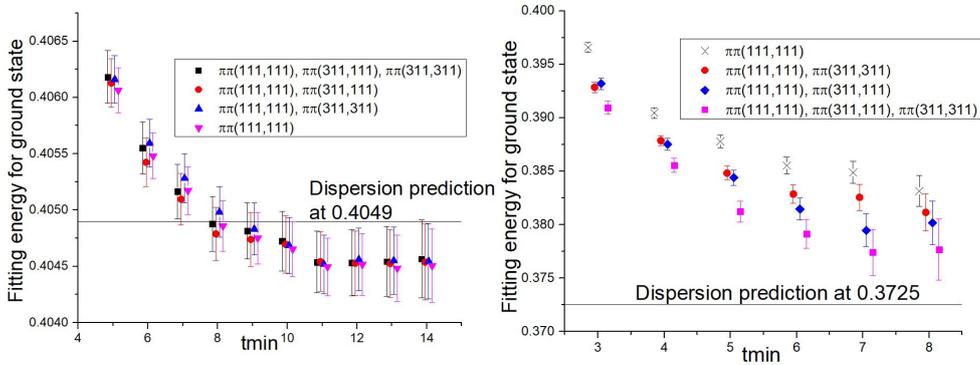


Figure 2: Left: the ground state energy as we vary t_{\min} for 4 different fitting setups in a moving frame calculation with $p_{tot} = (2, 0, 0)\frac{\pi}{L}$. Left: $I=2$ $\pi\pi$ correlator, right: $I=0$ $\pi\pi$ correlator. The solid line in both plots represents the dispersive prediction.

The last case is $I=0$ scattering in a moving frame. We have the same three operators as in the moving $I=2$ case. We perform the same fitting as we did in the stationary $I=0$ case, leaving out the constant term for the same reason, and plot the result with $p_{tot} = (2, 0, 0)\frac{\pi}{L}$ in Figure 2. Comparing those four plots we can see that the extra two operators improve the ground state energy by roughly 2σ , similar to what we get in the stationary $\pi\pi_{I=0}$ calculation. We can get the same conclusion by looking at the normalized overlap matrix in table 2, here the overlap between $\pi\pi(311, 111)$ and $\pi\pi(111, 111)$ is 0.1, which is not as small as $I=2$. Also the overlap between $\pi\pi(111, 111)$ operator

$\pi\pi_{I=0}$	state ₀	state ₁	state ₂	$\pi\pi_{I=2}$	state ₀	state ₁	state ₂
op ₀	1.0(0.0)	0.049(3)	0.037(8)	op ₀	1.0(0.0)	-0.31(5)	0.14(2)
op ₁	0.032(0.000)	1.0(0.0)	0.043(11)	op ₁	0.09(2)	1.0(0.0)	-0.30(20)
op ₂	$-13(0) \times 10^{-4}$	0.069(2)	1.0(0.0)	op ₂	0.01(1)	0.09(5)	1.0(0.0)

Table 2: Normalized overlap between operators and states in a moving frame calculation with $p_{tot} = (2, 0, 0) \frac{\pi}{L}$. For each row, the biggest overlap is normalized to 1. Operators with a higher index are constructed with a larger number of $\pi(311)$. Left: $\pi\pi_{I=2}$; right: $\pi\pi_{I=0}$

and the first excited state is roughly 0.3, which means if we only fit with a single operator, our result will be affected substantially by excited state contamination. This effect becomes smaller as we move to the larger total momenta, $(2, 2, 0) \frac{\pi}{L}$ and $(2, 2, 2) \frac{\pi}{L}$. We believe this is because the generation of states with different pion momentum from those of the constituent single-pion operators requires the exchange of momentum between those pions. The interaction of the pions is parameterized by the phase shift, which becomes smaller as the relative momentum decreases, hence the couplings are expected to decrease as we increase the center of mass momentum.

4. Phase shift and excited state contamination error

Using the energies we found in the last section, we can calculate the $\pi\pi$ scattering phase shifts at 4(3 in $I=0$) different energies. The results are plotted in Figure 3. Also plotted are the phase shifts calculated based on the energies obtained using the GEVP technique. We can see that our results for the $I=2$ scattering are consistent with the dispersive prediction, while for $I=0$ scattering our results are slightly lower. Also the fitting and GEVP results are consistent for most cases except the $I=0$ moving frame calculation.

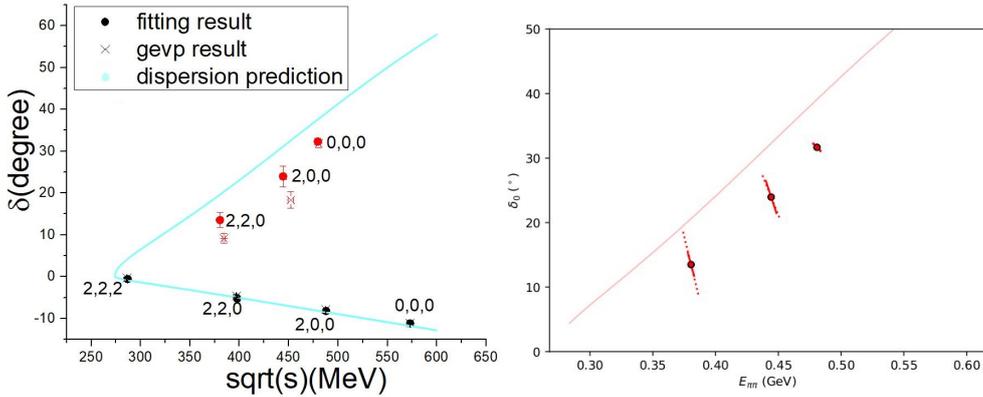


Figure 3: Left: Phase shifts for $I=2$ (black points) and $I=0$ (red points) $\pi\pi$ scattering at 4(3) different energies. Those energies are calculated from both multi-state fitting and GEVP. Only statistical errors are included. Right: Phase shift results where excited state contamination error is included. Solid error bars represent the statistical error and dash error bars show the combined error. The $I=2$ channel is unaffected so their results are not plotted here.

From the discussion in last section, we see that for all 4 cases, there could be 1 or 2 operators whose introduction doesn't improve the final result. Does that mean we can trust our results and

say they are unlikely to suffer from excited state contamination? Are there any excited state contamination errors in the results that are bigger than statistical error that we failed to recognize in the calculation? This is possible if all the operators we introduce have little overlap. Then it will be difficult for us to get information about the ground state from those extra operators. This lack of overlap does happen in our $I=2$ calculation.

To answer this question, we develop a new technique to estimate the remaining systematic error. For each case, we start by performing a n -state n -operator fitting as we did in last section, where n is the maximum number of operators we have for that case. Then we perform a frozen fit on $\pi\pi(111, 111)$ operator to $n + 1$ states, where the ground state energy and coupling are free, but those of the next $n - 1$ states are frozen to the results of the first fit. The energy of the $n+1^{th}$ state is frozen to the prediction of a model (e.g. the dispersive prediction). The difference between the two fit results is treated as the excited state contamination error. Based on this technique, we update our phase shift plots and the results are shown in Figure 3. The reason why $I=2$ channel is not included is because excited state contamination estimated by this method for that case is negligible. We can see that the excited state contamination is still obvious in moving $I=0$ results, while it is no longer important in stationary $I=0$ calculation.

5. Conclusion and outlook

We have described our lattice calculation for the $\pi\pi$ scattering phase shifts for both $I=0$ and $I=2$ at 3 and 4 different energies, respectively. We introduce multiple operators to control the excited state contamination. For different isospin channels and different total momenta, the effects of these extra operators are different. A new technique has been developed to estimate the remaining excited state contamination error. Our results are consistent with the dispersive predictions for $I=2$, and slightly different from dispersive prediction for $I=0$ moving frame. For $I=0$ stationary frame, after combining the statistical error, finite lattice spacing error, finite volume error, slightly unphysical pion mass error we get a result of $32.4(2.3)^\circ$. Our new technique shows excited state contamination is still important in $I=0$ moving frame calculation, and one thing to do in the future is to introduce a σ operator in the moving frame calculation, likely an important addition considering its effect in the stationary frame calculation.

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