Studies of I=0 and I=2 $\pi\pi$ scattering with physical pion mass

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We report a direct lattice calculation of both the I=0 and I=2 $\pi\pi$ scattering phase shifts using G-parity boundary conditions on an ensemble of $32^3 \times 64$ gauge configurations at physical quark mass. This extends an earlier calculation of the RBC/UKQCD Collaboration [1] by including additional operators and more statistics. We apply both multistate fitting and the generalized eigenvalue treatment to this set of operators in order to understand and reduce excited state contamination and to study $\pi\pi$ scattering at energies in the energy region around the kaon mass. These results are compared with predictions from dispersion theory.

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1. Introduction

An understanding of CP violation is one of the most important goals in physics. The standard measure of direct CP violation, $\text{Re}(\varepsilon'/\varepsilon)$, has been experimentally measured, but its predicted value from standard model is hard to analytically calculate due to the non-perturbative nature of QCD sector. Lattice QCD enables us to calculate this quantity with controlled errors, and whether the lattice calculation agrees with experimental value is a good test of the correctness of Standard Model.

In order to calculate $\text{Re}(\varepsilon'/\varepsilon)$, the quantity we need to compute is the kaon to two pion($K \to \pi\pi$) matrix element of the first-order weak Hamiltonian. During its calculation, an interesting process, $\pi\pi$ scattering, plays an important role: we not only need energy and amplitude of the $\pi\pi$ state when calculating the matrix element on lattice, we also need the Lellouch-Lüscher(LL) factor which is related to the derivative of $\pi\pi$ scattering phase shift with respect to energy.

The $\pi\pi$ scattering phase shift calculation is important for us for another reason: Different from most lattice groups who use a lattice with perodic/anti-perodic boundary conditions, we use a lattice with G-parity boundary condition(GPBC)[2] which likely increases the statistical accuracy of our results (especially those for $I = 0$ $K \to \pi\pi$ decay) by increasing the energy of the two-pion ground state to that of the kaon mass. This makes a comparison of our GPBC results for $\pi\pi$ scattering with the present theory of low-energy $\pi\pi$ scattering especially interesting.

The $\pi\pi$ scattering phase shift has been measured on lattice by many groups, but to date these calculations have been performed with unphysical pion mass or have ignored the effect of disconnected diagrams[4][5]. Now with the ingredients from the calculation of $K \to \pi\pi$ with physical pion mass, together with techniques to suppress the statistical error, we are able to perform a lattice calculation of $\pi\pi$ scattering with physical pion mass for a center of mass energy equals to kaon mass. In $\pi\pi_{I=2}$ scattering, we find a phase shift of $\delta = -11.0(2.9)(1.2)$ at 573MeV. Our 2015 result for the I=0, $\pi\pi$ state was calculated with single $\pi\pi$ interpolating operator and gave the phase shift of $\delta = 19.1(2.5)(1.2)$ at 508MeV. Now, after including a second $\pi\pi$ interpolating operator, the σ operator, we update our result to $\delta_{I=0} = 30.9(1.5)(3.0)$ at 483MeV, which substantially suppressed the excited state contamination present in our original calculation.

This proceeding summarizes the details of our calculation, and our efforts to suppress the statistical error and excited state contamination.

2. Computational methods

The isospin I $\pi\pi$ two-point function is determined from Euclidean Green's function

$$C^I(t_{src}, t_{snk}) = \text{Tr}\{O^I_{\pi\pi}(t_{src})O^I_{\pi\pi}(t_{snk})\} \tag{2.1}$$

After inserting two complete sets of intermediate states, we find

$$\begin{aligned}
C^I(t_{src}, t_{snk}) = &\langle\pi|O^I_{\pi\pi}|\pi\rangle\langle\pi|O^I_{\pi\pi}|\pi\rangle e^{-Lt\times E_\pi} + \langle 0|O^I_{\pi\pi}|\pi\pi\rangle\langle\pi\pi|O^I_{\pi\pi}|0\rangle e^{-t\times E_{\pi\pi}} \\
&+ \langle\pi\pi|O^I_{\pi\pi}|0\rangle\langle 0|O^I_{\pi\pi}|\pi\pi\rangle e^{-(Lt-t)\times E_{\pi\pi}} + \langle 0|O^I_{\pi\pi}|0\rangle\langle 0|O^I_{\pi\pi}|0\rangle \times \delta_{I,0}
\end{aligned} \tag{2.2}$$

in the limit where a) $t \equiv t_{src} - t_{snk}$ and b) $L_t - t$ are both large (L_t is the time extent of the lattice). Notice the first term describes the "around the world effect", which is a small but constant term. The

second and third terms, which can be combined together into a cosh function of the time separation, describe the ground state $\pi\pi$ scattering. The last term, which only shows up in $I = 0$ scattering, describes the vacuum piece that we are not interested in. It is the biggest source of error because it is constant which introduces a decreasing signal-to-noise ratio as we increase time separation to suppress excited state contamination.

The most significant difference between our calculation and those of other groups is the boundary condition: the lattice we use has a G-parity boundary condition[2]. Under this boundary condition, ground state pion is no longer stationary, instead it moves with momentum component π/L along each direction where we impose GPBC, while the ground state of kaon is still a stationary one. In our calculation, we impose GPBC along all three space directions, so the momentum of the ground state pion becomes $(\frac{\pi}{L}, \frac{\pi}{L}, \frac{\pi}{L})$, and by tuning the lattice, we have $E_{\pi\pi} \approx m_K$.

In order to suppress the systematic error, we use all-to-all propagator[3] to construct finite-sized pion interpolating operator so that our pion operator has better overlap with pion state, and our $\pi\pi$ operator has better overlap with the lattice $\pi\pi$ ground state. Here we use 900 low modes plus 1536 random modes from time/flavor/color/spin dilution to construct an all-to-all propagator, and choose a 1s hydrogen wave function as smearing function.

Another technique in order to suppress the statistical error in the $I = 0$ calculation is to use a time-separated $\pi\pi$ operator. Rather than putting the two pions at the same time slice, we put them on time slices with a separation of $t_{sep} = 4$. This suppresses the vacuum noise (the last term in equation (2.2)) by a factor of 2[6].

In our calculation, we use gauge field ensemble generated with the Iwasaki+DSDR gauge action and $\beta = 1.75$. We use $2 + 1$ flavor Möbius domain wall fermions (DWF) with a strange quark mass $m_s = 0.045$ and a light quark mass $m_l = 0.0001$. The size of our lattice is $32^3 \times 64$, with a fifth dimension length of 12. The inverse lattice spacing is $a^{-1} = 1.3784(68)$GeV, and pion mass is $m_\pi = 143.1(2.0)$MeV, which suggests that we are doing a calculation with physical pion mass. We published our original results based on an analysis of 216 configurations in 2015[1], and now we have generated 1386 configurations.

In addition to the usual $\pi\pi$ interpolating operator, we also include the σ operator which has the same quantum numbers as the $\pi\pi$ $I = 0$ state to reduce the effects of excited state contamination in the I=0 scattering. The $\pi\pi$ and σ operators we choose are (written for simplicity in infinite volume)

$$\sigma(t) = \int d^3 r_1 \int d^3 r_2 \bar{q}(\vec{r}_1, t) q(\vec{r}_2, t) \times h(\vec{r}_1 - \vec{r}_2) \tag{2.3}$$

$$\pi^i \pi^j(t, t+4) = \int d^3 r_1 \int d^3 r_2 \int d^3 r_3 \int d^3 r_4 \bar{q}(\vec{r}_1, t) \tau^i \gamma^5 q(\vec{r}_2, t) \bar{q}(\vec{r}_3, t) \tau^j \gamma^5 q(\vec{r}_4, t)$$
$$\times h(\vec{r}_1 - \vec{r}_2) h(\vec{r}_3 - \vec{r}_4) \tag{2.4}$$

where q and $\bar{q}$ are isodoublet quark fields and $h(\vec{r})$ is smearing function.

There are four types of $\pi\pi$ scattering diagrams that contribute to the Greens functions constructed from the $\pi^i \pi^j$ operator defined in Eq. (2.4). The $\pi\pi$, $I = 0$ and $I = 2$ correlators are linear combinations of these four diagrams in the following ways:

$$\langle \pi\pi(t) \pi\pi(0) \rangle^{I=2} = 2D - 2C$$
$$\langle \pi\pi(t) \pi\pi(0) \rangle^{I=0} = 2D + C - 6R + 3V \tag{2.5}$$

There are also four types of diagrams involved in $\pi\pi/\sigma$ Green's functions that are shown in Figure 2. The I=0 scattering, $\pi\pi/\sigma$ correlators are linear combinations of these four diagrams in the following ways:

$$\langle \sigma(t)\sigma(0) \rangle = \frac{1}{2}V_{\sigma\sigma} - \frac{1}{2}C_{\sigma\sigma}$$

$$\langle \sigma(t)\pi\pi(0) \rangle = \frac{\sqrt{6}}{4}\cdot V_{\sigma\pi\pi} - \frac{\sqrt{6}}{2}\cdot C_{\sigma\pi\pi}$$
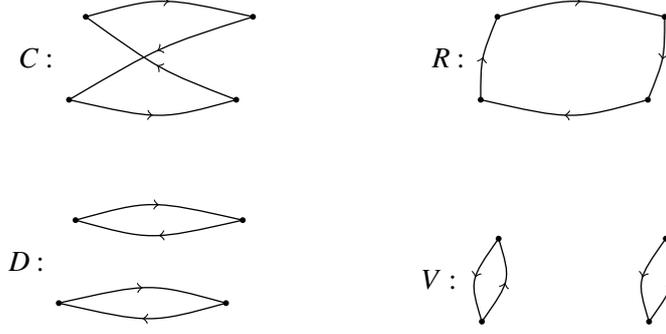
(2.6)

Figure 1: Four types of diagrams which contribute to $\pi\pi$ scattering Green's functions constructed from the $\pi^i\pi^j$ operator defined in Eq. (2.4). The two vertices on the left represent the two source pions and the two vertices on the right correspond to two sink pions.
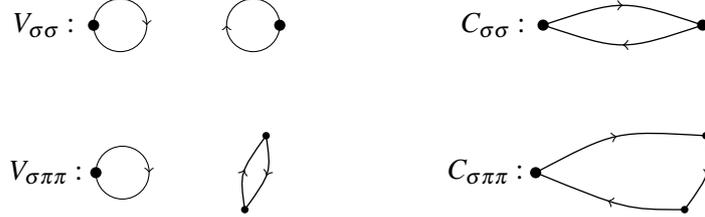

Figure 2: Four types of diagrams contribute to $\pi\pi/\sigma$ correlator. The large vertex represent σ operator

With GPBC, pion operator carries momentum of $(\pm\pi/L, \pm\pi/L, \pm\pi/L)$. Since we are interested in $\pi\pi$ scattering with a specific angular momentum, we need to evaluate a superposition of $\pi\pi$ states to obtain an angular momentum eigenstate. Since our lattice with GPBC has cubic symmetry at the meson level, we first calculate $\pi\pi$ correlators with 64 specific momentum combinations(that is, 8 choices for both source and sink operators), and project them to the A1 representation to obtain an S-wave correlator, and to the T2 representation to obtain a D-wave correlator. The σ operator carries zero momentum. We generated 8 different kinds of σ operator by constructing quark/anti-quark products with eight different relative momentum, and then averaged them to make an operator which is more rotational symmetric and used that as the σ operator.

After we calculated the lattice correlator, we performed a fit to determine the lattice energy. The fitting details will be explained in the next section. We then use Lüscher's formula[7] to convert lattice energy into a scattering phase shift, and compare it with the dispersion relation prediction. In this proceeding, we compare our lattice calculation result with Schenk's parametrization formula[8] and using the parameters of Colangelo *et al* [9].

3. Analysis and result

3.1 I=2 scattering

For I=2 scattering, we don't have the vacuum term, and from equation (2.1) we can see that the correlator has two terms: a constant term plus a cosh function. The effective mass plot in Figure 3 shows that there is a plateau starting from t=6. So we perform a correlated fit with the fitting function

$$C(t) = A \cdot \left(e^{-Et} + e^{-E \cdot (L_t - 2 \cdot t_{sep} - t)} \right) + C \tag{3.1}$$

with 3 parameters A(amplitude), E(energy) and C(around the world constant). We choose the fit range as (6-25) since the plateau in effective mass plot starts at $t = 6$. The results based on 216 configurations (old) and 1386 configurations (new) are summarized in table 1. It is clear that our
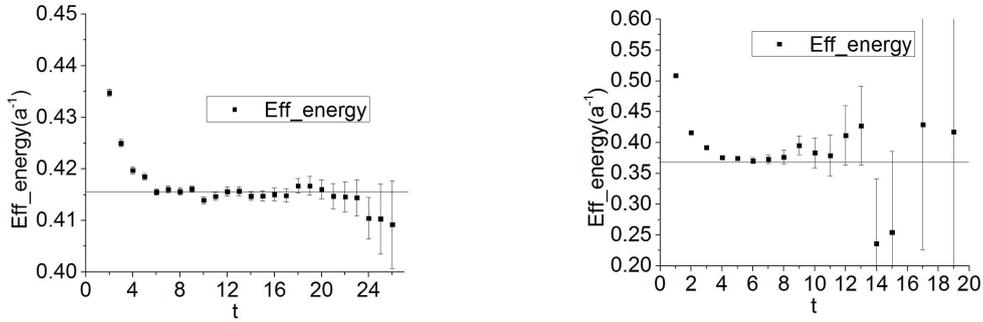

Figure 3: Left: effective mass plot for I=2 $\pi\pi$ correlator; right: effective mass plot for I=0 $\pi\pi$ correlator.

S-wave phase shift agrees perfectly with the dispersive predictions, also consistent with multi-state fitting result(not listed here), and the agreement between D-wave energy and twice the pion energy is also consistent with the expectation that the D-wave phase shift is small. The huge reduction in statistical error of energy is consistent with the $1/\sqrt{N}$ prediction since we increased the number of configurations by a factor of 2.5^2. This suggests one single operator is sufficient for us to obtain the $\pi\pi$ I=2 ground state energy, considering the relatively large a^{-1} error.

3.2 I=0 scattering: Single operator results

In I=0 scattering, the vacuum term shows up, so before we start fitting, we perform a vacuum subtraction. This means we explicitly calculate the fourth term in equation (2.1) and subtract that from our correlator. After performing the vacuum subtraction, we repeat the same procedure we applied to the $\pi\pi$ I=2. The effective mass plot in Figure 3 shows the relatively large increase in the error as the time increases compared with I=2, which is the consequence of the large statistical error in vacuum term. Since there is a plateau starting from t=6, we perform a correlated fit with the fitting function

$$C(t) = A \cdot \left(e^{-Et} + e^{-E \cdot (L_t - 2 \cdot t_{sep} - t)} \right) + C \tag{3.2}$$

with 3 parameters A(amplitude), E(energy) and C(around the world constant), and we choose the fit range as (6-25). The results based on 216 configurations (old) and 1386 configuration (new) are summarized in table 2.

	E(MeV)(Old)	δ(Old)	E(MeV)(New)	δ(New)
S-wave	573.2(0.6)(2.8)	-11.0(0.3)	573.9(0.2)(2.8)	-11.3(0.1)
Dispersion	574.1	-11.4	574.1	-11.4
$2E_\pi$	549.2(0.8)(2.8)		549.0(0.3)(2.8)	
D-wave	549.4(0.4)(2.8)		549.9(0.2)(2.8)	

Table 1: The $\pi\pi$ I=2 scattering results, χ^2/dof is 1.6 with the old data and 1.3 with the new data. The first error in the energy is statistical error and the second comes from propagating the inverse lattice spacing error, the error in phase shift is statistical error. E_π is the energy of pion with GPBC, so it differs from pion mass. The quantity labeled 'dispersion' is the prediction for the finite-volume $\pi\pi$ energy obtained by combining Lüscher's formula and the Schenk parameterization

	E(MeV)(Old)	δ(Old)	E(MeV)(New)	δ(New)
S-wave	498(11)(3)	23.8(5.2)	508(5)(3)	19.1(2.3)
Dispersion	474.6	35.0	474.6	35.0
$2E_\pi$	549.2(0.8)(2.8)		549.0(0.3)(2.8)	
D-wave	548.6(0.9)(2.8)		548.1(0.4)(2.8)	

Table 2: The $\pi\pi$ I=0 scattering results, χ^2/dof is 1.5 with old data and 1.6 with new data. The definition of the errors is the same as in Table 1. These results were obtained from the correlator of a single I=0 operator.

In this table, we can see the inconsistency between our calculation and the dispersive prediction: the phase shift we calculated is 3σ different from dispersive predictions for our old data, and after including more statistics, the discrepancy increases to 5σ. One possible reason is excited state contamination, so we performed a two state (cosh) fit to our data, but the ground state energy we find is the same as the one state fit energy. We conclude that the statistical error at large time have made it impossible to use a single operator to detect the nearby excited state identified below using two operators.

3.3 I=0 scattering: Two operator results

In order to control the excited state contamination, we included another operator, the σ operator, and we performed a correlated two-state simultaneous fit to the $\pi\pi/\sigma$ 2×2 Green's function using the fitting function

$$C_{ij} = A_{i0} \cdot A_{j0} \cdot (e^{-m_0 t} + e^{-m_0(Lt-t)}) + A_{i1} \cdot A_{j1} \cdot (e^{-m_1 t} + e^{-m_1(Lt-t)}) \tag{3.3}$$

where i,j can be the $\pi\pi$ or σ operator. We choose the fitting range to be (5-10). This gives results that are consistent with results from nearby ranges, and have good statistics and χ^2. The results are listed in table 3. Also we compare that result with the one from a GEVP[10] analysis. Now we can see the fitting result, the GEVP result and the dispersive prediction are all consistent with each other. That means adding the new σ operator allows us to distinguish the ground state from the excited state. By comparing this result with the previous single operator result, we can see that the introduction of the second operator also reduces the statistical error of the ground state energy.

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	E0(MeV)	δ
sim-fit(5-10)	483.1(1.4)(2.7)	31.0(0.7)(3.0)
GEVP: $t = 6, t_0 = 3$	475.6(2.6)(2.7)	34.7(1.2)(3.0)
Dispersion	474.6	35.0

Table 3: The $\pi\pi$ I=0 simultaneous fit results, χ^2/dof is 1.7. The definition of the errors is the same as in Table 1. The second error in phase shift is systematic error from excited state contamination. The results are from analysing the 2×2 $\pi\pi/\sigma$ Green's function.

The ability of these two operators to distinguish the ground and excited states can be seen directly by computing the determinant of the 2×2 correlation matrix. At t=6 we obtain a determinant of $(1.9 \pm 0.4) \times 10^{16}$, a quantity that would be zero if only one state were present.

4. Conclusion and outlook

We have described our lattice calculation of the $\pi\pi$ I=2 and I=0 scattering phase shifts at the kaon mass with a physical pion mass. For the I=2 channel, by using a single $\pi\pi$ operator, we obtain a phase shift which is consistent with the dispersive predictions. For I=0 channel, one single $\pi\pi$ operator can not distinguish the ground state and the first excited state. However when we add a σ operator, we are able to remove the excited state contamination.

At this moment we are ready to include a third operator[11], a $\pi\pi$ operator with larger relative $\pi\pi$ momentum, to help further suppress the excited state contamination in both the I=0 and I=2 calculation. By constructing a $\pi\pi$ operator from two all-to-all pion "mesonfields" with momenta that are not opposite but with a non-zero sum makes a moving frame calculation possible. By introducing this third operator, we are looking forward to seeing a similar suppression of excited state contamination in such a moving frame calculation.

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