S-Wave πK Scattering Length in 2+1 Flavor Lattice QCD

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The S-wave πK scattering lengths are calculated for both the isospin 1/2 and 3/2 channels in the lattice QCD by using the finite size formula. We perform the calculation with $N_f = 2+1$ gauge configurations generated on $32^3 \times 64$ lattice using the Iwasaki gauge action and nonperturbatively $O(a)$-improved Wilson action at $1/a = 2.17$ GeV. The quark masses correspond to $m_\pi = 0.29 - 0.70$ GeV. For $I = 1/2$, to separate the contamination from excited states, we construct a 2×2 matrix of the time correlation function and diagonalize it. Here, we adopt the two kinds of operators, $\bar{s}u$ and πK. It is found that the signs of the scattering lengths are in agreement with experiment, namely attraction in $I = 1/2$ and repulsion in $I = 3/2$. We investigate the quark-mass dependence of the scattering lengths and also discuss the limitation of chiral perturbation theory.

§1. Introduction

The scattering length is a key quantity for understanding the basic properties of the low-energy interaction. Many lattice calculations of the hadron-hadron scattering lengths have been reported in past years. Most of them, however, do not treat the scattering system with attractive interactions due to the computational cost. Handling the attractive interaction would be indispensable in scattering studies of the future.

Here, we focus on the S-wave πK system. This system has two isospin channels ($I = 3/2,\ 1/2$). The low-energy interaction is repulsive (attractive) for $I = 3/2$ ($I = 1/2$). In addition, the existence of a broad resonance, called κ state, is suggested in $I = 1/2$. Until now, three studies in lattice QCD have been reported[1)–3)] for these channels. The first study was performed by Miao et al.[1)] They calculated the $I = 3/2$ scattering length within the quenched approximation. The first calculation with dynamical quarks ($N_f = 2+1$) was reported by the NPLQCD Collaboration.[2)] They calculated the $I = 3/2$ scattering length for $m_\pi = 0.3 - 0.6$ GeV. They further determined the low energy constants in the $SU(3)$ chiral perturbation theory (ChPT) and evaluated the $I = 1/2$ scattering length by using ChPT. The first direct calculation on $I = 1/2$ has been done by Nagata et al.[3)] They, however, used the quenched approximation, and ignored the effect of ghost mesons which is nonnegligible in $I = 1/2$. In addition, their results do not reproduce the repulsive interaction even for $I = 3/2$, whose calculation is relatively easier, at their simulation points. The reliability of their calculations remains controversial. In conclusion, no satisfactory direct calculation for $I = 1/2$ has been carried out.

In the present work, we calculate the S-wave πK scattering lengths for both the isospin channels. We use a technique with a fixed kaon sink operator to reduce the computational cost of the calculation of the πK for $I = 1/2$. To separate the contamination from excited states for $I = 1/2$, we construct a 2×2 matrix of the time correlation function and diagonalize it. After obtaining the scattering lengths at each simulation points, we investigate the quark-mass dependence of the scattering lengths and also discuss the limitation of the $\mathcal{O}(p^4)$ $SU(3)$ ChPT in our results. A preliminary report of this work has been already presented.[4)] All calculations have been done on PACS-CS and T2K-Tsukuba at University of Tsukuba, and TSUBAME at Tokyo Institute of Technology.

§2. Details of simulation

The S-wave πK scattering length is defined by

$$a_0 = \lim_{k \to 0} \tan \delta_0(k)/k \ . \tag{2·1}$$

k is the scattering momentum related to the total energy by $E = \sqrt{m_\pi^2 + k^2} + \sqrt{m_K^2 + k^2}$. $\delta_0(k)$ is the S-wave scattering phase shift and can be evaluated by the Lüscher's finite size formula,[5)]

$$(\tan \delta_0(k)/k \ )^{-1} = \frac{1}{\pi L} \cdot \mathcal{Z}_{00} \left(1, \frac{k^2}{(2\pi/L)^2} \right) \ , \tag{2·2}$$

where the zeta function $\mathcal{Z}_{00}$ is an analytic continuation of

$$\mathcal{Z}_{00}(s, \bar{n}) \equiv \sum_{\vec{m} \in \boldsymbol{Z}^3} \frac{1}{(\vec{m}^2 - \bar{n})^s} \tag{2·3}$$

defined for $\mathrm{Re}(s) > 3/2$. In the case of attractive interaction, k^2 on the lowest state has a negative value, so k is pure imaginary. $\delta_0(k)$ at the unphysical k is no longer physical scattering phase shift. $\mathcal{Z}_{00}(1, k^2/(2\pi/L)^2)$, however, have a real value even for this case, so $\tan \delta_0(k)/k$ obtained by Eq. (2·2) is also real. If $|k^2|$ is enough small, we can regard $\tan \delta_0(k)/k$ as the physical scattering length at the πK threshold $(k = 0)$.

For $I = 3/2$, one can extract E from the time correlation function

$$G(t) = \langle 0 | \ K^+(t_1) \pi^+(t) \ (W_{K^+}(t_0 + 1) W_{\pi^+}(t_0))^\dagger \ |0\rangle \cdot e^{m_K(t_1 - t)} \ , \tag{2·4}$$

where $K^+ = \bar{s}\gamma_5 u$, $\pi^+ = -\bar{d}\gamma_5 u$, and W_{K^+}, W_{π^+} are the wall-source operators for the corresponding mesons. The time slice of the kaon source is shifted from that of the pion source t_0 to avoid the Fierz mixing of the wall-source operators.[6)] The time slice of the kaon sink operator t_1 is fixed as $t_1 \gg t$. The exponential factor $e^{m_K(t_1 - t)}$ is introduced to drop the unnecessary t-dependence appearing due to the fixed t_1.

For $I = 1/2$, the existence of the κ resonance is suggested in the low energy, and so that it might be necessary to separate the ground state contribution from the contamination coming from the excited states to obtain the scattering length. For this purpose, we use the two types of operators Ω_0 and Ω_1 ($\overline{\Omega}_0$ and $\overline{\Omega}_1$),

$$\begin{aligned}\Omega_0(t) &= \frac{1}{\sqrt{3}}\Big(K^+(t_1)\pi^0(t) - \sqrt{2}\,K^0(t_1)\pi^+(t)\Big)\cdot e^{m_K(t_1-t)}\ ,\\ \Omega_1(t) &= \kappa(t)\ ,\\ \overline{\Omega}_0(t_0) &= \frac{1}{\sqrt{3}}\Big(W_{K^+}(t_0+1)W_{\pi^0}(t_0) - \sqrt{2}\,W_{K^0}(t_0+1)W_{\pi^+}(t_0)\Big)\ ,\\ \overline{\Omega}_1(t_0) &= W_\kappa(t_0+1)\ ,\end{aligned} \quad (2{\cdot}5)$$

where, $K^0 = \bar{s}\gamma_5 d$, $\pi^0 = \frac{1}{\sqrt{2}}(\bar{u}\gamma_5 u - \bar{d}\gamma_5 d)$, $\kappa = \bar{s}u$, and W_{K^0}, W_{π^0}, W_κ are the wall-source operators for the corresponding mesons. The exponential factor in $\Omega_0(t)$ is introduced by the same reason as for $I = 3/2$. We construct the 2×2 matrix of the time correlation function,

$$G_{ij}(t) = \langle 0|\ \Omega_i(t)\ \overline{\Omega}^\dagger_j(t_0)\ |0\rangle\ , \qquad (\ i,\ j = 0,1\ ) \quad (2{\cdot}6)$$

and with a reference time t_R we extract the energy of the ground state by the diagonalization of $G^{-1}(t_R)\ G(t)$.[7)]

The calculations are carried out with $N_f = 2+1$ full QCD configurations generated by the PACS-CS Collaboration[8)] using the Iwasaki gauge action at $\beta = 1.90$ and nonperturbatively $\mathcal{O}(a)$-improved Wilson quark action with $C_{SW} = 1.715$ on $32^3\times 64$ lattice. The quark propagators in this work are calculated with the same quark action. The corresponding lattice cutoff is $1/a = 2.176(31)$ GeV ($a = 0.0907(13)$ fm) and the spatial extent of the lattice is $La = 2.902(41)$ fm. The quark mass parameters and corresponding hadron masses are listed in Table I. The Dirichlet (periodic) boundary condition is imposed to the temporal direction (spatial directions) in the quark propagators. The coulomb gauge fixing is employed for the use of the wall source. The time slice of the source is $t_0 = 12$ ($t_0 + 1 = 13$) for the π operator (K and κ operators) and the fixed sink time slice is $t_1 = 53$ for K operator. We calculate the time correlation functions on the gauge configurations shifted in the temporal direction by $T_{\rm shift}$ in Table I and take an average of them to improve the statistics.[*)] We adopt $t_R = 18$ as the reference time for the diagonalization for $I = 1/2$. The statistical errors are evaluated by the jackknife analysis with a binsize of 125 MD time. Here, the MD time is the number of trajectories multiplied by the trajectory length τ, and $\tau = 0.25$ ($\tau = 0.5$) for $\kappa_{ud} = 0.13770$ (others).

§3. Numerical results

k^2 and $\tan\delta_0(k)/k$ on the lowest state are shown in Table. II. For $I = 3/2$ ($I = 1/2$), k^2 is positive (negative), so we confirm the interaction is repulsive (attractive). The scattering length is defined as the constant term in the k^2-expansion

*) As mentioned later, data of $\pi\pi(I = 2)$ and $KK(I = 1)$ are also discussed in addition to those of πK. We do not include the time correlation function with $T_{\rm shift} = 0$ for $KK(I = 1)$ in the analysis.

Table I. The quark mass parameters and corresponding hadron masses.

κ_{ud}	κ_s	m_π [GeV]	m_K [GeV]	$N_{\rm conf}$	$T_{\rm shift}$
0.13770	0.13640	0.2949(23)	0.5925(17)	800	$0, 16, 32$
0.13754	0.13640	0.4110(16)	0.6348(13)	450	$0, 16, 32, 48$
0.13727	0.13640	0.5699(13)	0.7131(12)	400	$0, 16, 32, 48$
0.13700	0.13640	0.7010(12)	0.7887(12)	400	$0, 16, 32, 48$

Table II. k^2 and $\tan\delta_0(k)/k$ on the lowest state for $I = 3/2$ and $I = 1/2$.

	$I = 3/2$		$I = 1/2$	
m_π [GeV]	k^2 [GeV^2]	$\tan\delta_0(k)/k$ [fm]	k^2 [GeV^2]	$\tan\delta_0(k)/k$ [fm]
0.29	0.00272(16)	−0.1205(61)	−0.00678(48)	0.524(59)
0.41	0.00323(22)	−0.1402(82)	−0.01001(77)	1.08 (18)
0.57	0.00307(20)	−0.1340(76)	−0.0205 (28)	−5.9 (69)
0.70	0.00308(16)	−0.1343(62)	−0.063 (10)	−0.833(90)

of $\tan\delta_0(k)/k$ as in Eq. (2·1). Therefore, $\tan\delta_0(k)/k$ can be regarded as the scattering length if $|k^2|$ is small enough to neglect the $\mathcal{O}(k^2)$ term in the expansion. $|k^2|$ for $I = 1/2$ is, however, not so small in the heavy quark mass region. We especially find an extreme situation in $m_\pi > 0.41$ GeV. Due to the strong attraction, $\tan\delta_0(k)/k$ changes the sign and we get $\tan\delta_0(k) \simeq -i$. This fact suggests that the appearance of an unphysical bound state of the πK system in $m_\pi > 0.41$ GeV. We cannot use $\tan\delta_0(k)/k$ near the bound state for the extrapolation toward the πK threshold because the analytical structure of $\tan\delta_0(k)/k$ is not clear. In the following discussion, we assume that $|k^2|$ is small enough that $\tan\delta_0(k)/k$ reflect information at the πK threshold for all m_π of $I = 3/2$ and $m_\pi \leq 0.41$ GeV of $I = 1/2$, and adopt them as the scattering lengths. The validity of this assumption must be investigated by studying the L-dependence of $\tan\delta_0(k)/k$ in the future.

We extrapolate the scattering lengths toward the physical point. For this purpose, we employ the formula predicted by $\mathcal{O}(p^4)$ $SU(3)$ ChPT.[9)] To improve the ChPT fit, we also include the data of $\pi\pi(I = 2)$ and $KK(I = 1)$, which is same scattering system as $\pi K(I = 3/2)$ except for the replacement of the light and strange quarks. In the $\mathcal{O}(p^4)$ $SU(3)$ ChPT, a_0 can be described as

$$
\begin{aligned}
a_0^{(\pi\pi,I=2)} &= \frac{m_\pi}{16\pi F^2}\left[\,-1+\frac{16}{F^2}\left[\,m_\pi^2\cdot L(\mu)+\frac{1}{2}(m_\pi^2+2m_K^2)\cdot L_4(\mu)+\chi^{(\pi\pi,I=2)}\,\right]\,\right]\,,\\
a_0^{(KK,I=1)} &= \frac{m_K}{16\pi F^2}\left[\,-1+\frac{16}{F^2}\left[\,m_K^2\cdot L(\mu)+\frac{1}{2}(m_\pi^2+2m_K^2)\cdot L_4(\mu)+\chi^{(KK,I=1)}\,\right]\,\right]\,,\\
a_0^{(\pi K,I=3/2)} &= \frac{\mu_{\pi K}}{8\pi F^2}\left[\,-1+\frac{16}{F^2}\left[\,m_\pi m_K\cdot L(\mu)+\frac{1}{2}(m_\pi^2+2m_K^2)\cdot L_4(\mu)+\chi^{(\pi K,I=3/2)}\,\right]\,\right]\,,\\
a_0^{(\pi K,I=1/2)} &= \frac{\mu_{\pi K}}{8\pi F^2}\left[\,2+\frac{16}{F^2}\left[\,m_\pi m_K\cdot L(\mu)-(m_\pi^2+2m_K^2)\cdot L_4(\mu)+\chi^{(\pi K,I=1/2)}\,\right]\,\right],
\end{aligned}
\tag{3·1}
$$

where $\mu_{\pi K}$ is the reduced mass of πK, F is the decay constant in the chiral limit, and L_4, $L \equiv 2L_1 + 2L_2 + L_3 - 2L_4 - L_5/2 + 2L_6 + L_8$ are the low energy constants defined in Ref. 10) at scale μ. $\chi^{(\pi\pi,I=2),(KK,I=1),(\pi K,I=3/2),(\pi K,I=1/2)}(\mu, m_\pi, m_K)$ are known functions with chiral logarithm terms and the explicit forms can be found in the above references.

The fitting results of $a_0^{(\pi\pi,I=2)}/m_\pi$, $a_0^{(KK,I=1)}/m_K$ and $a_0^{(\pi K,I=3/2,1/2)}/\mu_{\pi K}$ are plotted by dotted lines as a function of m_π^2 in Fig. 1. The filled (open) symbols represent the data used (omitted) in the fit. We use only the data in $m_\pi \le 0.41$ GeV for the $\pi\pi(I=2)$, $KK(I=1)$ and $\pi K(I=3/2)$, and at $m_\pi = 0.29$ GeV for $\pi K(I=1/2)$ to obtain a reasonable $\chi^2/N_{\rm df}$. In this fit $\chi^2/N_{\rm df} = 1.8$ is a little larger than 1.0. This suggests that the validity of the $\mathcal{O}(p^4)$ $SU(3)$ ChPT is controversial near $m_\pi = 0.41$ GeV. The fit parameters and the scattering lengths at the physical point ($m_\pi = 0.140$ GeV, $m_K = 0.494$ GeV) are listed in Table III, where the renormalization scale is set to $\mu = 0.770$ GeV. Our value of $10^3 \cdot L_4$ is smaller than $-0.04(10)$ evaluated by PACS-CS Collaboration.[8] While we confirm that our numerical results in $0.29 \le m_\pi \le 0.41$ GeV are consistent with those in the previous lattice studies[2),11)–13)] within statistical errors, the scattering lengths for $\pi\pi(I=2)$, $KK(I=1)$ and $\pi K(I=3/2)$ at the physical point tend to be slightly overestimated compared to the previous results.[2),11)–13)] This discrepancy at the physical point is caused by the chiral extrapolation. To understand the discrepancy we need the systematic studies of the chiral extrapolation such as treating the kaon as a heavy particle or including the higher terms of the ChPT. They remain as future tasks. On the other hands, our measured scattering length for $\pi K(I=1/2)$ is almost consistent with the value evaluated from the data of $\pi K(I=3/2)$ by using ChPT.[2)]

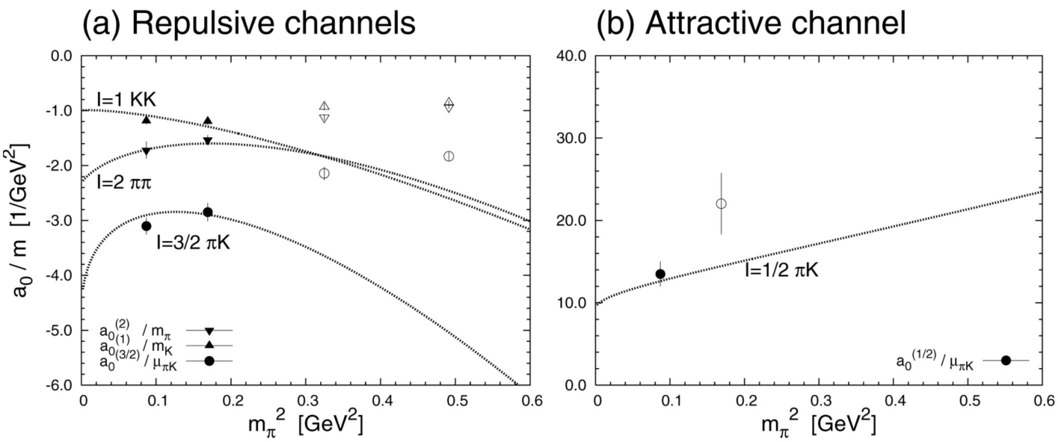

Fig. 1. m_π^2-dependence of $a_0/(m_\pi, m_K, \mu_{\pi K})$ and fit curves by the $\mathcal{O}(p^4)$ $SU(3)$ ChPT.

Table III. The fit parameters and $m_\pi a_0$ at the physical point ($m_\pi = 0.140$ GeV, $m_K = 0.494$ GeV).

F [GeV]	$10^3 \cdot L$	$10^3 \cdot L_4$	$m_\pi a_0^{(2)}$	$m_K a_0^{(1)}$	$m_\pi a_0^{(3/2)}$	$m_\pi a_0^{(1/2)}$
0.1020(62)	0.56(19)	−0.76(19)	−0.0376(54)	−0.224(49)	−0.0500(68)	0.154(25)

§4. Conclusion

Direct lattice QCD computation of the S-wave scattering length of πK ($I = 1/2,\ 3/2$) systems have been performed. The results have reproduced the correct signs of the scattering lengths for the first time. Therefore we have confirmed that the interaction is attractive (repulsive) in $I = 1/2$ ($I = 3/2$). We have found that the attraction in the $\pi K(I = 1/2)$ system becomes stronger at $m_\pi > 0.41$ GeV, and then the sign of $\tan\delta_0(k)/k$ becomes negative. We have compared the m_π^2-dependencies of the scattering lengths with those predicted by the $\mathcal{O}(p^4)$ $SU(3)$ ChPT. We use the data in $m_\pi \leq 0.41$ GeV for the $\pi\pi(I = 2)$, $KK(I = 1)$ and $\pi K(I = 3/2)$, and at $m_\pi = 0.29$ GeV for $\pi K(I = 1/2)$ to obtain a reasonable $\chi^2/N_{\rm df}$ in this fit. Due to the large value of $\chi^2/N_{\rm df}$, the validity of the $\mathcal{O}(p^4)$ $SU(3)$ ChPT remains controversial near $m_\pi = 0.41$ GeV. The systematic studies of the chiral extrapolation where the kaon is treated as a heavy particle or the higher terms of the ChPT are included, remain as future tasks.

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