S-wave πK scattering length from lattice QCD

Kiyoshi Sasaki[*]

Department of Physics, Tokyo Institute of Technology,
Tokyo 152-8551, Japan
E-mail: ksasaki@th.phys.titech.ac.jp

Naruhito Ishizuka

Graduate School of Pure and Applied Sciences, University of Tsukuba,
Tsukuba, Ibaraki 305-8571, Japan
and
Center for Computational Science, University of Tsukuba,
Tsukuba, Ibaraki 305-8577, Japan
E-mail: ishizuka@het.ph.tsukuba.ac.jp

Takeshi Yamazaki

Center for Computational Science, University of Tsukuba,
Tsukuba, Ibaraki 305-8577, Japan
E-mail: yamazaki@ccs.tsukuba.ac.jp

Makoto Oka

Department of Physics, Tokyo Institute of Technology,
Tokyo 152-8551, Japan
E-mail: oka@th.phys.titech.ac.jp

for PACS-CS Collaboration

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 $m_\pi = 0.30 - 0.70$ 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.

[*]Speaker.

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, existence of a broad resonance is suggested in $I = 1/2$. Until now, three studies in lattice QCD have been reported [1, 2, 3]. 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 for $I = 3/2$ 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 length at each simulation points, we investigate the quark-mass dependence and also discuss the limitation of $\mathcal{O}(p^4)$ $SU(3)$ ChPT. All calculations of this work have been done on the super parrarell computers, PACS-CS and T2K-Tsukuba, at the University of Tsukuba.

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 [4],

$$(\tan \delta_0(k)/k)^{-1} = \frac{1}{\pi L} \cdot \mathscr{Z}_{00} \left(1, \frac{k^2}{(2\pi/L)^2} \right) \ , \tag{2.2}$$

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

$$\mathscr{Z}_{00}(s, \bar{n}) \equiv \sum_{\vec{m} \in \mathbf{Z}^3} \frac{1}{(\vec{m}^2 - \bar{n})^s} \tag{2.3}$$

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. $\mathscr{Z}_{00}(1, k^2/(2\pi/L)^2)$, 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

$$G(t) = \langle 0| \, K^+(t_1)\pi^+(t) \, (W_{K^+}(t_0+1)W_{\pi^+}(t_0))^\dagger \, |0\rangle \cdot \mathrm{e}^{m_K(t_1-1)} \,, \tag{2.4}$$

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 [5]. The time slice of the kaon sink operator t_1 is fixed as $t_1 \gg t$. The exponential factor $\mathrm{e}^{m_K(t_1-t)}$ 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 are suggested in the low energy, and then it might be necessary to separate the contamination from the excited states. For this purpose, we use the two types of operators Ω_0 and Ω_1 ($\overline{\Omega}_0$ and $\overline{\Omega}_1$),

$$\Omega_0(t) = \frac{1}{\sqrt{3}}\left(K^+(t_1)\pi^0(t) - \sqrt{2}\, K^0(t_1)\pi^+(t)\right) \cdot \mathrm{e}^{m_K(t_1-t)} \,,$$
$$\Omega_1(t) = \kappa(t) \,,$$
$$\overline{\Omega}_0(t_0) = \frac{1}{\sqrt{3}}\left(W_{K^+}(t_0+1)W_{\pi^0}(t_0) - \sqrt{2}\, W_{K^0}(t_0+1)W_{\pi^+}(t_0)\right) \,,$$
$$\overline{\Omega}_1(t_0) = W_\kappa(t_0+1) \,, \tag{2.5}$$

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,

$$G_{ij}(t) = \langle 0| \, \Omega_i(t) \, \overline{\Omega}_j^\dagger(t_0) \, |0\rangle \qquad (\, i,\, j = 0,1\,) \,, \tag{2.6}$$

and with a reference time t_R we extract the energy of the ground state by the diagonalization of $G^{-1}(t_R)\, G(t)$ [6].

The calculations are carried out with $N_f = 2+1$ full QCD configurations generated by the PACS-CS Collaboration [7] using the Iwasaki gauge action at $\beta = 1.90$ and nonperturbatively $\mathscr{O}(a)$-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 1. The Dirichlet (periodic) boundary condition are 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 slice is $t_1 = 53$ for K operator. 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 250 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).

κ_{ud}	κ_s	m_π [GeV]	m_K [GeV]	N_{conf}
0.13770	0.13640	0.2971(29)	0.5935 (17)	800
0.13754	0.13640	0.4101(27)	0.6362 (19)	450
0.13727	0.13640	0.5707(16)	0.7135 (14)	400
0.13700	0.13640	0.7032(11)	0.79086(97)	400

Table 1: The quark mass parameters and corresponding hadron masses.

3. Numerical results

In Fig. 1, we show the time correlation functions for both the channels at $m_\pi \simeq 0.30$ GeV as an example. In the right panel, the absolute values of each component $G_{ij}(t)$ in $I = 1/2$ are presented. The open (filled) symbols represent the (off-)diagonal elements of $G_{ij}(t)$ and the signs are positive (negative). We find that the signals of $G(t)$ are very clean even in $I = 1/2$.
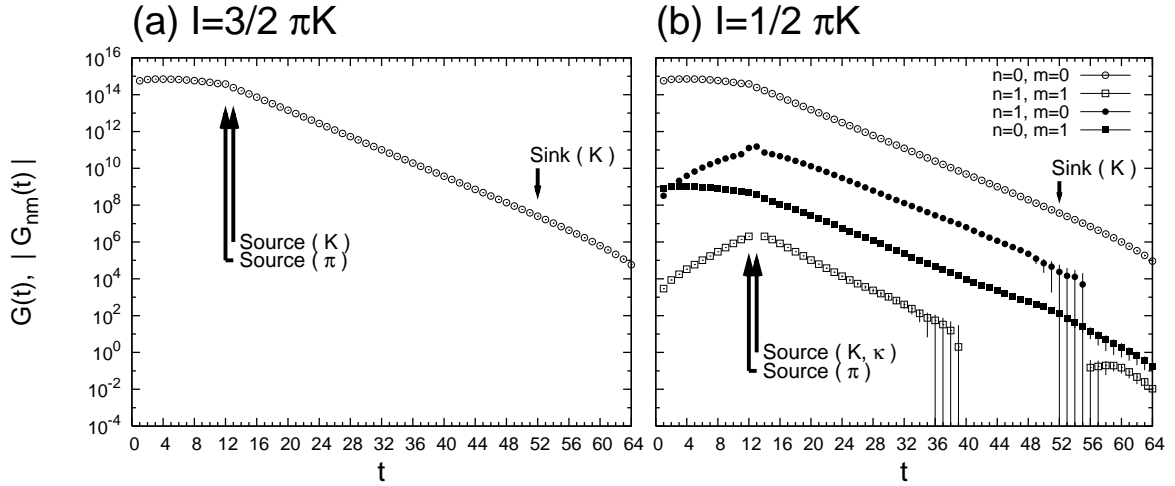
Figure 1: (a) $G(t)$ for $I = 3/2$ and (b) $|G_{ij}(t)|$ for $I = 3/2$ at $m_\pi \simeq 0.30$ GeV.

To see effects of the contaminations from excited states for the $I = 1/2$ πK system, we consider the ratios of $G_{00}(t)$ and EV$[\, G^{-1}(t_R)\, G(t)\,]_0$, the lowest eigenvalue of $G^{-1}(t_R)\, G(t)$, to the free πK propagator,

$$R_0(t) \equiv \frac{G_{00}(t)}{G_{00}(t_R)} \cdot \left[\, e^{-(m_\pi + m_K)\cdot(t - t_R)} \,\right]^{-1},$$

$$D_0(t) \equiv \text{EV}\left[\, G^{-1}(t_R)\, G(t)\, \right]_0 \cdot \left[\, e^{-(m_\pi + m_K)\cdot(t - t_R)} \,\right]^{-1}. \tag{3.1}$$

In the left panel of Fig. 2, $R_0(t)$ (open symbols) and $D_0(t)$ (filled symbols) at $m_\pi \simeq 0.30$ GeV are plotted. The difference of the two ratios is small. This means that the contamination from the excited states is negligible at this quark mass parameter. On the other hand, the right panel of 2 shows that the contamination is not so small at $m_\pi \simeq 0.70$ GeV. The diagonalization significantly
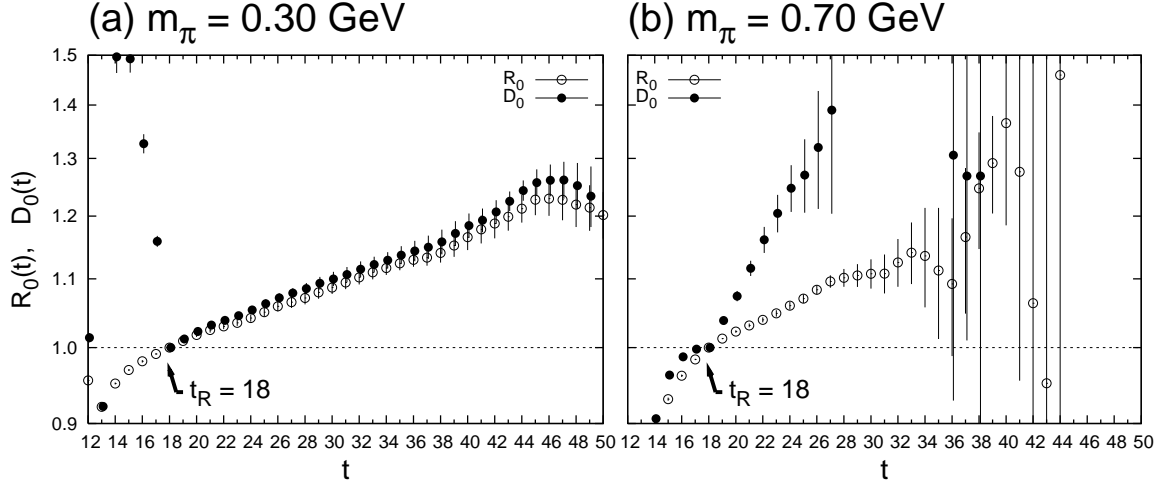
Figure 2: $R_0(t)$ and $D_0(t)$ at (a) $m_\pi \simeq 0.30$ GeV and (b) 0.70 GeV for $I = 1/2$.

changes the behavior of the ratio, because the πK-type operator (Ω_0) has a large overlap with the excited states. Therefore, separating the contamination is indispensable for the heavy quark masses.

k^2 and $\tan \delta_0(k)/k$ on the lowest state is shown in Table. 2. 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 of $\tan \delta_0(k)/k$. 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 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.

	$I = 3/2$		$I = 1/2$	
m_π [GeV]	k^2 [GeV^2]	$\tan \delta_0(k)/k$ [fm]	k^2 [GeV^2]	$\tan \delta_0(k)/k$ [fm]
0.30	0.00326(30)	$-0.141(11)$	$-0.00596(71)$	0.431(76)
0.41	0.00404(82)	$-0.170(29)$	$-0.0100\ (25)$	1.11 (75)
0.57	0.0029 (10)	$-0.130(38)$	$-0.0162\ (32)$	$-13.\ \ (120)$
0.70	0.00328(39)	$-0.142(15)$	$-0.060\ \ (12)$	$-\ 0.87\ (11)$

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

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 [8]. To improve the ChPT fit, we also include the data of $\pi\pi(I=2)$, 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

$$a_0^{(\pi\pi,I=2)} = \frac{m_\pi}{16\pi F^2}\left[-1 + \frac{16}{F^2}\left[m_\pi^2 \cdot L(\mu) + \frac{1}{2}(m_\pi^2 + 2m_K^2)\cdot L_4(\mu) + \chi^{(\pi\pi,I=2)}\right]\right],$$

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

$$a_0^{(\pi K,I=1/2)} = \frac{\mu_{\pi K}}{8\pi F^2}\left[2 + \frac{16}{F^2}\left[m_\pi m_K \cdot L(\mu) - (m_\pi^2 + 2m_K^2)\cdot L_4(\mu) + \chi^{(\pi K,I=1/2)}\right]\right], \quad (3.2)$$

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.[9] at scale μ. $\chi^{(\pi\pi,I=2),(\pi K,I=3/2),(\pi K,I=1/2)}(\mu,m_\pi,m_K)$ are known functions with chiral logarithm terms and the explicit forms can be found in the above references.

The fitting results of $a_0^{(\pi\pi,I=2)}/m_\pi$, $a_0^{(\pi K,I=3/2)}/\mu_{\pi K}$ and $a_0^{(\pi K,I=1/2)}/\mu_{\pi K}$ are plotted as a function of m_π^2 in Fig. 3. The filled symbols represent the data used in the fit. The fit with the data in $m_\pi \geq 0.57$ GeV significantly increases χ^2/N_{df}, so we only use the data in $m_\pi \leq 0.41$ GeV. The dotted lines are the fitting lines. The fit parameters and $m_\pi a_0$ at the physical point ($m_\pi = 0.140$ GeV, $m_K = 0.494$ GeV) are also listed in Table 3, where the renormalization scale is set to $\mu = 0.770$ GeV. The numerical results in $m_\pi \leq 0.41$ GeV are described by the ChPT within the statistical errors. $10^3 \cdot L_4$ is consistent with $-0.04(10)$ evaluated by PACS-CS Collaboration [7]. The scattering lengths for $\pi\pi(I=2)$ and $\pi K(I=3/2)$ are consistent with the previous lattice studies [2, 10]. Our measured scattering length for $\pi K(I=1/2)$ is also consistent with the value evaluated from the data of $\pi K(I=3/2)$ by using ChPT [10].

Our evaluation on the scattering length, however, has some issues to be solved. First, the statistical errors are not so small. The simple solution is to add calculations with different source points and improve the statistics. Second, the behavior near the chiral limit is strongly affected by the chiral logarithm term, so giving an evaluation without the long chiral extrapolation is desirable. For this purpose, the calculations in $m_\pi < 0.30$ GeV are now in progress. Third, $\tan\delta_0(k)/k$ in the low-momentum limit must be evaluated by systematic studies with the different volumes and boundary conditions. These are important issues in the future.

χ^2/N_{df}	F [GeV]	$10^3 \cdot L$	$10^3 \cdot L_4$	$m_\pi a_0^{(\pi\pi,I=2)}$	$m_\pi a_0^{(\pi K,I=3/2)}$	$m_\pi a_0^{(\pi K,I=1/2)}$
0.3	0.114(26)	0.6(18)	$-1.4(19)$	$-0.037(26)$	$-0.051(38)$	0.14(10)

Table 3: The fit parameters and $m_\pi a_0$ at the physical point ($m_\pi = 0.140$ GeV, $m_K = 0.494$ GeV) .

4. Conclusion

Direct lattice QCD computation of the *S*-wave scattering length of πK ($I = 1/2$ and $I = 3/2$) systems have been performed. The results have reproduced the correct signs of the scattering
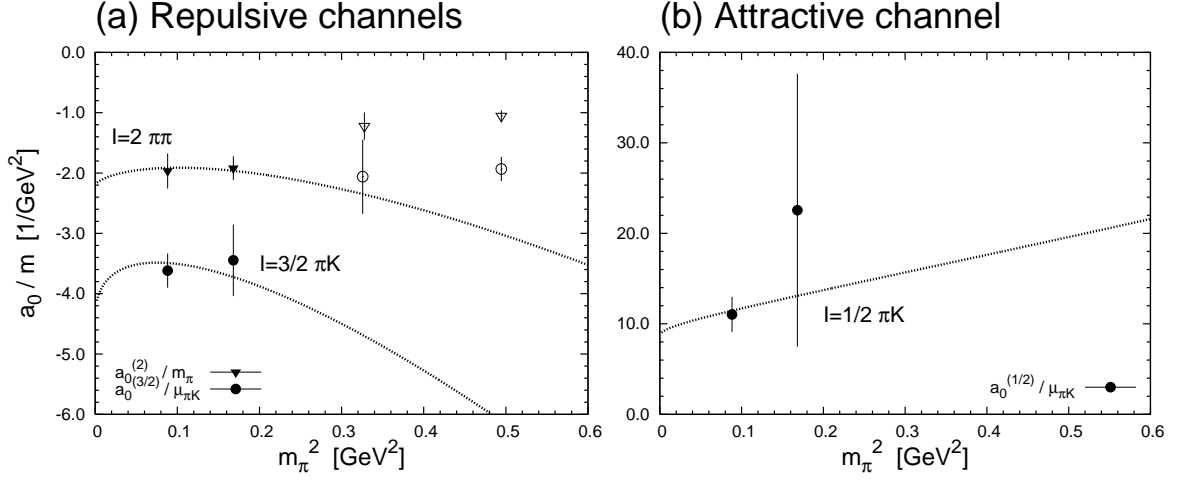
Figure 3: m_π^2-dependence of $a_0/(m_\pi, \mu_{\pi K})$ and fit curves by the $\mathcal{O}(p^4)$ $SU(3)$ ChPT.

lengths for the first time and therefore 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 there the sign of the scattering length becomes negative. We have compared the m_π-dependencies of the scattering lengths with those predicted by the $\mathcal{O}(p^4)$ $SU(3)$ ChPT. The data of πK ($I = 1/2$ and $I = 3/2$), $\pi\pi(I = 2)$ for $m_\pi \leq 0.41$ GeV have been used in the fit. We have confirmed that the numerical results in $m_\pi \leq 0.41$ GeV are described by the ChPT. Our evaluation on the scattering length, however, has some issues to be solved, and those remain as future tasks.

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