Finite size effect on pseudoscalar meson sector in 2+1 flavor QCD at the physical point

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We investigate finite size effect on pseudoscalar meson masses and decay constants using a partial set of the “PACS10” configurations which are generated keeping the space-time volumes over (10 fm)$^4$ in 2+1 flavor QCD at the physical point. We have tried two kinds of analyses fixing $\kappa$ values or measured axial Ward identity quark masses. Comparing the results on (5.4 fm)$^4$ and (10.8 fm)$^4$ lattices we have found sizable finite size effect on the pseudoscalar meson sector in the former analysis: 2.1%, 4.8% and 0.36% finite size effect on $m_\pi$, $m_{\eta}$ and $f_\pi$, respectively, on the (5.4 fm)$^4$ lattice. For the latter analysis the finite size effect on the pseudoscalar meson decay constants is 0.67% for $f_\pi$ and 0.26% for $f_\eta$, which are roughly a factor of three larger than the prediction of the full one-loop SU(3) chiral perturbation theory, while the finite size effect on the pseudoscalar meson masses is hardly detected under the current statistical precision.

I. INTRODUCTION

Lattice QCD simulations on very large lattices, which are named master-field simulations by Lüscher [1], have various potential advantages: the statistical errors decrease thanks to the geometrical symmetries of the lattice [2], the accessible minimum momentum is reduced in proportion to $1/L$ with $L$ the lattice extent, and we could be free from the finite size effect on the low energy properties of the baryons which is potentially severe discussed in Ref. [3]. Since the systematic study of the finite size effect demands huge computational cost, lattice QCD practitioners have been heavily depending on the analytic estimations so far [1] [4].

PACS Collaboration is now generating 2+1 flavor QCD configurations on very large lattices over (10 fm)$^4$ in 2+1 flavor QCD at the physical point using the Wilson-type quarks. These are called “PACS10” configurations. This project is the successor to the PACS-CS project which mainly focused on reducing the up-down quark masses up to the physical point [6] [7]. Since the PACS10 configurations have very large physical volumes, they should provide us a good opportunity to investigate the finite size effect in 2+1 flavor QCD. We have made a finite size study employing (10.8 fm)$^4$ and (5.4 fm)$^4$ lattices at a cutoff of $a^{-1} \approx 2.3$ GeV, the latter of which is a typical lattice size in current 2+1 flavor lattice QCD simulations at the physical point. The same hopping parameters are chosen for both lattices. We have performed two types of analyses: one is a comparison between the results for the pseudoscalar (PS) meson sector at the same hopping parameter on both lattices. The other is a comparison at the same axial Ward identity (AWI) quark masses on both lattices, where the quark masses on the smaller lattice is adjusted to those on the larger one by the reweighting method [7]. We have observed different types of finite size effects in two analyses. It is reasonable to make a comparison with the chiral perturbation theory (ChPT) in the second analysis with the quark mass fixed on both lattices.

In this paper we present details of two different types of analyses for finite size effect on the pseudoscalar meson sector. The results in the second analysis with the fixed quark mass are compared with the ChPT predictions. We conclude that the finite size effect on the PS meson decay constants is about 0.7% on the (5.4 fm)$^4$ lattice, which is roughly a factor of three larger than the expectation from ChPT. As for the PS meson masses it is difficult to detect the finite size effect beyond the statistical errors.

This paper is organized as follows. The simulation details are given in Sec. II. In Sec. III we present the results obtained with two kinds of analyses for the finite size effect and compare the results with the ChPT predictions. Our conclusions and outlook are summarized in Sec. IV.

II. SIMULATION DETAILS

A. Configuration generation

Following Ref. [8] we have generated 2+1 flavor QCD gauge configurations employing the stout-smeared $O(\alpha)$-improved Wilson-clover quark action and Iwasaki gauge action [9] on $V = L^3 \times T = 128^3$ and 64$^3$ lattices at $\beta = 1.82$. The corresponding lattice spacing is $a = 0.08457(67)$ fm ($a^{-1} = 2.333(18)$) GeV so that the physical lattice volumes reach (10.8 fm)$^4$ and (5.4 fm)$^4$, respectively. We use the stout smearing parameter $\rho = 0.1$ [10], and the number of the smearing is six. We adopt a value of the improvement coefficient $c_{SW} = 1.11$ which
is nonperturbatively determined by the Schrödinger functional (SF) scheme [11]. The hopping parameters for the light (up-down) and strange quarks \((\kappa^s_{ud}, \kappa^s_s) = (0.126117, 0.124902)\) are carefully adjusted to yield the physical pion and kaon masses \((m_{\pi}, m_K) = (135.0 \text{MeV}, 497.6 \text{MeV})\) on a \(128^4\) lattice within the cutoff error.

The degenerated up-down quarks are simulated with the domain-decomposed HMC (DDHMC) algorithm [12] both on \(64^4\) and \(128^4\) lattices. The ud quark determinant is separated into the UV and IR parts after the even-odd preconditioning. We also apply the twofold mass preconditioning [13, 14] to the IR part by splitting it into \(\tilde{F}_{\text{IR}}\), \(F'_{\text{IR}}\) and \(F''_{\text{IR}}\). This decomposition is controlled by two additional hopping parameters: \(\kappa''_{ud} = \rho_1 \kappa^s_{ud}\) with \(\rho_1 = 0.9997\) and \(\kappa''_{ud} = \rho_1 \rho_2 \kappa^s_{ud}\) with \(\rho_2 = 0.9940\). \(\tilde{F}_{\text{IR}}\) is derived from the action preconditioned with \(\kappa''_{ud}\). The ratio of two preconditioners with \(\kappa''_{ud}\) and \(\kappa''_{ud}\) gives \(F'_{\text{IR}}\). \(F''_{\text{IR}}\) is from the heaviest preconditioner with \(\kappa''_{ud}\). In the end the force terms consist of the gauge force \(F_g\), the UV force \(F_{\text{UV}}\) and the three IR forces \(F'_{\text{IR}}, F''_{\text{IR}}\) and \(\tilde{F}_{\text{IR}}\). We adopt the multiple time scale integration scheme [15] in the molecular dynamics (MD) steps. The associated step sizes are controlled by a set of integers \((N_0, N_1, N_2, N_3, N_4)\):

- \(\delta \tau_{\text{UV}} = \kappa_{\text{UV}} = \tau/N_0 N_1 N_2 N_3 N_4\),
- \(\delta \tau_{\text{IR}} = \kappa_{\text{IR}} = \tau/N_0 N_2 N_3 N_4\),
- \(\delta \tau_{\text{IR}} = \kappa_{\text{IR}} = \tau/N_0 N_2 N_3 N_4\) with \(\tau = 1.0\).

Our choice of \((N_0, N_1, N_2, N_3, N_4) = (8, 2, 2, 2, 12)\) and \((8, 2, 2, 2, 22)\) for the \(64^4\) and \(128^4\) lattices results in 80% and 72% acceptance rates, respectively.

The strange quark on a \(64^4\) lattice is simulated with the UVPHMC algorithm [16–19] where the action is UV-filtered [20] after the even-odd preconditioning without domain decomposition. We set the step size as \(\delta \tau_{s} = \delta \tau_{\text{IR}}''\) according to our observation \(|||F_{\text{IR}}''||| \approx |||F_{\text{IR}}''|||\). This algorithm is made exact by correcting the polynomial approximation with the global Metropolis test [21] at the end of each trajectory. We find that the choice of \(N_{\text{poly}} = 350\) yields 99% acceptance rate. On the other hand, we employ the RHMC algorithm [22] to save the memory in simulating the strange quark on a \(128^4\) lattice choosing the force approximation range of \([\min, \max] = [0.00025, 1.85]\) with \(N_{\text{RHMC}} = 8\) and \(\delta \tau_{s} = \delta \tau_{\text{IR}}''\) for the step size. After thermalization we generate 2000 and 200 trajectories on \(64^4\) and \(128^4\) lattices, respectively, and calculate hadronic observables at every 10 trajectories.

In Fig. 1 we present a jackknife analysis for the plaquette value averaged over the space-time volume on \(64^4\) and \(128^4\) lattices. The central values of the plaquette on both lattices show good consistency. An important observation is that the magnitude of the error on \(128^4\) lattice is saturated around 5 MD time, while the error for \(64^4\) lattice needs about 20 MD time to be independent of the binsize. This is because the correlation between successive configurations is reduced in proportion to \(1/\sqrt{V}\) thanks to the stochastic locality [1], once the physical extent of the lattice goes beyond the relevant scale for the target physical observable. We also point out that the error on \(128^4\) lattice is much smaller than that on \(64^4\) lattice.

**B. Reweighting technique**

When we investigate the finite size effect equalizing the AWI quark mass between \(64^4\) and \(128^4\) lattices, we need to make a tiny shift of the hopping parameters on the smaller lattice employing the reweighting technique. The reweighting factor for the ud quark is evaluated with a stochastic method introducing a set of independent Gaussian random noises \(\eta_i\) \((i = 1, \ldots, N_q)\):

\[
\text{det}[W_{\text{ud}}] = \left[ \lim_{N_q \rightarrow \infty} \frac{1}{N_q} \sum_{i=1}^{N_q} e^{-|W_{\text{ud}}^{-1}\eta_i|^2} \right],
\]

\[
W_{\text{ud}} = \frac{D(\kappa_{\text{ud}})}{D(\kappa_{\text{ud}})}
\]

where \(D(\kappa_{\text{ud}})\) is the Wilson-Dirac matrix with a target hopping parameter \(\kappa_{\text{ud}}^*\). For the strange quark we employ the square root trick,

\[
\text{det}[W_{s}] = \left[ \lim_{N_q \rightarrow \infty} \frac{1}{N_q} \sum_{i=1}^{N_q} e^{-|W_{s}^{-1}\eta_i|^2} \right]^{\frac{1}{2}},
\]

\[
W_{s} = \frac{D(\kappa_{s}^*)}{D(\kappa_{s})}
\]

To reduce the fluctuation in the stochastic evaluation [1 and 3], we employ the determinant breakup technique [23, 24], in which the interval between \(\kappa_{q}\) and \(\kappa_{q}^*\) is divided into \(N_B\) sub-intervals for \(q = \text{ud}, s\).

**C. Measurement of hadronic observables**

Since we are interested in the PS meson state with zero spatial momentum projection, we use the following local
PS operator and axial vector current:

\[ P(t) = \sum_{\bar{x}} \bar{q}_f(\bar{x}, t) \gamma_5 q_g(\bar{x}, t), \]  
\[ A_\mu(t) = \sum_{\bar{x}} \bar{q}_f(\bar{x}, t) \gamma_\mu \gamma_5 q_g(\bar{x}, t), \]  

where \( f \) and \( g \) (\( f, g = ud, s \)) label the valence quark flavors. We do not take account of the \( O(a) \) improvement of the axial vector current, because the coefficient \( c_A \) was evaluated to be consistent with zero within the statistical error \([11]\). The correlation functions are calculated by employing the wall source method without gauge fixing \([25]\). We make 8 measurements in each space-time direction, which amount to \( 8 \times 4 = 32 \) measurements in total for each gauge configuration both on \( 64^4 \) and \( 128^4 \) lattices. The statistical errors are estimated with the jackknife method. After investigating the bin size dependence we have chosen 50 and 10 trajectories for \( 64^4 \) and \( 128^4 \) lattices, respectively. The correlation between successive configurations on \( 128^4 \) lattice is reduced by about \( \sqrt{\frac{128^4}{64^4}} = 4 \) compared to that on \( 64^4 \) lattice.

The PS meson masses are extracted from the correlation function of \( \langle P(t) P^\dagger(0) \rangle \), whose \( t \) dependence is given by

\[ \langle P(t) P^\dagger(0) \rangle = L^3 C_{PP} W(m_{PS} T) \times \exp(-m_{PS} T) \exp(-m_{PS} (T - t)), \]  

where \( W(m_{PS} T) \) with \( T = 64 \) and 128 denotes the contribution from the PS meson propagation wrapping around the lattice in the time direction:

\[ W(m_{PS} T) = 1 + \exp(-m_{PS} T) + \exp(-2m_{PS} T) + \cdots = \frac{1}{1 - \exp(-m_{PS} T)}. \]  

The PS meson decay constant is defined by

\[ Z_A \sqrt{2 \kappa_f} \sqrt{2 \kappa_g} \langle 0 | A_4 | PS \rangle = f_{PS} m_{PS} \]  

with \( |PS\) the PS meson state at rest and \( Z_A \) the renormalization factor of the axial current. We evaluate \( f_{PS} \) with the following combination:

\[ f_{PS} = Z_A \sqrt{2 \kappa_f} \sqrt{2 \kappa_g} \frac{\sqrt{2} |C_{AP}|}{m_{PS} \sqrt{|C_{PP}|}}, \]  

where we extract \( m_{PS}, C_{AP}, C_{PP} \) from a simultaneous fit of Eq. (7) and

\[ \langle A_4(t) P^\dagger(0) \rangle = L^3 C_{AP} W(m_{PS} T) \times \exp(-m_{PS} T) - \exp(-m_{PS} (T - t)) \]  

with a common fit range of \([t_{\min}, t_{\max}] = [17, 60] \) and \([20, 60] \) for \( \pi \) and \( K \) mesons, respectively, on the \( 128^4 \) lattice and \([t_{\min}, t_{\max}] = [17, 30] \) and \([20, 30] \) on the \( 64^4 \) lattice. Since we are interested in the finite size effect, we use the central value of \( Z_A = 0.9650(68)(95) \), which was nonperturbatively determined by the Schrödinger functional scheme \([20]\).

We define the bare AWI quark mass as

\[ m^A_{\text{AWI}} + m^g_{\text{AWI}} = \frac{\langle 0 | \nabla_4 A_4 | PS \rangle}{\langle 0 | P | PS \rangle}. \]  

The AWI quark masses are evaluated with

\[ m^A_{\text{AWI}} + m^g_{\text{AWI}} = m_{PS} \frac{|C_{AP}|}{|C_{PP}|}, \]  

where \( m_{PS}, C_{AP}, C_{PP} \) are extracted from a simultaneous fit of Eqs. (7) and (12) with \([t_{\min}, t_{\max}] = [17, 60] \) and \([20, 60] \) for \( \pi \) and \( K \) mesons, respectively, on the \( 128^4 \) lattice and \([t_{\min}, t_{\max}] = [17, 30] \) and \([20, 30] \) on the \( 64^4 \) lattice.

### III. NUMERICAL RESULTS

#### A. Finite size effect at the fixed hopping parameters

We first compare the results on \( 64^4 \) and \( 128^4 \) lattices at the same hopping parameters \((\kappa_{ud}, \kappa_s) = (0.126117, 0.124902)\). Figure 2 shows the effective masses for the PS mesons. We observe that the effective \( \pi \) meson mass on the \( 64^4 \) lattice is clearly heavier than that on the \( 128^4 \) lattice beyond the error bars. On the other hand, the effective mass for the \( K \) meson shows little finite size effect. In Table II we summarize the fit results for the PS meson masses \( m_{\pi,K} \) choosing the fit range of \([t_{\min}, t_{\max}] = [17, 60] \) and \([20, 60] \) for \( \pi \) and \( K \) mesons, respectively, on the \( 128^4 \) lattice and \([t_{\min}, t_{\max}] = [17, 30] \) and \([20, 30] \) on the \( 64^4 \) lattice. The deviation in the \( \pi \) meson channel is found to be about 2%. We also list the AWI quark masses \( m_{ud,s} \) in Table II. The ud quark mass on the \( 64^4 \) lattice is heavier than that on the \( 128^4 \) lattice by 4.8% in accordance with the finite size effect found for \( m_\pi \). Essentially, what makes the \( \pi \) meson mass heavier on \( 64^4 \) lattice is the increment of the ud quark mass, which is caused by the shift of the critical kappa \( \kappa_c \) due to the finite size effect. For the decay constants we plot the results on \( 64^4 \) and \( 128^4 \) lattices in Fig. 1, which are obtained by the method explained in Sec. II C. Their numerical values are presented in Table III. The small (0.36%) finite size effect is observed in the \( \pi \) meson channel, though it is hardly detected in the \( K \) meson channel. It should be noted that our results show an expected feature from ChPT that the finite size effect makes the values of the decay constants smaller as the spatial volume decreases.

#### B. Finite size effect at the fixed AWI quark masses

Let us turn to the analysis with the fixed AWI quark masses. In the previous subsection we have found that the AWI quark masses on \( 64^4 \) and \( 128^4 \) lattices show deviation by 4.8%. We adjusted the AWI quark masses on
the 64\textsuperscript{4} lattice to those on the 128\textsuperscript{4} lattice with the use of the reweighting technique explained in Sec. II B. The target hopping parameter is \((\kappa_{\text{ud}}^*,\kappa_s^*) = (0.126119,0.124902)\), which is obtained by a tiny shift of \((\Delta \kappa_{\text{ud}}^*, \Delta \kappa_s^*) = (+0.000002, \pm 0)\) from the simulation point. We choose \(N_B^\text{ud} = 4\) for the number of the determinant breakup and introduce 12 noise vectors for each determinant breakup. Figure 4 shows the configuration dependence of the reweighting factor from \((\kappa_{\text{ud}}^*,\kappa_s^*) = (0.126117,0.124902)\) to \((\kappa_{\text{ud}}^*,\kappa_s^*) = (0.126119,0.124902)\), which is normalized by the configuration average. The fluctuations are less than 60\% around the average. In Fig. 5 we plot the reweighting factor as a function of the stout-smeared plaquette value on each configuration. We observe that the reweighting factor takes larger values as the pla-
quette value increases. This is an expected correlation, due to which the reweighted plaquette value at \((\kappa_{ud},\kappa_s) = (0.126119,124902)\) should be larger than the original one at \((\kappa_{ud},\kappa_s) = (0.126117,0.124902)\). Figure 4 tells us how many noise vectors are necessary to make the reweighted values converged. We observe that the values of \(m_{ud}, m_\pi\) and \(f_\pi\) with the error bars show little dependence. Similar behaviors are obtained for other physical quantities. So \(N_\eta = 12\) in our choice is sufficient.

In Table [I] we present the results for the reweighted AWI quark masses on 64\(^4\) lattice, which show good agreement with those on 128\(^4\) lattice both for the ud and s quarks. This assures that the target hopping parameters are properly chosen. In Fig. 2 the red triangle represents the reweighted effective pseudoscalar meson masses on 64\(^4\) lattice. We find that they are degenerate with those on 128\(^4\) lattice within the error bars for both the \(\pi\) and \(K\) mesons. The numerical values for the fit results in Table [I] give quantitative confirmation of the consistency. It is hard to detect the finite size effect on \(m_\pi\) and \(m_K\) between 64\(^4\) and 128 lattices. On the other hand, the results for the PS meson decay constants are plotted in Fig. 3. We find that the reweighted \(f_\pi\) and \(f_K\) show clear finite size effect, whose magnitude is 0.67% for \(f_\pi\) and 0.26% for \(f_K\).

![Fig. 4. Configuration dependence of the reweighting factor from \((\kappa_{ud},\kappa_s) = (0.126119,124902)\) to \((\kappa_{ud},\kappa_s) = (0.126119,124902)\).](image)

**C. Comparison with ChPT prediction**

In SU(3) ChPT the full one-loop expressions for the finite size effects defined by \(R_X = (X_0 - X(\infty))/X(\infty)\)

are given by [6]:

\[
R_{m_\pi} = \frac{1}{4} \xi_\pi \tilde{g}_1(\lambda_\pi) - \frac{1}{12} \xi_\eta \tilde{g}_1(\lambda_\eta),
\]

\[
R_{m_K} = \frac{1}{6} \xi_\eta \tilde{g}_1(\lambda_\eta),
\]

\[
R_{f_\eta} = -\xi_\pi \tilde{g}_1(\lambda_\pi) - \frac{1}{2} \xi_K \tilde{g}_1(\lambda_K),
\]

\[
R_{f_K} = -\frac{3}{8} \xi_\pi \tilde{g}_1(\lambda_\pi) - \frac{3}{4} \xi_K \tilde{g}_1(\lambda_K) - \frac{3}{8} \xi_\eta \tilde{g}_1(\lambda_\eta),
\]

with

\[
\xi_{PS} \equiv \frac{2m_{PS}^2}{(4\pi f_\pi)^2},
\]

\[
\lambda_{PS} \equiv m_{PS} L,
\]

\[
\tilde{g}_1(x) \equiv \sum_{n=1}^{\infty} \frac{4m(n)}{\sqrt{n}x} K_1(\sqrt{n}x),
\]

where \(K_1\) is the modified Bessel function of the second kind and \(m(n)\) denotes the multiplicity of the partition.

**Fig. 5.** Reweighting factor from \((\kappa_{ud},\kappa_s) = (0.126119,0.124902)\) to \((\kappa_{ud},\kappa_s) = (0.126119,124902)\) as a function of stout-smeared plaquette value.

**Fig. 6.** Reweighted values for \(m_{ud}\) (top), \(m_s\) (middle) and \(f_\pi\) (bottom) as a function of \(N_\eta\).
\( n = n_x^2 + n_y^2 + n_z^2 \). In Fig. 7, we draw the \( L \) dependence of \( |R_X| \) (\( X = m_\pi, m_K, f_\pi, f_K \)) at the physical point. Since we have special interest in the values of \( R_X \) at \( L = 5.4 \) fm and 10.8 fm, they are summarized in Table IV. At \( L = 10.8 \) fm the expected finite size effect is at most 0.001\% found in \( f_\pi \) channel, which is completely negligible magnitude in current numerical simulations. On the other hand, the lattice with \( L = 5.4 \) fm can yield detectable finite size effect, whose magnitude is expected to be 0.2\% for \( f_\pi \) and 0.08\% for \( f_K \). Actually, our simulation results support this feature semi-quantitatively; 0.67\% finite size effect for \( f_\pi \) and 0.26\% for \( f_K \), though they are roughly a factor of three larger than the ChPT predictions. The discrepancy may be due to the higher-order effects in SU(3) ChPT, which are shown to enhance the magnitude of the finite size effects for \( f_\pi \) and \( f_K \) in Ref. [5].

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
\( L \) & 64 (rewighted) & 128 \\
\hline
\( m_\pi L \) & 3.74 & 7.48 \\
\hline
\( R_{m_\pi} \) & \( 5.067 \times 10^{-4} \) & \( 3.405 \times 10^{-6} \) \\
\hline
\( R_{m_K} \) & \( 3.317 \times 10^{-9} \) & \( 1.912 \times 10^{-16} \) \\
\hline
\( R_{f_\pi} \) & \( -2.027 \times 10^{-3} \) & \( -1.362 \times 10^{-5} \) \\
\hline
\( R_{f_K} \) & \( -7.602 \times 10^{-4} \) & \( -5.108 \times 10^{-6} \) \\
\hline
\end{tabular}
\caption{\( R_X (X = m_\pi, m_K, f_\pi, f_K) \) with \( L = 5.4 \) fm and 10.8 fm at the physical point.}
\end{table}

\section{Conclusions and Outlook}

We have investigated the finite size effect on the PS meson sector using (5.4 fm)\(^2\) and (10.8 fm)\(^2\) lattices in 2+1 flavor QCD at the physical point. The analysis at the fixed hopping parameters reveals 2.1\%, 4.8\% and 0.36\% finite size effect on \( m_\pi, m_{ud} \) and \( f_\pi \), respectively. On the other hand, in the analysis at the fixed AWI quark masses with the aid of the reweighting technique we detect 0.67\% and 0.26\% finite size effect on \( f_\pi \) and \( f_K \), respectively, which are roughly a factor of three larger than the ChPT prediction. We plan to make a similar finite size study for the baryon sector using the PACS10 configurations.

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