

$l = 2$ two-pion wave function and scattering phase shift

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$I = 2$ two-pion wave function and scattering phase shiftKiyoshi Sasaki^{1,*} and Naruhito Ishizuka^{1,2}¹*Center for Computational Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8577, Japan*²*Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan*

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We calculate a two-pion wave function for the $I = 2$ S -wave two-pion system with a finite scattering momentum and estimate the interaction range between two pions, which allows us to examine the validity of a necessary condition for the finite size formula presented by Rummukainen and Gottlieb. We work in the quenched approximation employing the plaquette gauge action for gluons and the improved Wilson action for quarks at $1/a = 1.63$ GeV on the $32^3 \times 120$ lattice. The quark masses are chosen to give $m_\pi = 0.420, 0.488$, and 0.587 GeV. We find that the energy dependence of the interaction range is small and the necessary condition is satisfied for our range of the quark mass and the scattering momentum, $k \leq 0.16$ GeV. We also find that the scattering phase shift can be obtained with a smaller statistical error from the two-pion wave function than from the two-pion time correlator.

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I. INTRODUCTION

Calculations of the scattering phase shift represent an important step for expanding our understanding of the strong interaction based on lattice QCD to dynamical aspects of hadrons. For the simplest case of the $I = 2$ S -wave two-pion system, several calculations have been reported in Refs. [1–6]. These calculations employ the finite size formula presented by Lüscher [7] and the extension to the system with a nonzero total momentum by Rummukainen and Gottlieb [8], in which the scattering phase shift is related to the energy eigenvalue in a finite volume. In previous applications of the formula the energy was calculated from an asymptotic time behavior of the two-pion time correlator.

The derivation of the finite size formula assumes a condition $R < L/2$ for the two-pion interaction range R and the lattice size L , so that the boundary condition does not distort the shape of the two-pion interaction. It is important to examine the validity of this necessary condition for reliable results of the scattering phase shift. The CP-PACS Collaboration calculated the two-pion wave function for the ground state of the $I = 2$ S -wave two-pion system and estimated the interaction range from it [9]. In this case the scattering momentum is very small; thus their work is an examination of the condition for the scattering length. They found that the interaction range is $R \sim 1.3\text{--}1.6$ fm for the pion mass $m_\pi = 0.520\text{--}0.860$ GeV. They also evaluated the scattering length and found it can be given with a smaller statistical error from the wave function than from the two-pion time correlator.

In the present paper we extend their work of the necessary condition for the scattering length (the scattering momentum $k \sim 0$) to that for the scattering phase shift

($k \neq 0$) for the $I = 2$ S -wave two-pion system. In order to set a finite momentum for the ground state, we consider a system having the total momentum $\mathbf{P} = (2\pi/L)\mathbf{e}_x$. We calculate the two-pion wave function and evaluate the scattering phase shift from it, as carried out by the CP-PACS Collaboration for the scattering length.

This article is organized as follows. In Sec. II we briefly review the derivation of the finite size formula presented by Rummukainen and Gottlieb [8], with emphasis on the role of the condition for the interaction range. The calculation method of the wave function and the simulation parameters are given in Sec. III. In Sec. IV A we present our results for the wave function and estimate the interaction range. The scattering phase shift from the wave function is provided and compared to those with the two-pion time correlator in Sec. IV B. Our results for the scattering length and the scattering phase shift at the physical quark mass are presented in Sec. IV C. Our conclusions are given in Sec. V. Preliminary reports of the present work were presented in Ref. [10]. The calculation was carried out on VPP5000/80 at the Academic Computing and Communications Center of University of Tsukuba.

II. FINITE SIZE FORMULA

We briefly review the derivation of the finite size formula presented by Rummukainen and Gottlieb [8], with emphasis on the role of the condition for the interaction range. We restrict ourselves to the formula for the $I = 2$ S -wave two-pion system, but the generalization can be easily carried out. The formula has also been derived from other approaches in Refs. [11,12]. We follow, however, the original derivation in Ref. [8].

First we consider a wave function in the infinite volume in Minkowski space defined by

$$\Psi(x_1; x_2) = \langle 0 | \pi^+(x_1) \pi^+(x_2) | \pi^+(p_1), \pi^+(p_2); \text{in} \rangle, \quad (1)$$

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in the spacelike region $(x_1 - x_2)^2 < 0$. The state $|\pi^+(p_1), \pi^+(p_2); \text{in}\rangle$ is an asymptotic two-pion state with the four-dimensional momenta p_1 and p_2 . $\pi^+(x)$ is an interpolating operator for π^+ at the four-dimensional position $x = (x^0, \mathbf{x})$. We assume that the two-pion interaction range R is finite and the wave function satisfies

$$(\square_j + m_\pi^2)\Psi(x_1; x_2) = 0 \quad \text{for } j = 1, 2, \quad (2)$$

for $-(x_1 - x_2)^2 > R^2$, where \square_j is the d'Alembertian with respect to the coordinate x_j .

In order to remove a trivial dependence of the center of mass coordinate $X = (x_1 + x_2)/2$, we introduce a relative wave function defined by

$$\phi(x) = \Psi(x_1; x_2) \cdot e^{iP \cdot X}, \quad (3)$$

where $x = x_1 - x_2$ is the relative coordinate and $P = p_1 + p_2 = (E, \mathbf{P})$ is the total four-dimensional momentum. From (2) $\phi(x)$ satisfies

$$(\square - k^2)\phi(x) = 0, \quad (4)$$

$$P \cdot \partial \phi(x) = 0, \quad (5)$$

for $-x^2 > R^2$, where k^2 is the scattering momentum defined by

$$k^2 = P^2/4 - m_\pi^2 = (E^2 - \mathbf{P}^2)/4 - m_\pi^2. \quad (6)$$

Equations (4) and (5) also yield

$$[\nabla^2 - (\mathbf{P} \cdot \nabla)^2/E^2 + k^2]\phi(x) = 0. \quad (7)$$

We can obtain a relation between the wave function and the scattering phase shift by introducing a center of mass frame. The wave function in the center of mass frame $\phi_{\text{CM}}(x_{\text{CM}})$ is related to that in the original frame $\phi(x)$ by the Lorentz transformation,

$$\phi_{\text{CM}}(x_{\text{CM}}) = \phi(x). \quad (8)$$

x_{CM} is the coordinate in the center of mass frame given by

$$x_{\text{CM}}^0 = \gamma(x^0 - \mathbf{v} \cdot \mathbf{x}), \quad (9)$$

$$\mathbf{x}_{\text{CM}} = \hat{\gamma}[\mathbf{x} - \mathbf{v}x^0], \quad (10)$$

where \mathbf{v} is the velocity $\mathbf{v} = \mathbf{P}/E$ and γ is the Lorentz boost factor $\gamma = 1/\sqrt{1 - \mathbf{v}^2} = E/\sqrt{P^2}$. The operation $\hat{\gamma}[\mathbf{x}]$ is defined by

$$\hat{\gamma}[\mathbf{x}] = \gamma \mathbf{x}_{\parallel} + \mathbf{x}_{\perp}, \quad (11)$$

where \mathbf{x}_{\parallel} and \mathbf{x}_{\perp} are components of \mathbf{x} parallel and perpendicular to the velocity \mathbf{v} , i.e., $\mathbf{x}_{\parallel} = \mathbf{v}(\mathbf{x} \cdot \mathbf{v})/\mathbf{v}^2$ and $\mathbf{x}_{\perp} = \mathbf{x} - \mathbf{x}_{\parallel}$.

From (4) and (5), $\phi_{\text{CM}}(x)$ satisfies

$$(\square - k^2)\phi_{\text{CM}}(x) = 0, \quad (12)$$

$$\frac{\partial}{\partial x^0} \phi_{\text{CM}}(x) = 0, \quad (13)$$

for $-x^2 > R^2$. Thus, $\phi_{\text{CM}}(x^0, \mathbf{x})$ is independent of x^0 and

$$\phi(0, \mathbf{x}) = \phi_{\text{CM}}(-\gamma(\mathbf{v} \cdot \mathbf{x}), \hat{\gamma}[\mathbf{x}]) = \phi_{\text{CM}}(0, \hat{\gamma}[\mathbf{x}]) \quad (14)$$

for $|\mathbf{x}| > R$.

In the following we always consider the wave function at $x^0 = 0$ and omit the argument for the relative time, for example, $\phi(\mathbf{x}) = \phi_{\text{CM}}(\hat{\gamma}[\mathbf{x}])$ for (14). We also know that the Helmholtz equation is satisfied:

$$(\nabla^2 + k^2)\phi_{\text{CM}}(\mathbf{x}) = 0 \quad \text{for } |\mathbf{x}| > R. \quad (15)$$

We can expand $\phi_{\text{CM}}(\mathbf{x})$ in terms of the spherical Bessel $j_l(x)$ and the Neumann function $n_l(x)$ as

$$\begin{aligned} \phi_{\text{CM}}(\mathbf{x}) = & \sum_{l=0}^{\infty} \sum_{m=-l}^l b_{lm}(k) \cdot Y_{lm}(\Omega)(\alpha_l(k) \cdot j_l(k|\mathbf{x}|) \\ & + \beta_l(k) \cdot n_l(k|\mathbf{x}|)), \end{aligned} \quad (16)$$

with some constant $b_{lm}(k)$, where Ω is the spherical coordinate for \mathbf{x} . The conventions of $j_l(x)$, $n_l(x)$, and $Y_{lm}(\Omega)$ agree with those of Ref. [13]. The coefficients $\alpha_l(k)$ and $\beta_l(k)$ yield the scattering phase shift as $\tan \delta_l(k) = \beta_l(k)/\alpha_l(k)$.

Next we consider a wave function on a periodic box L^3 in Euclidian space (on the lattice), which is defined by

$$\Psi^L(\mathbf{x}_1, \tau; \mathbf{x}_2, \tau) = \langle 0 | \pi^+(\mathbf{x}_1, \tau) \pi^+(\mathbf{x}_2, \tau) | \pi^+ \pi^+; E, \mathbf{P} \rangle, \quad (17)$$

where $|\pi^+ \pi^+; E, \mathbf{P}\rangle$ is an eigenstate with the total energy E and momentum \mathbf{P} on the lattice. The wave function is periodic with respect to the position of either of the pions:

$$\begin{aligned} \Psi^L(\mathbf{x}_1 + \mathbf{n}_1 L, \tau; \mathbf{x}_2 + \mathbf{n}_2 L, \tau) &= \Psi^L(\mathbf{x}_1, \tau; \mathbf{x}_2, \tau) \\ &\quad \text{for } \mathbf{n}_1, \mathbf{n}_2 \in \mathbb{Z}^3. \end{aligned} \quad (18)$$

We introduce a relative wave function like in Minkowski space by

$$\phi^L(\mathbf{x}) = \Psi^L(\mathbf{x}_1, \tau; \mathbf{x}_2, \tau) \cdot e^{E\tau - i\mathbf{P} \cdot \mathbf{X}}, \quad (19)$$

with $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$ and $\mathbf{X} = (\mathbf{x}_1 + \mathbf{x}_2)/2$. Equations (18) and (19) yield

$$\phi^L(\mathbf{x}) = (-1)^{L/(2\pi) \mathbf{P} \cdot \mathbf{n}} \cdot \phi^L(\mathbf{x} + \mathbf{n}L) \quad \text{for } \mathbf{n} \in \mathbb{Z}^3. \quad (20)$$

In the derivation of the finite size formula, it is assumed that the two-pion interaction range R is smaller than one-half the lattice extent, so that the boundary condition does not distort the shape of the two-pion interaction. With this assumption, $\phi^L(\mathbf{x})$ satisfies the same equation as for $\phi(\mathbf{x})$:

$$\begin{aligned} [\nabla^2 - (\mathbf{P} \cdot \nabla)^2/E^2 + k^2]\phi^L(\mathbf{x}) &= 0 \\ &\quad \text{for } R < |\hat{\gamma}[\mathbf{x}]| < L/2. \end{aligned} \quad (21)$$

The finite size formula is given by solving (21) under the boundary condition (20). It is convenient to change the variable from \mathbf{x} to $\mathbf{y} = \hat{\gamma}[\mathbf{x}]$ and define a new function by

$$\phi_{\text{CM}}^L(\mathbf{y}) = \phi^L(\mathbf{x}), \quad (22)$$

to solve the differential equation (21). $\phi_{\text{CM}}^L(\mathbf{x})$ satisfies

$$(\nabla^2 + k^2)\phi_{\text{CM}}^L(\mathbf{x}) = 0 \quad \text{for } R < |\mathbf{x}| < L/2, \quad (23)$$

$$\phi_{\text{CM}}^L(\mathbf{x}) = (-1)^{L/(2\pi)\mathbf{P}\cdot\mathbf{n}} \cdot \phi_{\text{CM}}^L(\mathbf{x} + \hat{\gamma}[\mathbf{n}]L) \quad \text{for } \mathbf{n} \in \mathbb{Z}^3. \quad (24)$$

Note that (22) is not the Lorentz transformation on the lattice, but it is merely a definition of the function with a change of the variable from \mathbf{x} to $\mathbf{y} = \hat{\gamma}[\mathbf{x}]$ to solve (21).

The general solution of (23) under (24) can be written by

$$\phi_{\text{CM}}^L(\mathbf{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l v_{lm}(k) \cdot G_{lm}(\mathbf{x}; k), \quad (25)$$

with some constant $v_{lm}(k)$. $G_{lm}(\mathbf{x}; k)$ is given by the periodic Green function:

$$G(\mathbf{x}; k) = \frac{1}{\gamma L^3} \sum_{\mathbf{q} \in \Gamma_{\mathbf{P}}} \frac{1}{\mathbf{q}^2 - k^2} e^{i\mathbf{q}\cdot\mathbf{x}}, \quad (26)$$

$$\Gamma_{\mathbf{P}} = \left\{ \mathbf{q} | \mathbf{q} = \hat{\gamma}^{-1} \left[\frac{2\pi}{L} \mathbf{n} + \mathbf{P}/2 \right], \mathbf{n} \in \mathbb{Z}^3 \right\}, \quad (27)$$

as

$$G_{lm}(\mathbf{x}; k) = \mathcal{Y}_{lm}(\nabla) G(\mathbf{x}; k), \quad (28)$$

where $\mathcal{Y}_{lm}(\mathbf{x}) = |\mathbf{x}|^l \cdot Y_{lm}(\Omega)$ with the spherical coordinate Ω for \mathbf{x} . The expansion of $G(\mathbf{x}; k)$ in terms of $j_l(x)$ and $n_l(x)$ is given by

$$G(\mathbf{x}; k) = \frac{k}{4\pi} n_0(k|\mathbf{x}|) + \sum_{l=0}^{\infty} \sum_{m=-l}^l g_{lm}(k; 1) \cdot Y_{lm}(\Omega) j_l(k|\mathbf{x}|). \quad (29)$$

The function $g_{lm}(k; 1)$ is an analytic continuation of

$$g_{lm}(k; z) = \left(\frac{i}{k} \right)^l \frac{4\pi}{\gamma L^3} \sum_{\mathbf{q} \in \Gamma_{\mathbf{P}}} \mathcal{Y}_{lm}(\mathbf{q}) \cdot (\mathbf{q}^2 - k^2)^{-z}, \quad (30)$$

which is defined for $\text{Re}(z) > (l+3)/2$, where the region $\Gamma_{\mathbf{P}}$ is defined by (27). The explicit expansion for $G_{lm}(\mathbf{x}; k)$ with general l and m is not needed. Note, however, that $G_{lm}(\mathbf{x}; k)$ contains $j_{l'}(k|\mathbf{x}|)$ for a whole range of l' and $n_{l'}(k|\mathbf{x}|)$ with only $l' = l$ as known from (28) and (29).

The wave function in Euclidian space is related to that in Minkowski space by the analytic continuation of the relative time $ix^0 \rightarrow x^4$. It seems that $\phi^L(\mathbf{x}) = \phi(\mathbf{x})$ at $x^0 = x^4 = 0$ and

$$\phi_{\text{CM}}^L(\mathbf{x}) = \phi_{\text{CM}}(\mathbf{x}), \quad (31)$$

from (14) and (22). But this is not true, because the

degeneracies of the energy eigenstate in the infinite and the finite volumes are different. Equation (31) should be changed to

$$\phi_{\text{CM}}^L(\mathbf{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l C_{lm}(k) \cdot Y_{lm}(\Omega) \phi_{\text{CM}}^{(lm)}(|\mathbf{x}|), \quad (32)$$

with some constant $C_{lm}(k)$, where Ω is the spherical coordinate for \mathbf{x} . $\phi_{\text{CM}}^{(lm)}(|\mathbf{x}|)$ is the lm component of $\phi_{\text{CM}}(\mathbf{x})$ defined by

$$\phi_{\text{CM}}^{(lm)}(|\mathbf{x}|) = \int d\Omega Y_{lm}^*(\Omega) \phi_{\text{CM}}(\mathbf{x}). \quad (33)$$

Substituting (16) and (25) into (32), we obtain

$$\begin{aligned} \phi_{\text{CM}}^L(\mathbf{x}) &= \sum_{l=0}^{\infty} \sum_{m=-l}^l v_{lm}(k) \cdot G_{lm}(\mathbf{x}; k) \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^l D_{lm}(k) \cdot Y_{lm}(\Omega) (\alpha_l(k) \cdot j_l(k|\mathbf{x}|) \\ &\quad + \beta_l(k) \cdot n_l(k|\mathbf{x}|)), \end{aligned} \quad (34)$$

where $D_{lm}(k) = C_{lm}(k) b_{lm}(k)$.

In the present work we consider only the two-pion state in the \mathbf{A}_1^+ representation of the rotational group on the lattice, which is equal to the S wave up to the angular momentum $l = 2$. If the scattering phase shift for $l \geq 2$ is very small in the energy range under consideration, $\beta_l(k) \sim 0$ for $l \geq 2$ in (34). This also means that $v_{lm}(k) \sim 0$ for $l \geq 2$, because $G_{lm}(\mathbf{x}; k)$ contains $n_l(k|\mathbf{x}|)$ as discussed before. This expectation is supported by our numerical simulation as shown later.

We use the expansion form of $G(\mathbf{x}; k)$ in (29) to determine the allowed values of k , $D_{lm}(k)$, and $v_{00}(k)$ in (34). Comparing the coefficients of $j_0(k|\mathbf{x}|)$ and $n_0(k|\mathbf{x}|)$ in both lines of (34), we find

$$D_{00}(k) \cdot \alpha_0(k) = v_{00}(k) \cdot \frac{1}{\sqrt{4\pi}} g_{00}(k; 1), \quad (35)$$

$$D_{00}(k) \cdot \beta_0(k) = v_{00}(k) \cdot \frac{k}{4\pi}, \quad (36)$$

where $g_{00}(k; 1)$ is defined from (30). Finally we obtain the finite size formula by taking the ratio of (35) and (36):

$$\frac{\alpha_0(k)}{\beta_0(k)} = \frac{1}{\tan \delta_0(k)} = \frac{\sqrt{4\pi}}{k} g_{00}(k; 1). \quad (37)$$

The other components of (34) give only information for $D_{lm}(k)$. In the case of $\mathbf{P} = \mathbf{0}$, this formula turns out to be the formula presented by Lüscher in Ref. [7].

III. METHOD OF CALCULATIONS

A. Calculation of the wave function

In the present work we consider the ground state of the $I = 2$ S -wave two-pion system with the total momentum $\mathbf{P} = \mathbf{0}$ and $\mathbf{P} = (2\pi/L)\mathbf{e}_x$. When the interaction between two pions is turned off, the scattering momentum k defined by (6) takes

$$\begin{aligned} k &= 0 \quad \text{for } \mathbf{P} = \mathbf{0}, \\ k &= \pi/(\gamma L) \quad \text{for } \mathbf{P} = (2\pi/L)\mathbf{e}_x. \end{aligned} \quad (38)$$

These values of k are changed by the two-pion interaction.

In order to calculate the wave function we construct the correlation function:

$$F_{\pi\pi}(\mathbf{x}, \tau, \tau_s) = \langle 0 | \Omega(\mathbf{x}, \tau) \bar{\Omega}(\mathbf{P}, \tau_s) | 0 \rangle. \quad (39)$$

The operator $\Omega(\mathbf{x}, \tau)$ is defined by

$$\Omega(\mathbf{x}, \tau) = \sum_{\hat{R}} \frac{1}{L^3} \sum_{\mathbf{X}} e^{i\mathbf{P} \cdot \mathbf{X}} \pi^+(\mathbf{X} + \hat{R}[\mathbf{x}], \tau) \pi^+(\mathbf{X}, \tau), \quad (40)$$

where $\pi^+(\mathbf{x}, \tau)$ is an interpolating operator for π^+ at the position (\mathbf{x}, τ) . The operation \hat{R} represents an element of the cubic group (O_h) for $\mathbf{P} = \mathbf{0}$ and the tetragonal group (D_{4h}) for $\mathbf{P} = (2\pi/L)\mathbf{e}_x$. The summation over \hat{R} projects out the A_1^+ representation of these groups, which is equal to the S -wave state up to the angular momentum $l = 4$ for $\mathbf{P} = \mathbf{0}$ and $l = 2$ for $\mathbf{P} = (2\pi/L)\mathbf{e}_x$.

The operator $\bar{\Omega}(\mathbf{P}, \tau_s)$ in (39) is defined by

$$\bar{\Omega}(\mathbf{P}, \tau_s) = \frac{1}{N_R} \sum_{j=1}^{N_R} [\pi^+(\mathbf{P}, \tau_s; \xi_j) \pi^+(\mathbf{0}, \tau_s; \eta_j)]^\dagger, \quad (41)$$

where

$$\begin{aligned} \pi^+(\mathbf{P}, \tau_s; \xi_j) &= \frac{1}{L^3} \left[\sum_{\mathbf{x}} e^{i\mathbf{P} \cdot \mathbf{x}} \bar{d}(\mathbf{x}, \tau_s) \xi_j^*(\mathbf{x}) \right] \\ &\quad \times \gamma_5 \left[\sum_{\mathbf{y}} u(\mathbf{y}, \tau_s) \xi_j(\mathbf{y}) \right]. \end{aligned} \quad (42)$$

The operator $\pi^+(\mathbf{P}, \tau_s; \eta_j)$ is defined as $\pi^+(\mathbf{P}, \tau_s; \xi_j)$ by changing $\xi_j(\mathbf{x})$ to $\eta_j(\mathbf{x})$. The functions $\xi_j(\mathbf{x})$ and $\eta_j(\mathbf{x})$ are $U(1)$ noise whose property is

$$\lim_{N_R \rightarrow \infty} \frac{1}{N_R} \sum_{j=1}^{N_R} \xi_j^*(\mathbf{x}) \xi_j(\mathbf{y}) = \delta^3(\mathbf{x} - \mathbf{y}). \quad (43)$$

In the present work we set $N_R = 2$.

Neglecting the contributions from excited states, we can extract the wave function by

$$\phi^L(\mathbf{x}) = \frac{F_{\pi\pi}(\mathbf{x}, \tau_0, \tau_s)}{F_{\pi\pi}(\mathbf{x}_0, \tau_0, \tau_s)}, \quad (44)$$

in the large τ_0 region, introducing a reference position \mathbf{x}_0 .

We note that $\phi^L(\mathbf{x})$ at all positions \mathbf{x} are not independent. The number of independent positions is $(L+2)(L+4) \times (L+6)/48$ for $\mathbf{P} = \mathbf{0}$ and $(L+2)^2(L+4)/16$ for $\mathbf{P} = (2\pi/L)\mathbf{e}_x$, owing to the boundary condition (20) and the rotational symmetry on the lattice, $\phi^L(\mathbf{x}) = \phi^L(\hat{R}[\mathbf{x}])$.

In the present work we attempt to extract the energy of the two-pion system and the scattering phase shift from the wave function. For a comparison, we also evaluate them from the two-pion time correlator:

$$G_{\pi\pi}(\tau, \tau_s) = \frac{1}{L^3} \sum_{\mathbf{x}} F_{\pi\pi}(\mathbf{x}, \tau, \tau_s), \quad (45)$$

as done in the previous works of the scattering phase shift. We also calculate the time correlator for the pion and the ρ meson,

$$G_{\pi}(\tau, \tau_s) = \frac{1}{N_R} \sum_{j=1}^{N_R} \frac{1}{L^3} \sum_{\mathbf{x}} \langle 0 | \pi^+(\mathbf{x}, \tau) (\pi^+(\mathbf{0}, \tau_s; \xi_j))^\dagger | 0 \rangle, \quad (46)$$

$$\begin{aligned} G_{\rho}(\tau, \tau_s) &= \frac{1}{N_R} \sum_{j=1}^{N_R} \frac{1}{L^3} \sum_{\mathbf{x}} \sum_{a=1,2,3} \langle 0 | \rho_a(\mathbf{x}, \tau) \\ &\quad \times (\rho_a(\mathbf{0}, \tau_s; \xi_j))^\dagger | 0 \rangle, \end{aligned} \quad (47)$$

which are used to extract the masses. In (47) $\rho_a(\mathbf{x}, \tau)$ is an interpolating operator for the ρ meson with the polarization a at the position (\mathbf{x}, τ) and $\rho_a(\mathbf{0}, \tau_s; \xi_j)$ is given by substituting γ_a for γ_5 in (42).

B. Simulation parameters

Our simulation is carried out in the quenched approximation with the plaquette gauge action at $\beta = 5.9$. Gauge configurations are generated with the 5-hit pseudo-heat-bath algorithm and the over-relaxation algorithm mixed in the ratio of 1:4. This combination is called a sweep, and the physical quantities are measured every 200 sweeps after 2000 sweeps for the thermalization.

We use the improved Wilson action for quarks [14]. The clover coefficient C_{SW} is chosen for the mean-field improved value defined by

$$C_{\text{SW}} = \langle U_{\square} \rangle^{-3/4} = (1 - 2/\beta)^{-3/4} = 1.364, \quad (48)$$

where $\langle U_{\square} \rangle$ is the 1×1 Wilson loop which is evaluated in one-loop perturbation theory. The quark propagators are calculated with the Dirichlet boundary condition imposed in the time direction and the periodic boundary condition in the spatial one. The source operator $\bar{\Omega}(\mathbf{P}, \tau_s)$ in (39) is set at $\tau_s = 20$ to avoid effects from the time boundary.

The lattice cutoff is estimated as $1/a = 1.631(45)$ GeV [$a = 0.1208(33)$ fm] from m_{ρ} . The lattice size is $32^3 \times 120$, which corresponds to the spatial extent 3.87 fm in physical units. We choose three quark masses to give $m_{\pi} = 0.420, 0.488$, and 0.587 GeV. The numbers of configura-

TABLE I. Masses of the pion and the ρ meson calculated from the time correlator.

κ	N_{conf}	m_π (GeV)	m_ρ (GeV)	m_π/m_ρ
0.1413	400	0.419 64(66)	0.837(12)	0.5012(71)
0.1410	212	0.488 29(95)	0.8598(95)	0.5679(62)
0.1405	212	0.587 49(74)	0.9007(67)	0.6522(48)

tions are 400, 212, and 212 for each quark mass, which are generated independently. The masses of the pion and ρ meson calculated from the time correlator are listed in Table I.

IV. RESULTS

A. Wave functions

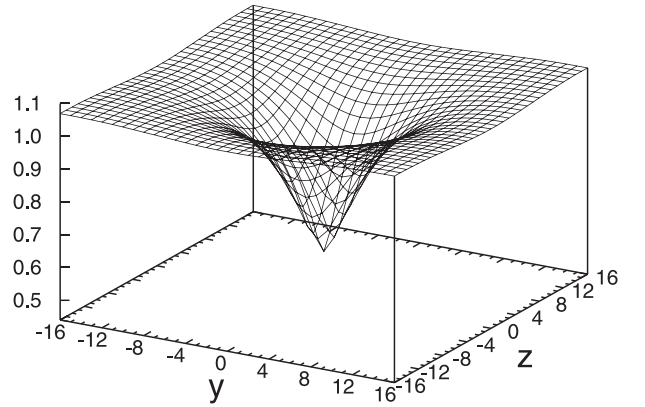
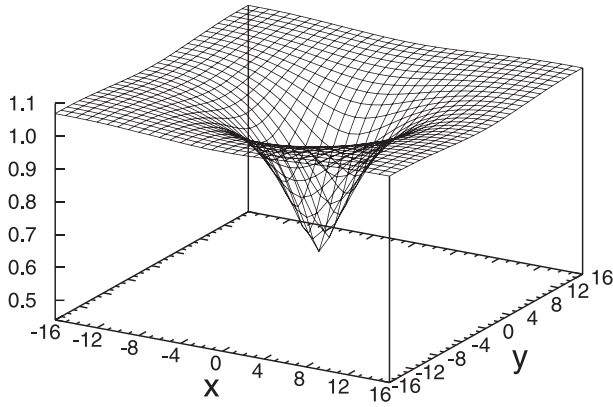
We obtain the wave function $\phi^L(\mathbf{x})$ from (44) and transform it to $\phi_{\text{CM}}^L(\mathbf{x}) = \phi^L(\hat{\gamma}^{-1}[\mathbf{x}])$. In the transformation we

calculate the Lorentz boost factor by $\gamma = \sqrt{E^2 - \mathbf{P}^2}$ with the energy E extracted from the two-pion time correlator. In Fig. 1 we show $\phi_{\text{CM}}^L(\mathbf{x})$ at $m_\pi = 0.420$ GeV for the total momentum $\mathbf{P} = \mathbf{0}$ and $\mathbf{P} = (2\pi/L)\mathbf{e}_x$. Here we set the reference position $\mathbf{x}_0 = (7, 5, 2)$ and $\tau_0 - \tau_s = 40$ in (44), confirming that the wave function does not depend on the choice of τ_0 for $\tau_0 - \tau_s > 32$. In the figure, the left and right panels for each momentum show the wave functions on the xy plane at $z = 0$ and on the yz plane at $x = 0$. While the boundary conditions for $\mathbf{P} = \mathbf{0}$ are the periodic conditions in all directions, those for $\mathbf{P} = (2\pi/L)\mathbf{e}_x$ are antiperiodic in the x direction and periodic in the other directions as known from (24). These features are clearly shown in the figure.

We consider the two-pion interaction from the ratio

$$V_{\text{CM}}^L(\mathbf{y}) = \frac{\nabla_y^2 \phi_{\text{CM}}^L(\mathbf{y})}{\phi_{\text{CM}}^L(\mathbf{y})} = \frac{1}{\phi^L(\mathbf{x})} (\nabla^2 - (\mathbf{P} \cdot \nabla)^2 / E^2) \phi^L(\mathbf{x}), \quad (49)$$

(a) $\mathbf{P} = \mathbf{0}$



(b) $\mathbf{P} = (2\pi/L)\mathbf{e}_x$

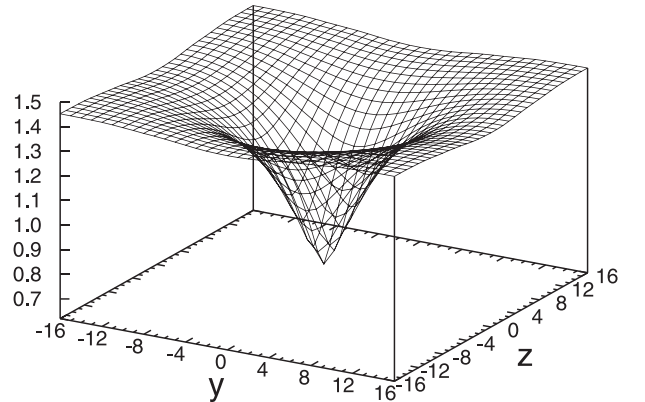
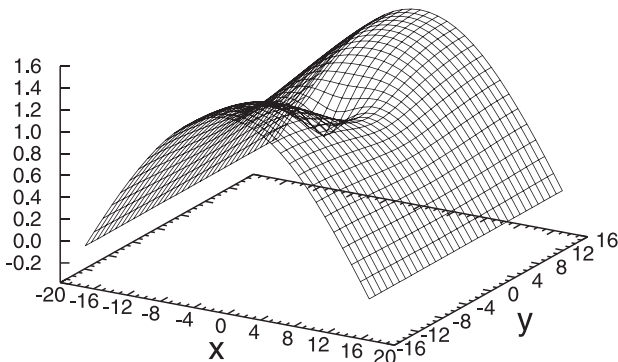


FIG. 1. Two-pion wave functions $\phi_{\text{CM}}^L(\mathbf{x})$ at $m_\pi = 0.420$ GeV for the total momentum $\mathbf{P} = \mathbf{0}$ and $\mathbf{P} = (2\pi/L)\mathbf{e}_x$. The left and right panels for each momentum show $\phi_{\text{CM}}^L(\mathbf{x})$ on the xy plane at $z = 0$ and on the yz plane at $x = 0$.

where $\mathbf{y} = \hat{\gamma}[\mathbf{x}]$ and $\nabla_{\mathbf{y}}^2$ is the Laplacian with respect to \mathbf{y} . Away from the two-pion interaction range, we expect that $V_{\text{CM}}^L(\mathbf{x})$ is independent of \mathbf{x} and equal to $-k^2$. In the calculation of the ratio, we rewrite (49) by

$$V_{\text{CM}}^L(\mathbf{y}) = \frac{1}{\phi^L(\mathbf{x})} \left(\frac{1}{\gamma^2} \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right) \phi^L(\mathbf{x}), \quad (50)$$

and adopt the naive numerical derivative

$$\frac{\partial^2}{\partial x_i^2} f(\mathbf{x}) = f(\mathbf{x} + \hat{i}) + f(\mathbf{x} - \hat{i}) - 2f(\mathbf{x}), \quad (51)$$

where the Lorentz boost factor γ is calculated with E extracted from the two-pion time correlator. In Fig. 2 $V_{\text{CM}}^L(\mathbf{x})$ is plotted for the same parameters as for Fig. 1. We find that the ratio is almost constant for $|\mathbf{x}| > 10$, both for $\mathbf{P} = \mathbf{0}$ and $\mathbf{P} = (2\pi/L)\mathbf{e}_x$. We also observe a strong repulsive interaction near the origin consistent with the negative scattering phase of the $I = 2$ two-pion system.

Here, we note a physical meaning of $V_{\text{CM}}^L(\mathbf{x})$ in (49). It seems that $V_{\text{CM}}^L(\mathbf{x})$ is equal to the corresponding ratio in Minkowski space defined by

$$V_{\text{CM}}(\mathbf{x}) = \frac{\nabla^2 \phi_{\text{CM}}(\mathbf{x})}{\phi_{\text{CM}}(\mathbf{x})}, \quad (52)$$

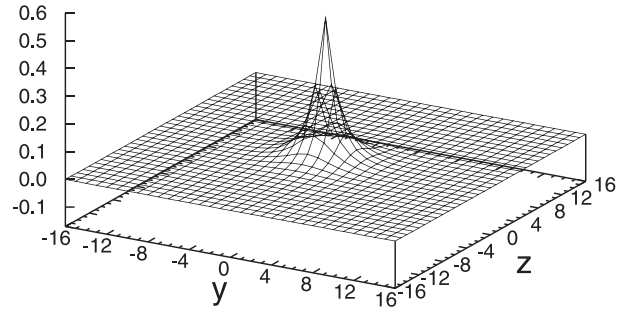
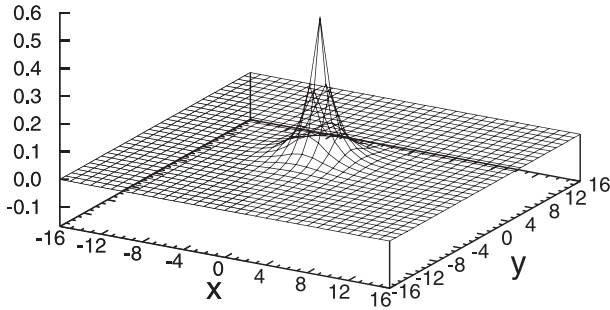
which approximately takes the potential of the two-pion interaction in the nonrelativistic limit. This, however, is not true for $\mathbf{P} \neq \mathbf{0}$ in the interaction region $|\mathbf{x}| < R$. Ignoring the difference of the degeneracy of the energy eigenstate in the infinite and the finite volumes, the wave function in Euclidian space, which is calculated in the present work, is related to that in Minkowski space by the analytic continuation as $\phi^L(\mathbf{x}) = \phi(\mathbf{x})$ at the relative time $x^0 = 0$. But a relation between $\phi_{\text{CM}}^L(\mathbf{x})$ and $\phi_{\text{CM}}(\mathbf{x})$ is

$$\phi_{\text{CM}}^L(\hat{\gamma}[\mathbf{x}]) = \phi^L(\mathbf{x}) = \phi(\mathbf{x}) = \phi_{\text{CM}}(-\gamma(\mathbf{v} \cdot \mathbf{x}), \hat{\gamma}[\mathbf{x}]), \quad (53)$$

which is not a relation at $x^0 = 0$. Thus, there is no simple relation between $V_{\text{CM}}^L(\mathbf{x})$ in (49) and $V_{\text{CM}}(\mathbf{x})$ in (52) for $\mathbf{P} \neq \mathbf{0}$. Only for the region $|\mathbf{x}| > R$, we give a simple relation: $V_{\text{CM}}^L(\mathbf{x}) = V_{\text{CM}}(\mathbf{x}) = -k^2$, due to the x^0 independence of the wave function, $\phi_{\text{CM}}(x^0, \mathbf{x}) = \phi_{\text{CM}}(0, \mathbf{x})$.

We now consider the two-pion interaction range R . In quantum field theory the wave function does not strictly

(a) $\mathbf{P} = \mathbf{0}$



(b) $\mathbf{P} = (2\pi/L)\mathbf{e}_x$

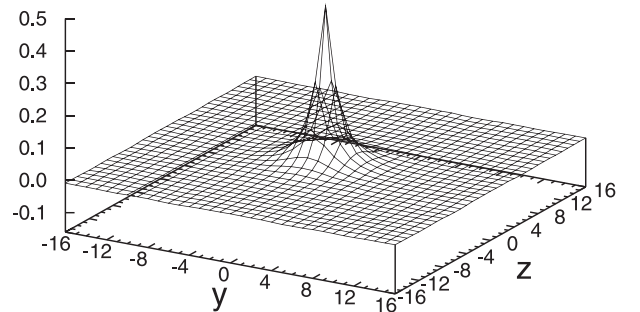
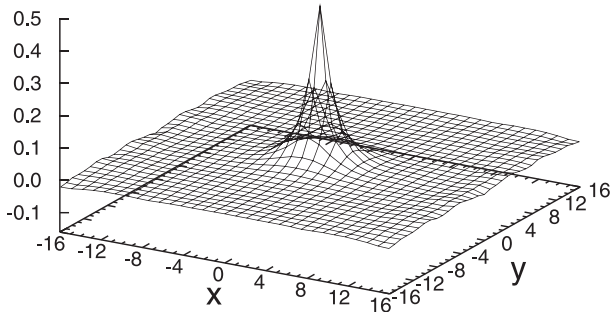


FIG. 2. $V_{\text{CM}}^L(\mathbf{x})$ at $m_\pi = 0.420$ GeV for the total momentum $\mathbf{P} = \mathbf{0}$ and $\mathbf{P} = (2\pi/L)\mathbf{e}_x$. The left and right panels for each momentum show $V_{\text{CM}}^L(\mathbf{x})$ on the xy plane at $z = 0$ and on the yz plane at $x = 0$.

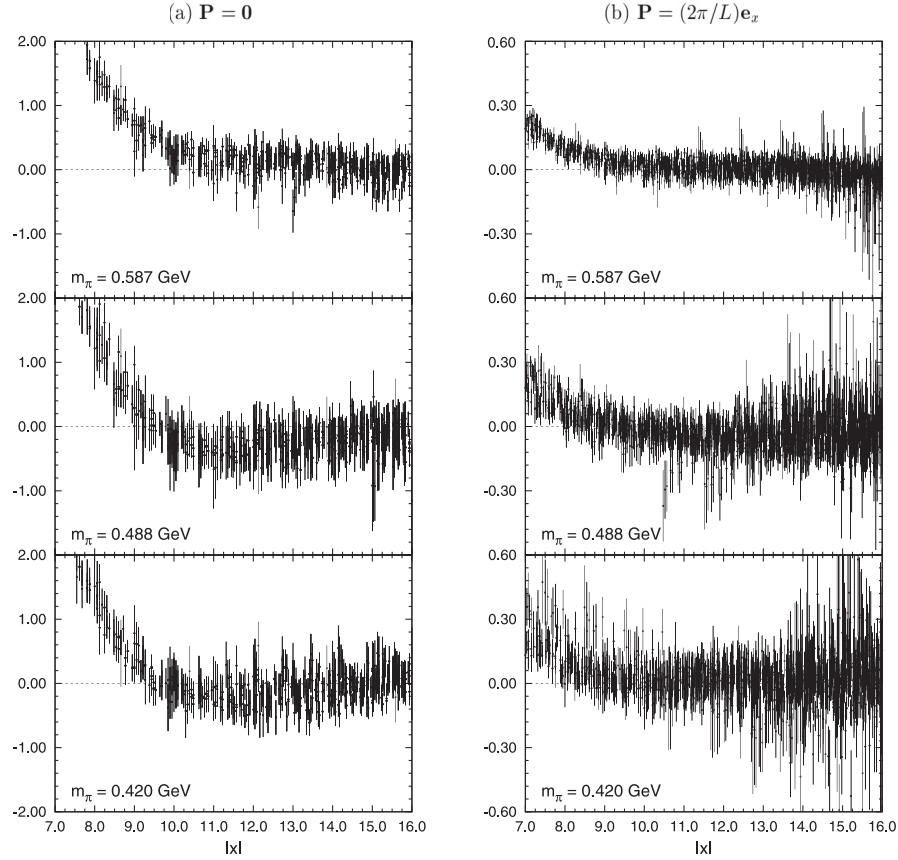


FIG. 3. $U_{\text{CM}}^L(\mathbf{x})$ as the function of $|\mathbf{x}|$ for the total momentum $\mathbf{P} = \mathbf{0}$ and $\mathbf{P} = (2\pi/L)\mathbf{e}_x$.

satisfy the Helmholtz equation (23), even for the large $|\mathbf{x}|$ region. Hence, with k obtained from the two-pion time correlator, $V_{\text{CM}}^L(\mathbf{x}) + k^2$ shows a small tail at large $|\mathbf{x}|$. We may take the wave function as satisfying the Helmholtz equation, if $V_{\text{CM}}^L(\mathbf{x}) + k^2$ is sufficiently small compared with k^2 . In the present work we take an operational definition of the range R as the scale, where

$$U_{\text{CM}}^L(\mathbf{x}) = \frac{V_{\text{CM}}^L(\mathbf{x}) + k^2}{k^2} = \frac{(\nabla^2 + k^2)\phi_{\text{CM}}^L(\mathbf{x})}{k^2\phi_{\text{CM}}^L(\mathbf{x})} \quad (54)$$

is small enough compared with the statistical error. With this definition we expect that the systematic error of the scattering phase shift from the interaction tail is smaller than the statistical error of the scattering phase shift.

We show $U_{\text{CM}}^L(\mathbf{x})$ as the function of $|\mathbf{x}|$ in Fig. 3. We find $R < L/2 (= 16)$ in all cases. This means that the necessary condition for the finite size formula is satisfied on the 32^3 lattice for our range of the quark mass $m_\pi = 0.420\text{--}0.587$ GeV and the momentum $k \sim 0 - \pi/(\gamma L) \times (\sim 0.16$ GeV) with the current statistics of the simulations.

B. Scattering phase shift from the wave function

We attempt to calculate the scattering phase shift by substituting the momentum k obtained from three methods

into the finite size formula (37). The first method is the conventional one, where we calculate the momentum k by (6) with the energy of the two-pion system E extracted from the two-pion time correlator. Our results for k and the scattering phase shift $\delta_0(k)$ are tabulated in Table II for $\mathbf{P} = \mathbf{0}$ and Table III for $\mathbf{P} = (2\pi/L)\mathbf{e}_x$ (labeled “From T ”).

In the second method, we extract k by fitting the wave function $\phi^L(\mathbf{x})$ to the Green function (26) with the form

$$\phi^L(\mathbf{x}) = C \cdot G(\hat{\gamma}[\mathbf{x}]; k), \quad (55)$$

taking k and an overall constant C as free parameters. This method was introduced by the CP-PACS Collaboration in Ref. [9] for the evaluation of the scattering length, where they found that the statistical error can be reduced with this method. The numerical evaluation of $G(\hat{\gamma}[\mathbf{x}]; k)$ and an explicit procedure of the fitting are discussed in Appendix A. We choose the fitting range $|\mathbf{x}| \geq x_m$ with x_m tabulated in Tables II and III. An example of the fitting is shown in Fig. 4 at $m_\pi = 0.420$ GeV, where the data points are shown with open circles and the values for the fits with cross symbols. We find that the fit works well both for $\mathbf{P} = \mathbf{0}$ and $\mathbf{P} = (2\pi/L)\mathbf{e}_x$. This means that the contribution of $G_{lm}(\mathbf{x}; k)$ with $l \geq 2$ is negligible as expected.

TABLE II. Results for the total momentum $\mathbf{P} = \mathbf{0}$ from the two-pion time correlator (“From T ”), fitting the wave function (“From ϕ ”), and fitting $V(\mathbf{x}; \gamma)$ (“From V ”).

κ m_π (GeV)		0.1413 0.419 64(66)	0.1410 0.488 29(95)	0.1405 0.587 49(74)
x_m k (GeV)		13.0	14.0	12.0
$\delta_0(k)$ (deg)	From T	0.0383(14)	0.0360(19)	0.0396(14)
	From ϕ	0.037 60(91)	0.0363(12)	0.038 10(92)
	From V	0.037 62(46)	0.037 50(57)	0.038 75(33)
a_0/m_π (GeV $^{-2}$)	From T	−1.71(18)	−1.44(22)	−1.88(18)
	From ϕ	−1.63(11)	−1.48(14)	−1.70(11)
	From V	−1.636(56)	−1.621(69)	−1.776(42)
$A(m_\pi, k)$	From T	−1.86(12)	−1.43(14)	−1.415(87)
	From ϕ	−1.808(79)	−1.460(88)	−1.322(58)
	From V	−1.809(40)	−1.546(42)	−1.363(21)
	From T	−0.330(22)	−0.343(34)	−0.489(30)
	From ϕ	−0.320(14)	−0.349(21)	−0.457(20)
	From V	−0.3198(70)	−0.370(10)	−0.4709(72)

Our results for k and $\delta_0(k)$ are tabulated in Tables II and III (labeled “From ϕ ”). These are consistent with those of the conventional method (“From T ”). We also find that the statistical errors are reduced. Thus the method with the wave function is also efficient for the evaluation of the scattering phase shift.

As discussed in Sec. IVA, the ratio $V_{\text{CM}}^L(\mathbf{x})$ in (49) is equal to $-k^2$ away from the interaction range. For simplicity, we write the ratio by

$$V(\mathbf{x}; \gamma) \equiv V_{\text{CM}}^L(\hat{\gamma}[\mathbf{x}]) = \frac{1}{\phi^L(\mathbf{x})} \left(\frac{1}{\gamma^2} \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right) \phi^L(\mathbf{x}), \quad (56)$$

with (50). We extract k by minimizing the chi-square:

$$\chi^2(k) = \sum_{|\mathbf{x}| \geq x_m} \left(\frac{V(\mathbf{x}; \gamma) + k^2}{\delta V(\mathbf{x}; \gamma)} \right)^2, \quad (57)$$

TABLE III. Results for the total momentum $\mathbf{P} = (2\pi/L)\mathbf{e}_x$ from the two-pion time correlator (“From T ”), fitting the wave function (“From ϕ ”), and fitting $V(\mathbf{x}; \gamma)$ (“From V ”).

κ m_π (GeV)		0.1413 0.419 64(66)	0.1410 0.488 29(95)	0.1405 0.587 49(74)
x_m k (GeV)		10.0	11.0	12.0
γ	From T	0.1610(14)	0.1594(21)	0.1634(12)
	From ϕ	0.160 15(96)	0.161 17(82)	0.163 69(54)
	From V	0.159 56(40)	0.161 97(38)	0.163 94(28)
$\delta_0(k)$ (deg)	From T	1.061 59(22)	1.047 49(23)	1.033 921(92)
	From ϕ	1.061 68(19)	1.047 39(17)	1.033 944(82)
	From V	1.061 73(17)	1.047 34(16)	1.033 937(82)
$A(m_\pi, k)$	From T	−8.4(12)	−5.5(17)	−7.20(98)
	From ϕ	−7.69(78)	−6.92(69)	−7.46(46)
	From V	−7.21(33)	−7.59(31)	−7.67(24)
	From T	−0.412(55)	−0.308(94)	−0.472(62)
	From ϕ	−0.379(37)	−0.387(37)	−0.488(29)
	From V	−0.356(15)	−0.423(17)	−0.501(15)

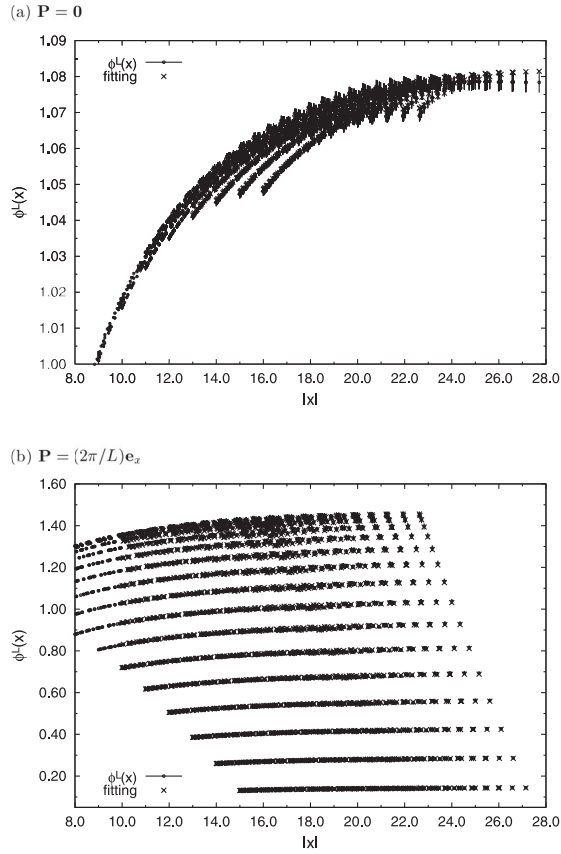


FIG. 4. Results of fitting the wave function $\phi^L(\mathbf{x})$ to the Green function at $m_\pi = 0.420$ GeV for the total momentum $\mathbf{P} = \mathbf{0}$ and $\mathbf{P} = (2\pi/L)\mathbf{e}_x$. Open circles refer to the data points and cross symbols to the results of the fitting.

taking k as a free parameter, where $\delta V(\mathbf{x}; \gamma)$ is the statistical error at fixed γ . This method is an extension of that introduced by the CP-PACS Collaboration in Ref. [9] for $\mathbf{P} = \mathbf{0}$ to the system with $\mathbf{P} \neq \mathbf{0}$. As known in (56), $V(\mathbf{x}; \gamma)$ depends on k through γ . This fact makes the analysis difficult. We use a similar procedure as for fitting the wave function (see Appendix B). We choose the same fitting range x_m for fitting the wave function. Our results for k and $\delta_0(k)$ are tabulated in Tables II and III (labeled “From V”). As shown in the tables, the results are consistent with those from the two-pion time correlator (“From T”) and fitting the wave function (“From ϕ ”). We also find that the statistical error is significantly reduced.

C. Scattering length and phase shift at physical quark mass

For $\mathbf{P} = \mathbf{0}$, the momentum k is very small as shown in Table II. Thus the scattering length a_0 can be calculated by

$$a_0 = \frac{\tan \delta_0(k)}{k}. \quad (58)$$

In Fig. 5 we plot the scattering length a_0/m_π obtained from

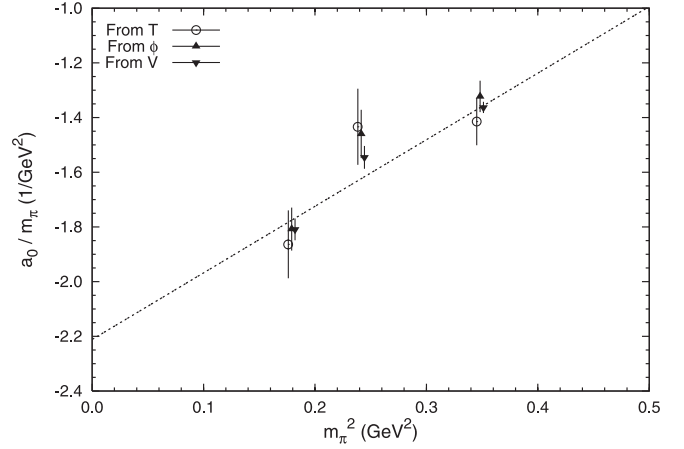


FIG. 5. Scattering length a_0/m_π obtained from the two-pion time correlator (“From T”), fitting the wave function (“From ϕ ”), and fitting $V(\mathbf{x}; \gamma)$ (“From V”). The result of chiral extrapolation for the data of “From V” is also plotted.

three methods discussed in the previous section. They are consistent, but the statistical errors are significantly reduced by using the two methods with the wave function (“From ϕ ” and “From V”). We carry out the chiral extrapolation with the fit form, $a_0/m_\pi = A + B \cdot m_\pi^2$, and obtain

$$a_0/m_\pi = -2.211(77) \text{ GeV}^{-2}, \quad (59)$$

in the chiral limit, for the data of fitting $V(\mathbf{x}, \gamma)$ (“From V”). The result of chiral extrapolation is also plotted in Fig. 5. We note that the prediction from chiral perturbation theory is $a_0/m_\pi = -2.265(51) \text{ GeV}^{-2}$ [15].

We obtain the scattering phase shift at the physical quark mass for the various momenta k from the scattering amplitude defined by

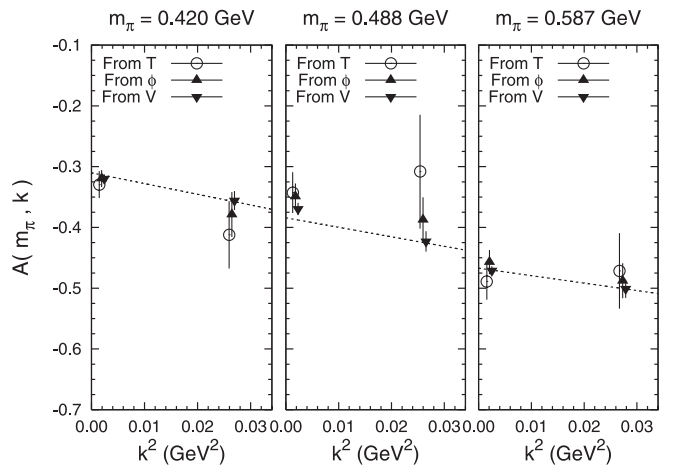


FIG. 6. Scattering amplitude $A(m_\pi, k)$ for three quark masses obtained from the two-pion time correlator (“From T”), fitting the wave function (“From ϕ ”), and fitting $V(\mathbf{x}; \gamma)$ (“From V”). The fit curves for the data of “From V” are also plotted.

TABLE IV. Results of the coefficients A_{ij} in (61).

	A_{10} (GeV^{-2})	A_{20} (GeV^{-4})	A_{01} (GeV^{-2})	A_{11} (GeV^{-4})
From T	-2.10(27)	2.02(92)	-7.7(56)	26(22)
From ϕ	-2.17(17)	2.52(59)	-3.2(34)	6(12)
From V	-2.187(80)	2.42(26)	-2.3(15)	3.2(56)

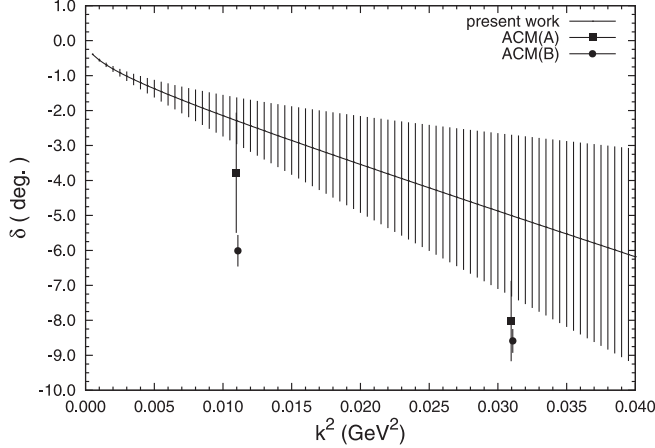


FIG. 7. Results of the scattering phase shift at the physical pion mass and the experiments in Ref. [16].

$$A(m_\pi, k) = \frac{\tan \delta_0(k)}{k} \sqrt{m_\pi^2 + k^2}, \quad (60)$$

which is normalized as $A(m_\pi, k) = a_0 m_\pi$ at $k = 0$. We show the results in Tables II and III, and plot them in Fig. 6. We fit these amplitudes with a fitting form:

$$A(m_\pi, k) = A_{10} \cdot m_\pi^2 + A_{20} \cdot m_\pi^4 + A_{01} \cdot k^2 + A_{11} \cdot m_\pi^2 k^2. \quad (61)$$

The results of the fitting are also plotted in Fig. 6 and summarized in Table IV. We find that $A_{10}(=a_0/m_\pi)$ is consistent with (59).

Finally, we estimate the scattering phase shift $\delta_0(k)$ at the physical quark mass by putting $m_\pi = 0.140$ GeV in (61). In Fig. 7 our results are plotted as a function of k^2 and compared with the experiments [16]. Our results are larger than the experiments. We consider that this disagreement arises from the effect of the finite lattice spacing. We must leave this issue for studies in the future.

V. CONCLUSION

We have calculated the two-pion wave function for the ground state of the $I = 2$ S -wave two-pion system both for $\mathbf{P} = \mathbf{0}$ and $\mathbf{P} = (2\pi/L)\mathbf{e}_x$. We have investigated the validity of the necessary condition for the finite size formula and found that it is satisfied on the 32^3 lattice for the quark mass range $m_\pi = 0.420$ – 0.587 GeV and the scattering momentum $k \leq 0.16$ GeV. We have also found that the scattering phase shift can be extracted from the wave

function with a smaller statistical error than from the two-pion time correlator, which has been used in the studies to date.

An implication of the present work is the feasibility to calculate the decay width of the ρ meson through studies of the $I = 1$ two-pion system. We can extract the energy eigenvalue from the wave function at a single time slice, so the method with the wave function is effective for investigating the scattering system. While the evaluation of the disconnected diagrams with a good precision has been a computational problem, our method could lend tactics that can be used to evaluate such complicated diagrams with a modest cost.

ACKNOWLEDGMENTS

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APPENDIX A: FITTING THE WAVE FUNCTION TO THE GREEN FUNCTION

We introduce

$$\bar{k}^2 = (\hat{\gamma}^{-1}[\mathbf{P}/2])^2, \quad (A1)$$

and expand the Green function around $k^2 = \bar{k}^2$ as

$$G(\hat{\gamma}[\mathbf{x}]; k) = \sum_{j=0}^{\infty} (k^2 - \bar{k}^2)^{j-1} \cdot F(\hat{\gamma}[\mathbf{x}]; j, \bar{k}). \quad (A2)$$

The coefficient $F(\mathbf{x}; j, \bar{k})$ is defined by

$$F(\mathbf{x}; 0, \bar{k}) = -\frac{1}{\gamma L^3} \sum_{\mathbf{q}^2 = \bar{k}^2} e^{i\mathbf{q} \cdot \mathbf{x}}, \quad (A3)$$

and

$$F(\mathbf{x}; j, \bar{k}) = \frac{1}{\gamma L^3} \sum_{\mathbf{q}^2 \neq \bar{k}^2} \frac{1}{(\mathbf{q}^2 - \bar{k}^2)^j} e^{i\mathbf{q} \cdot \mathbf{x}}, \quad (A4)$$

for $j \geq 1$, where $\mathbf{q} \in \Gamma_{\mathbf{P}}$ [defined by (27)]. We evaluate $F(\mathbf{x}; j, \bar{k})$ for $j \geq 1$ from

$$\begin{aligned} (\gamma L^3) \cdot F(\mathbf{x}; j, \bar{k}) &= -\frac{1}{j!} \sum_{\mathbf{q}^2 = \bar{k}^2} e^{i\mathbf{q} \cdot \mathbf{x}} + \sum_{r=1}^j \frac{1}{(j-r)!} \\ &\quad \times \sum_{\mathbf{q}^2 \neq \bar{k}^2} \frac{e^{-(\mathbf{q}^2 - \bar{k}^2)}}{(\mathbf{q}^2 - \bar{k}^2)^r} e^{i\mathbf{q} \cdot \mathbf{x}} \\ &\quad + \frac{2\pi^{3/2}\gamma}{(j-1)!} \left(\frac{2\pi}{L}\right)^{-3} \\ &\quad \times \int_0^1 d\eta \eta^{2j-4} e^{(\eta \bar{k})^2} \cdot f(\mathbf{x}; \eta), \end{aligned} \quad (A5)$$

where

$$f(\mathbf{x}; \eta) = \sum_{\mathbf{n} \in \mathbb{Z}^3} (-1)^{L/(2\pi)\mathbf{P} \cdot \mathbf{n}} \cdot e^{-((\mathbf{x} + \hat{\gamma}[\mathbf{n}]L)/(2\eta))^2}. \quad (\text{A6})$$

Equation (A5) is obtained by the same technique discussed in Ref. [9]. $F(\hat{\gamma}[\mathbf{x}]; j, \bar{k})$ in (A2) depends on k through γ . This fact makes the fitting of the wave function difficult. In the present work, we adopt the following procedure:

- (1) We calculate $\gamma_0 = E/\sqrt{E^2 - \mathbf{P}^2}$ with the energy E extracted from the two-pion time correlator and take it as the initial value of γ .
- (2) We fix \bar{k} and $F(\hat{\gamma}[\mathbf{x}]; j, \bar{k})$ in (A2) with a given γ and fit the wave function, taking k as the free parameter.
- (3) We update γ by $\gamma = \sqrt{1 + \mathbf{P}^2/[4(m_\pi^2 + k^2)]}$ with k obtained in the procedure (2).
- (4) We iterate the procedures (2) and (3) until the value of k becomes stable.

It is expected that k rapidly converges in this procedure, because the dependence of γ on k is very small. We confirm that k is stable within the single precision after five iterations for all our simulation parameters. We carry out the above procedure for each jackknife bin and estimate the statistical error of k by the jackknife method.

APPENDIX B: FITTING $V(\mathbf{x}; \gamma)$

The fit of $V(\mathbf{x}; \gamma)$ is performed by a similar procedure as for fitting the wave function discussed in Appendix A:

- (1) We calculate $\gamma_0 = E/\sqrt{E^2 - \mathbf{P}^2}$ with the energy E extracted from the two-pion time correlator and take it as the initial value of γ .
- (2) We fix $V(\mathbf{x}; \gamma)$ with a given γ and search for k that gives the least number of $\chi^2(k)$ in (57).
- (3) We update γ by $\gamma = \sqrt{1 + \mathbf{P}^2/[4(m_\pi^2 + k^2)]}$ with k obtained in the procedure (2).
- (4) We iterate the procedures (2) and (3) until the value of k becomes stable.

It is expected that k in this procedure rapidly converges, because the dependence of γ on k is very small. We confirm that k is stable within the single precision after five iterations, as for fitting the wave function. We carry out the above procedure for each jackknife bin and estimate the statistical error of k by the jackknife method.

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