

Using lattice chiral effective theory to study $\pi\pi$ scattering

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We use lattice field theory to study the finite-volume energy spectrum of the $\pi\pi$ system in $SU(2)$ chiral effective field theory (ChEFT) at leading order in the chiral expansion. This finite-volume spectrum can be directly related to the (infinite-volume) $\pi\pi$ scattering phase shifts by Lüscher's formula. We compare our results to the finite-volume spectrum obtained from lattice QCD by the RBC-UKQCD Collaboration. Our calculation and the lattice QCD calculation are both performed with the physical pion mass and the same lattice volume (as measured in physical units). However, we find significant differences between the two calculations in the isospin $I = 0$ channel. In particular, there is a nearly stable σ resonance in our lattice ChEFT calculation, which is absent in the lattice QCD calculation. This likely indicates that ChEFT does not converge well with a naive lattice regularization.

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I. INTRODUCTION

Chiral effective field theory (ChEFT) was introduced by Weinberg in 1979 as a low-energy effective theory for QCD [1]. While ChEFT is often employed in conjunction with perturbation theory, there are good reasons for studying ChEFT nonperturbatively. For example, we can use chiral symmetry through the partially conserved axial current relations to obtain many useful results. [2] We can get even more nonperturbative information using lattice Monte Carlo. There are many reasons to be interested in doing this.

- (1) First, lattice ChEFT could aid lattice QCD calculations. Perturbative ChEFT is used extensively to perform various extrapolations on lattice QCD results (for example, extrapolations to infinite volume or to physical pion mass; see Ref. [3] for a review). These extrapolations could also be performed using lattice ChEFT, which would allow direct comparison of the observables in the effective theory with QCD, even at the level of correlation functions.
- (2) Second, by matching lattice ChEFT with lattice QCD, we could determine the ChEFT low-energy constants in the lattice regularization, and, with some additional calculation, in perturbative renormalization schemes such as $\overline{\text{MS}}$.

- (3) Third, lattice ChEFT (involving only pion degrees of freedom) could provide useful insights for more complicated lattice simulations of nuclear ChEFT. In nuclear physics, lattice ChEFT has long been used to study the spectrum, structure, and scattering of atomic nuclei [4–28]. It should be noted that most of these calculations use instantaneous pions. (Reference [4] is one of the exceptions.) See Ref. [24] for a more recent proposal to introduce dynamical pions using the quantum Monte Carlo method.
- (4) Fourth, a more direct mapping between chiral effective theory and QCD could add insight into chiral effective theory. For example, it could contribute to understanding the nature of the σ resonance (see Ref. [29] for a review discussing recent progress on this question).

The leading-order [$\mathcal{O}(p^2/\Lambda^2)$] $SU(2)$ chiral effective theory is equivalent to the $O(4)$ nonlinear sigma model, which in turn is the strongly interacting limit of the $O(4)$ linear sigma model [30]. The $O(4)$ (non)linear sigma model has been frequently studied on the lattice with Monte Carlo calculations. It is often used as a “toy” model to test various algorithmic and theoretical techniques, such as Lüscher's formula [31,32] and the maximum entropy method [33]. It has also been employed to study the Higgs sector of the standard model [34,35]. In this work, we view it as the chiral effective theory at leading order in the effective field theory expansion. We choose its parameters to give the pions their physical mass and decay constant. To our knowledge, this is the first time that lattice ChEFT has been used to study $\pi\pi$ scattering and compared with first-principles lattice QCD calculations of the same process. The finite-volume $\pi\pi$ energy spectrum is directly related to

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(infinite-volume) scattering phase shifts by Lüscher's formula [36], and the lattice QCD calculations agree well with experimental measurements [37].

We find that our lattice simulation of the sigma model does *not* reproduce the low-energy spectrum of QCD. This is likely because the lattice regularization introduces power divergences which enhance higher-order terms in the normal power-counting for chiral effective theory (see Sec. IV). This problem might be solved by using a more sophisticated lattice regularization (for example, by introducing smearing).

In Sec. II, we introduce the linear sigma model and discuss its connection to $SU(2)$ chiral effective theory. In Sec. III, we present the results of our calculations. We show that we are indeed simulating in the nonlinear sigma model regime. We then show how various observables depend on our model parameters, demonstrating that the physical point is unique, and that it lies near a phase transition. Finally, we compare the energy spectrum of our theory to lattice QCD calculations, noting significant disagreement in the isospin $I = 0$ channel. Because the physical point is unique, the low-energy constants cannot be adjusted to fix this discrepancy. In Sec. IV, we discuss the likely reason for this discrepancy and a possible resolution.

II. CHIRAL EFFECTIVE THEORY AND THE LINEAR SIGMA MODEL

A. The linear sigma model

In principle, it is possible to construct an effective scalar field theory in terms of the pion fields which exactly reproduces the dynamics of QCD. In Appendix A, we show this is true by explicitly constructing such an effective action. The exponential of the resulting action is real, but it is not guaranteed to always be positive. While this construction is explicit and proves that a sufficiently sophisticated effective action can describe QCD to arbitrary high accuracy, it is not yet practical to obtain this sophisticated action in a form that is suitable for effective theory calculations. In the following numerical work, we instead approximate the effective action with the leading-order terms in the conventional chiral expansion, with the understanding that more accurate results can be obtained if more higher-order terms are included in the effective action.

In the standard treatment, “one writes down the most general possible Lagrangian, including all terms consistent with assumed symmetry principles” [1]. The resulting Lagrangian is in general nonlocal. However, we can expand this nonlocal function in terms of derivatives of the scalar fields. For a process involving energy scale E , most terms contribute corrections which are suppressed by powers of E/Λ , where Λ represents the cutoff scale of the effective theory. If we collect the pion degrees of freedom into an $SU(2)$ field U , the leading-order $SU(2)$ chiral effective Lagrangian (after Wick rotation to Euclidean time) is

$$\mathcal{L}_{\text{SU}(2)} = \frac{F_0^2}{4} \text{Tr} \left[\sum_{\mu} (\partial_{\mu} U) \partial_{\mu} U^{\dagger} \right] + \frac{F_0^2 B_0 M}{2} \text{Tr}(U^{\dagger} + U), \quad (1)$$

where F_0 , B_0 , and M are scalar parameters. This is also called the $SU(2)$ nonlinear sigma model. Because $SU(2)$ is diffeomorphic to the 3-sphere, we can replace our dynamical variable U with a set of four fields ϕ_i constrained so that the sum of their squares is constant. A convenient diffeomorphism is given by

$$U = \frac{\phi_0}{F_0} + i \sum_{j=1,2,3} \frac{\phi_j}{F_0} \tau_j, \quad (2)$$

where τ_j are the Pauli sigma matrices, and $\sum_{j=0}^3 \phi_j^2 = F_0^2$. In terms of these new dynamical variables,

$$\mathcal{L} = \frac{1}{2} \sum_{\mu} \sum_{j=0}^3 (\partial_{\mu} \phi_j)^2 + \alpha \phi_0, \quad \text{with} \quad \alpha \equiv 2F_0 B_0 M \quad \text{and} \quad \text{constraint} \quad \sum_{j=0}^3 \phi_j^2 = F_0^2. \quad (3)$$

There is a closely related model in which the four fields are no longer exactly constrained to lie on the surface of a 3-sphere: the $O(4)$ linear sigma model,

$$\mathcal{L} = \frac{1}{2} \sum_{\mu} \sum_{i=0}^3 (\partial_{\mu} \phi_i)^2 + \frac{m^2}{2} \sum_{i=0}^3 \phi_i^2 + \frac{\lambda}{4!} \left(\sum_{i=0}^3 \phi_i^2 \right)^2 + \alpha \phi_0. \quad (4)$$

The $O(4)$ symmetry of this model is broken both spontaneously (for $m^2 < 0$) and explicitly by the $\alpha \phi_0(x)$ term. In the symmetry-broken phase, the fields are dynamically constrained to lie close to the surface of a 3-sphere, with the strength of the constraint controlled by the parameter λ . Unlike the nonlinear sigma model, the linear sigma model is renormalizable. However, as Lüscher's work [38] proved, the theory still does not have a nontrivial continuum limit. Of course, this does not affect our use of the linear sigma model as an effective theory, which has an explicit cutoff. In the limit as $\lambda \rightarrow \infty$ (with $\frac{m^2}{\lambda}$ held fixed), we return to the nonlinear sigma model. In this paper, we study the linear sigma model numerically with very large λ ($\lambda = 10^4$). To discretize the theory for the lattice, we use the Lagrangian density

$$\mathcal{L}(x) = \frac{1}{2} \sum_{\mu} \sum_{i=0}^3 (\phi_i(x+\mu) - \phi_i(x))^2 + \frac{m^2}{2} \sum_{i=0}^3 \phi_i(x)^2 + \frac{\lambda}{4!} \left(\sum_{i=0}^3 \phi_i(x)^2 \right)^2 + \alpha \phi_0(x). \quad (5)$$

B. Particle identifications

In our theory, when there is no explicit symmetry breaking ($\alpha = 0$), the $O(4)$ symmetry can be spontaneously broken. The symmetry can break along any direction, described by some linear combination of the four fields. We may simply redefine the fields so that the direction of symmetry breaking lies along ϕ_0 . Then ϕ_0 will have a nonzero vacuum expectation value, while the other three fields will still have a vacuum expectation value of 0, respecting a reduced $O(3)$ symmetry. These three fields correspond to massless Goldstone bosons. When we add in explicit symmetry breaking ($\alpha \neq 0$), the explicit symmetry-breaking term $\alpha\phi_0$ ensures that the $O(4)$ symmetry will be broken in such a way that ϕ_0 takes on the nonzero vacuum expectation value without the need for redefinition. This means that the fields ϕ_1 , ϕ_2 , and ϕ_3 correspond to the pseudo-Goldstone bosons. As long as α is small, their masses will be small. Therefore, these fields are identified as pions. The remaining degree of freedom is the sigma field $\sigma = \phi_0 - \langle\phi_0\rangle$, where $\langle\phi_0\rangle$ is the vacuum expectation value of ϕ_0 . The sigma degree of freedom disappears in the $\lambda \rightarrow \infty$ limit, although the theory will still contain an associated resonance.

C. Pion decay constant

The pion decay constant F_π may be defined in the continuum by the matrix element of the axial current between the vacuum and a single-pion state:

$$\langle 0 | A_\mu^i(x, t) | \pi(p) \rangle = F_\pi p^\mu e^{-p_0 t - i\mathbf{p} \cdot \mathbf{x}}. \quad (6)$$

Here, we define $A_{\mu,i} \equiv \bar{\psi} \gamma_\mu \gamma_5 \frac{\tau_i}{2} \psi$, where τ_i is the i th Pauli sigma matrix acting on flavor space. With this definition, the physical pion decay constant is approximately 92 MeV. This definition implies

$$\langle 0 | A_0^i(x, t) | \pi(\mathbf{p} = 0) \rangle = F_\pi m_\pi e^{-m_\pi t} \quad (7)$$

and

$$\langle 0 | \partial_\mu A_\mu^i(x) | \pi^i(\mathbf{p} = 0) \rangle = m_\pi^2 F_\pi e^{-m_\pi t}. \quad (8)$$

We can calculate F_π directly by fitting correlation functions of the axial current with pion fields. We can also use Noether's theorem to replace $\partial_\mu A_\mu^i(x)$ so that we can fit correlation functions involving only pion fields.

On the lattice, we modify the definition of F_π to account for periodic boundary conditions. We define the axial current as the conserved current associated with rotations involving ϕ_0 . Specifically, we choose the discretization

$$A_i^\mu \equiv \phi_0(x - \mu) \phi_i(x) - \phi_0(x) \phi_i(x - \mu). \quad (9)$$

With this definition, the appropriate discrete version of Noether's theorem is

$$\sum_\mu [A_i^\mu(x + \mu) - A_i^\mu(x)] = -\alpha \phi_i. \quad (10)$$

D. Isospin channels

In QCD, we may define operators that couple to various pion states. For example, we could define

$$\pi^\pm = \frac{i}{\sqrt{2}} \bar{\psi} \gamma^5 \left(\pm \frac{\tau^1}{\sqrt{2}} + i \frac{\tau^2}{\sqrt{2}} \right) \psi \quad \text{and} \quad \pi^0 = i \bar{\psi} \gamma^5 \frac{\tau^3}{\sqrt{2}} \psi. \quad (11)$$

In our effective theory, we can build corresponding operators

$$\pi^\pm = \frac{1}{\sqrt{2}} (\pm \phi_1 + i \phi_2) \quad \text{and} \quad \pi^0 = \phi_3. \quad (12)$$

From these operators, we can create two-pion operators with specific angular momentum and isospin. In this paper, we consider only operators that are angularly symmetric. For our isospin-0 operator, we choose

$$\begin{aligned} \mathcal{O}^{I=0}(p) &= \frac{1}{\sqrt{3}N_p} \sum_{|\mathbf{p}|=p} [\pi^+(\mathbf{p})\pi^-(\mathbf{-p}) - \pi^0(\mathbf{p})\pi^0(\mathbf{-p}) \\ &\quad + \pi^-(\mathbf{p})\pi^+(\mathbf{-p})] \end{aligned} \quad (13)$$

$$\begin{aligned} &= -\frac{1}{\sqrt{3}N_p} \sum_{|\mathbf{p}|=p} [\phi_1(\mathbf{p})\phi_1(\mathbf{-p}) + \phi_2(\mathbf{p})\phi_2(\mathbf{-p}) \\ &\quad + \phi_3(\mathbf{p})\phi_3(\mathbf{-p})]. \end{aligned} \quad (14)$$

The sum is over all momenta $\mathbf{p}$ on the lattice with norm p , and N_p is the number of distinct lattice momenta that satisfy this condition. The pions that this operator couples to will have a relative momentum of $2p$. For our isospin-2 operator, we choose

$$\begin{aligned} \mathcal{O}^{I=2}(p) &= \frac{1}{\sqrt{6}N_p} \sum_{|\mathbf{p}|=p} [\pi^+(\mathbf{p})\pi^-(\mathbf{-p}) + 2\pi^0(\mathbf{p})\pi^0(\mathbf{-p}) \\ &\quad + \pi^-(\mathbf{p})\pi^+(\mathbf{-p})] \end{aligned} \quad (15)$$

$$\begin{aligned} &= \frac{1}{\sqrt{6}N_p} \sum_{|\mathbf{p}|=p} [-\phi_1(\mathbf{p})\phi_1(\mathbf{-p}) - \phi_2(\mathbf{p})\phi_2(\mathbf{-p}) \\ &\quad + 2\phi_3(\mathbf{p})\phi_3(\mathbf{-p})]. \end{aligned} \quad (16)$$

III. RESULTS

All the code to generate these results is available as part of the Qlattice library [39]. A sketch of the overall workflow is as follows:

- (1) We use the hybrid Monte Carlo algorithm [40] to simulate the linear sigma model for various choices of the parameters m^2 , λ , and α on a finite lattice with periodic boundary conditions. This results in an ensemble of random configurations of the scalar fields $\phi_i(x)$, with each random field configuration sampled according to the probability density $e^{-S_E[\phi]}$.
- (2) We measure correlation functions of the scalar fields by approximating the path integral as a sum over our ensemble of field configurations:

$$\begin{aligned} \langle T\{\mathcal{O}[\phi_i]\} \rangle &= \frac{1}{Z} \int D\phi_i \mathcal{O}[\phi_i] e^{-S[\phi]} \\ &\approx \frac{1}{N_{\text{conf}}} \sum_{\text{conf}} \mathcal{O}[\phi_i^{\text{conf}}], \end{aligned} \quad (17)$$

where N_{conf} is the number of configurations in the ensemble and we sum over the operator $\mathcal{O}$ evaluated on each configuration.

- (3) We use the identifications of Secs. II B and II C to connect these correlation functions to QCD matrix elements. See Appendix B for a discussion of how each observable was determined from the scalar field correlation functions.
- (4) Using the same method used in Ref. [37] for lattice QCD, we solve the generalized eigenvalue problem (GEVP) to get the energy spectrum of our theory in the isospin-0 and isospin-2 channels.

A. Lambda dependence

We want to study the linear sigma model in the large- λ limit, where it behaves like the nonlinear sigma model. In Fig. 1, we plot the probability distribution of $\sum_{i=0}^3 \phi_i^2(x)$ (by translational invariance, the point in space does not matter) for three different values of λ . In the $\lambda \rightarrow \infty$ limit, this distribution would be a delta function. These plots show that we have indeed chosen λ to be sufficiently large that the fields are being dynamically constrained to lie close to the surface of a 3-sphere. We can therefore expect our theory to behave similarly to the nonlinear sigma model.

In Fig. 2, we show how varying λ affects various observables. $\frac{m^2}{\lambda}$ and α are fixed so that we are near the physical ratio of m_π to F_π at $\lambda \approx 10^4$ (we define the physical ratio to be $m_\pi/F_\pi = 135/92 \approx 1.47$). Based on Figure 2, we note that further increasing past $\lambda = 10^4$ does not seem to have a significant effect on our results. Therefore, in subsequent sections, we will do all our calculations using $\lambda = 10^4$. As λ becomes larger, simulations become more

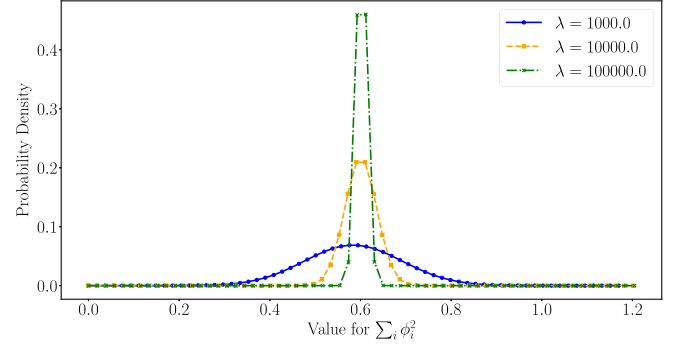


FIG. 1. The probability distribution of $\sum_i \phi_i^2(x)$ for various λ on a $16^3 \times 32$ lattice with $m^2/\lambda = -0.102$ and $\alpha = 0.007$. These parameters are chosen so that we are near the physical point (defined as the point where $m_\pi/F_\pi = 135/92 \approx 1.47$) when $\lambda = 10^4$ (see Table I for more information on the ensemble with $\lambda = 10^4$). As can be seen from the figure, at large λ , the values of the fields are dynamically constrained to lie near the surface of a 3-sphere.

difficult, since the dynamically-imposed constraint on $\sum_i \phi_i^2(x)$ becomes more stringent.

B. The phase transition and sigma stability

We fix $\lambda = 10^4$. The two remaining parameters, m^2 and α , can be tuned to find the physical point. For our purposes, we define the physical point as the point where $m_\pi = 135$ MeV and $F_\pi = 92$ MeV. With this definition, we tune m^2 and α until the ratio m_π/F_π is close to its physical value of $135/92 \approx 1.47$. We then use the requirement $F_\pi = 92$ MeV to define the lattice spacing.

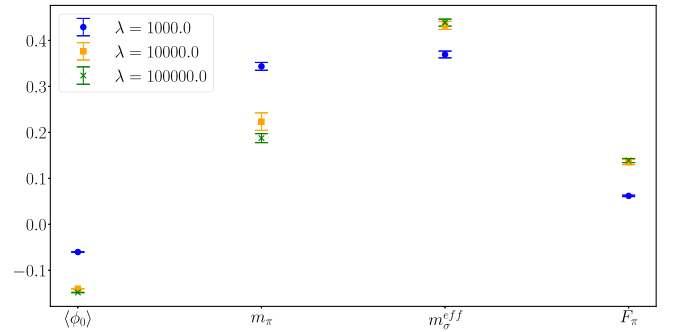


FIG. 2. The λ -dependence of the vacuum expectation value of ϕ_0 , the pion mass m_π , the effective sigma mass m_σ^{eff} , and the pion decay constant F_π on a $16^3 \times 32$ lattice. All values are in lattice units. We set $m^2/\lambda = -0.102$ and $\alpha = 0.007$ so that we are near the physical point (defined as the point where $m_\pi/F_\pi = 135/92 \approx 1.47$) when $\lambda = 10^4$ (see Table I for more information on the ensemble with $\lambda = 10^4$). The effective sigma mass is based on the values of the σ - σ correlation function at time separations 0 and 1. As can be seen from the figure, increasing λ from 10^4 to 10^5 does not significantly affect m_σ^{eff} .

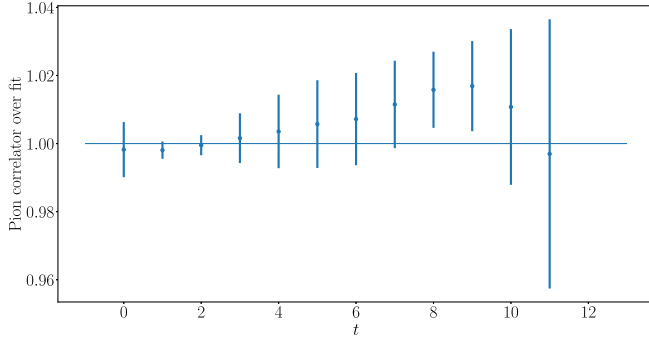


FIG. 3. The correlation function $\langle (\sum_{i=1}^3 \sum_{\mathbf{x}} \phi_i(\mathbf{x}, t)) \times (\sum_{j=1}^3 \sum_{\mathbf{x}'} \phi_j(\mathbf{x}', 0)) \rangle$ divided by a single-state fit $f(t) = \frac{A}{\cosh((N_t/2-1)m_\pi)} \cosh((\frac{N_t}{2}-t)m_\pi)$, where A and m_π are the fit parameters, and N_t is the time extent of the lattice (see Appendix B). This correlation function was calculated on the $16^3 \times 128$ ensemble with $m^2/\lambda = -0.102$, $\alpha = 0.007$, and $\lambda = 10^4$ (see Table II for more details on this ensemble). The fit gives $A = 7238(102)$ and $m_\pi = 0.2201(77)$. As can be seen from the figure, the single-state fit works well even at small t .

When we calculate the pion mass, we fit correlation functions $\langle \mathcal{O}_\pi(t) \mathcal{O}_\pi(0) \rangle$ of the pion-interpolating operator $\mathcal{O}_\pi(t) \equiv \sum_{i=1}^3 \sum_{\mathbf{x}} \phi_i(\mathbf{x}, t)$ (see Appendix B). As can be seen from Fig. 3, a simple single-state fit works even for small t . This stands in contrast to lattice QCD, where excited states of the pion can couple to the pion-interpolating operators (see, for example, Ref. [41]). In our effective theory, the pions have no internal degrees of freedom. Since G-parity forbids $\mathcal{O}_\pi$ from coupling to two-pion states, the first excited state contributions would have to come from three-pion states, which are numerically very small.

As shown in Fig. 4, when the parameter m^2/λ is sufficiently small in magnitude (in our convention, m^2 is negative), the theory is in the symmetric phase, where $m_\pi = m_\sigma$ and $F_\pi = 0$. The theory enters the symmetry-broken phase around $m^2/\lambda \approx -0.1$, which is consistent with the results of previous lattice studies using the non-linear sigma model [34]. In the symmetry-broken phase, F_π is no longer zero. Based on the tree-level formula $F_\pi = \sqrt{-m^2/\lambda}$, we expect F_π to continue increasing as we increase $|m^2/\lambda|$. This expectation is qualitatively supported by our results in Fig. 4, although we see significant departures from the tree-level formula. On the other hand, m_π starts with a large value in the symmetric phase ($m_\pi = m_\sigma$). As we transition into the symmetry-broken phase by increasing $|m^2/\lambda|$, m_π decreases significantly, because it is the mass of a pseudo-Goldstone boson. Based on Fig. 4, m_π continues to decrease after the phase transition as we increase $|m^2/\lambda|$.

Since we have F_π increasing and m_π decreasing as a function of $|m^2/\lambda|$, there is only one physical point for each given value of α . Note that we cannot tune F_π and m_π independently of each other, since a change in either m^2/λ

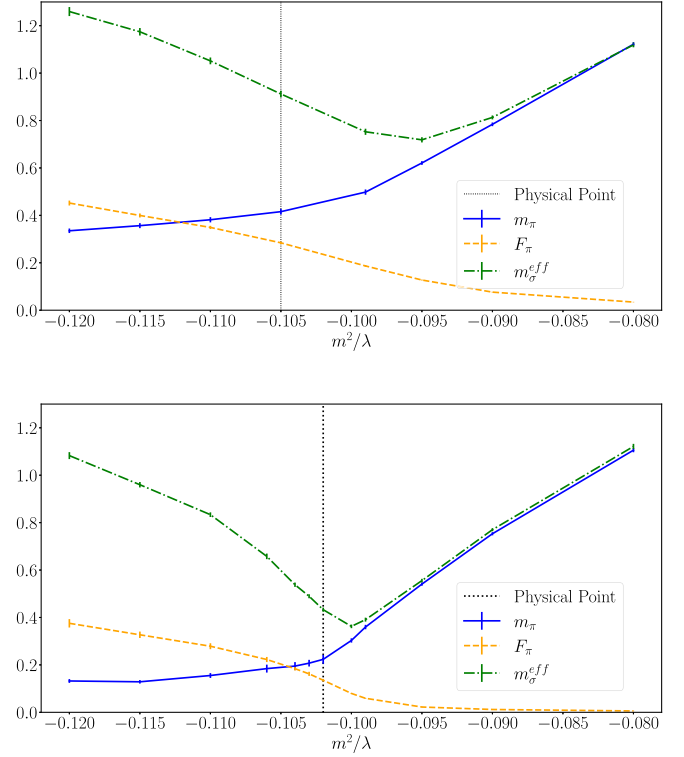


FIG. 4. The pion mass m_π , the effective sigma mass m_σ^{eff} , and the pion decay constant F_π (all measured in lattice units) versus $\frac{m^2}{\lambda}$ on a $8^3 \times 16$ lattice (top) and a $16^3 \times 32$ lattice (bottom). The value of m^2/λ closest to the physical point (defined as the point where $m_\pi/F_\pi = 135/92 \approx 1.47$) is marked by a vertical line. λ is held fixed at 10^4 , which we have determined is sufficiently large that further increases will not have a strong effect on the results. We set $\alpha = 0.05$ for the $8^3 \times 16$ lattice and $\alpha = 0.007$ for the $16^3 \times 32$ lattice. The resulting lattice spacing and spatial extent near the physical points are given in Table I. The effective sigma mass is based on the values of the σ - σ correlation function at time separations 0 and 1. Increasing the magnitude of $\frac{m^2}{\lambda}$ causes F_π to increase while m_π decreases, making it clear that the physical point is unique.

or α affects both F_π and m_π , as shown in Fig. 4. In fact, in all our calculations, the physical point occurs close to the symmetric phase at roughly the same value of m^2/λ , as shown in Table I. The parameter α serves mainly to control the lattice spacing.

As can be seen from Fig. 4, at the physical point, the effective sigma mass is about twice the pion mass, indicating that the sigma particle is on the border between being stable and unstable. Furthermore, if we were to simulate larger-than-physical pion masses, holding the pion decay constant at the same value, then the sigma would become a stable particle.

C. Energy spectrum from GEVP

We can determine the finite-volume spectrum of our theory by solving a generalized eigenvalue problem

TABLE I. Parameters and observables for the ensembles from Figure 4 closest to the physical point (defined as the point where $m_\pi/F_\pi = 135/92 \approx 1.47$). The inverse lattice spacing a^{-1} is defined by requiring $F_\pi = 92$ MeV. L is the length of the lattice volume along each of the three spacial dimensions. As usual, $\lambda = 10^4$ in all these ensembles.

Size	m^2/λ	α	a^{-1} (GeV)	L (fm)	$m_\pi a$	$F_\pi a$	m_π/F_π
$8^3 \times 16$	-0.105	0.05	0.3237(61)	4.876(92)	0.416(12)	0.2841(54)	1.462(43)
$12^3 \times 24$	-0.103	0.015	0.474(12)	4.99(13)	0.272(11)	0.1940(50)	1.427(59)
$16^3 \times 32$	-0.102	0.007	0.679(28)	4.64(19)	0.223(19)	0.1353(56)	1.65(14)

(GEVP). We create a list of operators $\{\mathcal{O}_i\}$ with a particular set of quantum numbers (e.g., $I = 0$) and define corresponding operator states

$$|\mathcal{O}_i\rangle \equiv \frac{1}{N_i}(\mathcal{O}_i - \langle\mathcal{O}_i\rangle)|0\rangle, \quad (18)$$

where $\langle\mathcal{O}_i\rangle$ is the vacuum expectation value of $\mathcal{O}_i$, and N_i is chosen to normalize the state to 1. We then approximate the energy eigenstates by writing them as linear combinations of the operator states

$$|E_{I,n}\rangle = \sum_i c_{I,n}^i |\mathcal{O}_i\rangle. \quad (19)$$

We can determine the energy eigenvalues $e^{-E_{I,n}}$ and the coefficients $c_{I,n}^i$ by requiring that

$$\langle E_{I,n} | e^{-H(t+1)} | \mathcal{O}_j \rangle = e^{-E_{I,n}} \langle E_{I,n} | e^{-Ht} | \mathcal{O}_j \rangle \quad (20)$$

for all j .

For the $I = 0$ GEVP, we have chosen the set of operators

$$\mathcal{O}_\pi^{I=0}(\mathbf{p} = 0) = -\sum_{\mathbf{x}} [\phi_1(\mathbf{x})^2 + \phi_2(\mathbf{x})^2 + \phi_3(\mathbf{x})^2], \quad (21)$$

$$\mathcal{O}_\sigma = -\sum_{\mathbf{x}} \phi_0(\mathbf{x})^2, \quad (22)$$

$$\begin{aligned} \mathcal{O}_\pi^{I=0}\left(\mathbf{p} = \frac{2\pi}{L}\right) = & -\sum_{|\mathbf{p}|=2\pi/L} [\phi_1(\mathbf{p})\phi_1(-\mathbf{p}) + \phi_2(\mathbf{p})\phi_2(-\mathbf{p}) \\ & + \phi_3(\mathbf{p})\phi_3(-\mathbf{p})], \end{aligned} \quad (23)$$

where $\phi_i(\mathbf{p}) \equiv \sum_{\mathbf{x}} \phi_i(\mathbf{x}) e^{-i\mathbf{p}\cdot\mathbf{x}}$. For the $I = 2$ GEVP, we have chosen

$$\mathcal{O}_\pi^{I=2}(\mathbf{p} = 0) = \sum_{\mathbf{x}} [-\phi_1(\mathbf{x})^2 - \phi_2(\mathbf{x})^2 + 2\phi_3(\mathbf{x})^2], \quad (24)$$

$$\begin{aligned} \mathcal{O}_\pi^{I=2}\left(\mathbf{p} = \frac{2\pi}{L}\right) = & \sum_{|\mathbf{p}|=2\pi/L} [-\phi_1(\mathbf{p})\phi_1(-\mathbf{p}) - \phi_2(\mathbf{p})\phi_2(-\mathbf{p}) \\ & + 2\phi_3(\mathbf{p})\phi_3(-\mathbf{p})]. \end{aligned} \quad (25)$$

See Sec. II D for the explanation behind the assignment of isospin to these operators.

In Fig. 5, we show the energy spectrum of the theory in the isospin-0 and isospin-2 channels and compare it to the spectrum in Ref. [37] from lattice QCD. To get our results, we solved the GEVP from Eq. (20) for various choices of time separations t . We chose the lattice spacing so that the volume of the lattice (as measured in physical units) is about the same as in Ref. [37] (see Table VI for a comparison).

In Fig. 6, we show the volume dependence of the $I = 0$ ground-state energy and first excited-state energy, respectively. Without changing any of the parameters in the Lagrangian, we simulate at different spatial volumes, starting with our $8^3 \times 128$ lattice with $L = 4.750(26)$ fm. As the volume increases, the ground-state energy increases, and, as shown in Table III, the ground state becomes more associated with the $\pi\pi$ operator at zero relative momentum. On the other hand, as the volume increases, the first excited-state energy decreases, and, as shown in Table IV, the first excited state becomes more associated with the σ operator. The second excited state is mostly associated with the $\pi\pi$ operator at one unit of relative momentum, as shown in Table V.

D. Comparison with other methods

The spectrum for the isospin-2 channel is similar to the spectrum of full QCD, as recently calculated on the lattice by the RBC/UKQCD Collaboration [37]. In the isospin-0 channel, however, the spectrum looks very different. The results from our theory and lattice QCD are compared side-by-side in Table VI. In our theory, there are two states at around twice the pion mass. These states are formed mainly from linear combinations of the $I = 0$ two-pion operator $\mathcal{O}^{I=0}(p = 0)$ and the sigma operator. Our second excited state is associated mainly with the operator $\mathcal{O}(p = \frac{2\pi}{L})$. It occurs at around the same energy as the first excited state in lattice QCD. We interpret this spectrum as indicating the sigma resonance happens at a much lower energy in our theory than in QCD. Lattice QCD shows that the sigma becomes stable when the pion mass is around 300 MeV [42–44].

We also note that our results show a different behavior for the sigma resonance than unitarized chiral perturbation theory. Unitarized two-loop chiral perturbation theory

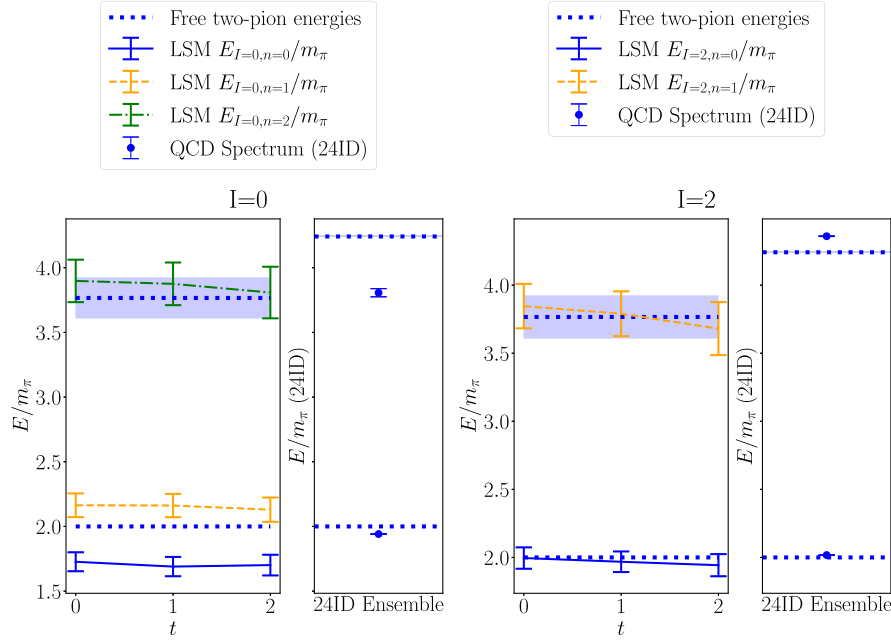


FIG. 5. The isospin-0 (left) and isospin-2 (right) energy spectrum. The dotted lines show the energies of a system of two free (noninteracting) pions with either zero momentum or one unit of momentum. The orange, green, and solid blue lines give the energy eigenvalues for the linear sigma model as determined by solving the GEVP from Eq. (20) using time separations t and $t+1$ on a $16^3 \times 128$ lattice with $m^2/\lambda = -0.102$ and $\alpha = 0.007$ (as usual, $\lambda = 10^4$). These parameters are chosen so that we are near the physical point with $a^{-1} = 0.6363(99)$ GeV and $L = 4.961(77)$ fm (see Table II for more details). The data points with error bars and marked with circles show the QCD spectrum, as calculated on the 24ID ensemble in Ref. [37] on a $24^3 \times 64$ lattice with similar physical volume [$L = 4.63(1)$ fm] and $a^{-1} = 1.023(2)$ GeV. The error bars on the QCD spectrum do not include the error in determining m_π .

predicts a sigma pole location of around 3 times the pion mass at the physical point, with the sigma becoming more stable as the pion mass increases until it finally becomes stable when the pion mass is around twice its physical value [46]. In contrast, in our results, the sigma is already nearly stable at the physical point.

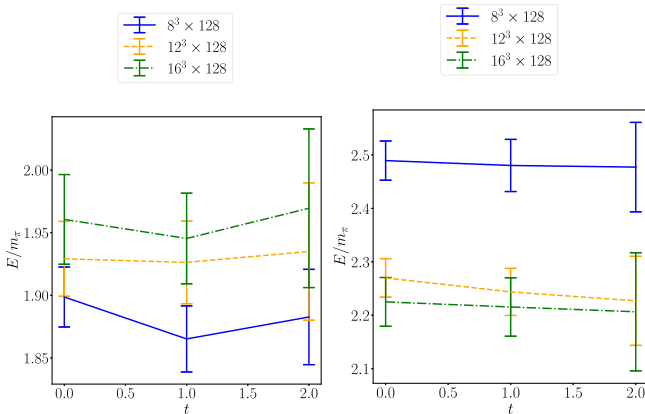


FIG. 6. The isospin-0 ground state (left) and first excited state (right), as determined by solving the generalized eigenvalue problem using time separations t and $t+1$, for three different lattice volumes. The simulations are done with $m^2/\lambda = -0.105$ and $\alpha = 0.05$ (as usual, $\lambda = 10^4$), so that we are near the physical point (see Table II for more details on these ensembles).

Finally, our results also differ from previously published results on the unitarized linear sigma model. Achasov and Shestakov [47] calculated the pole mass and width of the sigma resonance by unitarizing the two-flavor linear sigma model, using parameters that correspond to $\lambda \approx 300$ in our conventions. They set their other parameters so that the tree-level values of F_π and m_π are physical. They then employ a simple unitarization model and show that it gives results for the $\pi\pi$ phase shift that are consistent with experiment at low energies. They calculate the sigma pole mass to be around 417 MeV, in contrast to our results. It should be noted that both m_π and F_π differ significantly from their tree-level values at $\lambda = 300$, based on our calculations. The choice of parameters in Achasov and Shestakov's paper lies deep within the symmetric phase.

IV. POWER COUNTING WITH A LATTICE REGULARIZATION

In chiral perturbation theory (ChPT) with dimensional regularization, all corrections from loops and higher-order terms in the Lagrangian are suppressed by powers of $E/(4\pi F_0)$, where E is the relevant energy scale and F_0 is the tree-level pion decay constant. This allows ChPT to remain predictive for energies below $4\pi F_\pi \approx 1$ GeV. Now, if we instead study ChPT with lattice regularization, we will have power divergences in addition to the logarithmic

TABLE II. Parameters and observables for the ensembles used for the GEVP analysis. The inverse lattice spacing a^{-1} is defined by requiring $F_\pi = 92$ MeV. L is the length of the lattice volume along each of the three spacial dimensions. The physical value of m_π/F_π is about $135/92 \approx 1.47$. As usual, $\lambda = 10^4$ in all these ensembles.

Size	m^2/λ	α	a^{-1} (GeV)	L (fm)	$m_\pi a$	$F_\pi a$	m_π/F_π
$16^3 \times 128$	-0.102	0.007	0.6363(99)	4.961(77)	0.2201(77)	0.1445(23)	1.522(59)
$8^3 \times 128$	-0.105	0.05	0.3323(18)	4.750(26)	0.4196(43)	0.2769(15)	1.516(19)
$12^3 \times 128$	-0.105	0.05	0.3271(19)	7.238(41)	0.4151(35)	0.2812(16)	1.476(15)
$16^3 \times 128$	-0.105	0.05	0.3272(26)	9.649(77)	0.4118(74)	0.2812(22)	1.464(30)

TABLE III. The coefficients $c_{I,n}^i$ from Eq. (19) for the $I = 0$ ground state, as determined by the GEVP analysis using time separations 0 and 1. The simulations are done with $m^2/\lambda = -0.105$ and $\alpha = 0.05$ (as usual, $\lambda = 10^4$), so that we are near the physical point (see Table II for more details on these ensembles).

Lattice volume	$c_{I=0,n=0}^{\pi,p=0}$	$c_{I=0,n=0}^\sigma$	$c_{I=0,n=0}^{\pi,p=2\pi/L}$
$8^3 \times 128$	0.8110(92)	-0.585(13)	0.0219(53)
$12^3 \times 128$	0.9137(81)	-0.407(18)	0.0185(80)
$16^3 \times 128$	0.9466(84)	-0.321(24)	0.046(16)

TABLE IV. The coefficients $c_{I,n}^i$ from Eq. (19) for the $I = 0$ first excited state, as determined by the GEVP analysis using time separations 0 and 1. The simulations are done with $m^2/\lambda = -0.105$ and $\alpha = 0.05$ (as usual, $\lambda = 10^4$), so that we are near the physical point (see Table II for more details on these ensembles).

Lattice volume	$c_{I=0,n=1}^{\pi,p=0}$	$c_{I=0,n=1}^\sigma$	$c_{I=0,n=1}^{\pi,p=2\pi/L}$
$8^3 \times 128$	0.6269(89)	0.7740(72)	-0.0902(81)
$12^3 \times 128$	0.465(16)	0.8708(89)	-0.163(13)
$16^3 \times 128$	0.374(24)	0.899(10)	-0.232(18)

divergences that are present in dimensional regularization. As a result, we are no longer guaranteed that divergences will be suppressed by powers of $E/(4\pi F_0)$. For example, as calculated in Ref. [48], with lattice-regularized ChPT, there is a quadratic divergence from the one-loop correction to the pion mass squared:

TABLE V. The coefficients $c_{I,n}^i$ from Eq. (19) for the $I = 0$ second excited state, as determined by the GEVP analysis using time separations 0 and 1. The simulations are done with $m^2/\lambda = -0.105$ and $\alpha = 0.05$ (as usual, $\lambda = 10^4$), so that we are near the physical point (see Table II for more details on these ensembles).

Lattice volume	$c_{I=0,n=2}^{\pi,p=0}$	$c_{I=0,n=2}^\sigma$	$c_{I=0,n=2}^{\pi,p=2\pi/L}$
$8^3 \times 128$	0.1129(72)	0.2341(76)	0.9657(24)
$12^3 \times 128$	0.0923(85)	0.265(12)	0.9600(36)
$16^3 \times 128$	0.057(16)	0.308(17)	0.9499(57)

$$\frac{M^2 - M_0^2}{M_0^2} \approx \frac{0.2}{(F_0 a)^2} + \dots, \quad (26)$$

where M_0 is the tree-level pion mass. We see that the suppression of this divergence requires $(F_0 a)^2 \gg 0.2$. To avoid large discretization effects, we must have $a \ll \frac{1}{M_0}$. Therefore, we must have $\frac{F_0}{M_0} \gg F_0 a \gg \sqrt{0.2} \approx 0.45$. Since the physical value of $\frac{F_\pi}{M_\pi}$ is about $92/135 \approx 0.7$, we have good reason to be worried about the validity of power-counting arguments in lattice ChPT.

From our simulation results, we get nonperturbative confirmation that we are not justified in ignoring higher-order terms in the effective theory expansion. Our leading-order terms are not capable of reproducing the low-energy

TABLE VI. The spectrum of the SU(2) linear sigma model versus QCD. $E_{I,n}$ is the energy of the n th excited state in the isospin- I channel. a is the lattice spacing, and L is the length of the lattice volume along each of the three spatial dimensions. The linear sigma model results are based on a GEVP analysis using time separations 0 and 1 on a $16^3 \times 128$ lattice with $m^2/\lambda = -0.102$ and $\alpha = 0.007$ (as usual, $\lambda = 10^4$). These parameters are chosen so that we are near the physical point (defined as the point where $m_\pi/F_\pi = 135/92 \approx 1.47$). Noninteracting pion energy $2E_{\pi,p=2\pi/L}$ is shown for comparison.

	Linear sigma model	Lattice QCD [37,45]
$E_{I=0,n=0}/m_\pi$	1.727(73)	1.9413(29) ^a
$E_{I=0,n=1}/m_\pi$	2.164(92)	3.806(32) ^a
$E_{I=0,n=2}/m_\pi$	3.898(164)	4.984(86) ^a
$E_{I=2,n=0}/m_\pi$	1.995(78)	2.0174(24) ^a
$E_{I=2,n=1}/m_\pi$	3.846(163)	4.3595(22) ^a
$2E_{\pi,p=(2\pi/L)}/m_\pi$	3.767(156)	4.242(4) ^a
$m_\pi L$	3.52(12)	3.3466(43)
L/fm	4.961(77)	4.63(1)
a^{-1}/GeV	0.6363(99)	1.023(2)
m_π/MeV	140(5)	142.6(3)
F_π/MeV	92	94.44(8) ^b

^aThese errors on the QCD spectrum do not include the error in determining m_π .

^bThis error does not include the error in determining the lattice spacing.

physics of QCD. We could, of course, try to add more terms to the Lagrangian. However, even if we could get the effective theory expansion to converge on the correct physics with more terms, we would at best be relying on delicate cancellations between the lower-order and higher-order terms.

Since the origin of this problem is the lattice regularization, a potential solution would be to change the regularization so that power divergences are more strongly suppressed. For example, we could smear the pion fields over adjacent lattice sites, making the lattice cutoff less harsh.

V. CONCLUSION

We simulated the $O(4)$ linear sigma model on the lattice. These simulations were done at large values of the coupling constant, so that our theory behaves similarly to the nonlinear sigma model. We demonstrated that our coupling constant was sufficiently large by noting that the fields were dynamically confined to lie close to the surface of a 3-sphere, and that further increases in the coupling constant had little effect on our observables. We found that the physical point is near the phase transition between the symmetric and symmetry-broken phases.

We calculated the spectrum of our theory in the isospin-0 and isospin-2 channels. In the isospin-2 channel, we get similar results to those from lattice QCD. The first two states are two pions at rest and two pions with one unit of relative momentum, with energies similar to what we would get for noninteracting pions. However, we found that our results for the isospin-0 channel are very different from the same channel in QCD. In our calculations, the first excited state in the isospin-0 channel appears at a much lower energy than the first excited state in lattice QCD calculations. Our results also differ from results obtained for the linear sigma model by unitarization [47].

The discrepancy with lattice QCD likely indicates that the chiral effective expansion does not converge well with our lattice regularization. However, since we have proved that an accurate lattice chiral effective action exists in Appendix A, we think this discrepancy might be alleviated in future works using smearing. If smearing does indeed solve the discrepancy with QCD, lattice ChEFT could provide useful information for lattice QCD extrapolations at the level of correlation functions with the same finite volume treatment and in Euclidean time.

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for this work based on Qlattice [39]. The computational work for this project was conducted using resources provided by the Storrs High-Performance Computing (HPC) cluster. We extend our gratitude to the UConn Storrs HPC and its team for their resources and support, which aided in achieving these results.

DATA AVAILABILITY

All the code used to generate the results of this article is openly available [39].

APPENDIX A: EXACT EFFECTIVE THEORY FOR QCD

In this appendix, we demonstrate that it is possible to construct a lattice effective theory in terms of pions which exactly reproduces the dynamics of lattice QCD. Specifically, we construct a lattice field theory with four scalar fields whose correlation functions are exactly the same as the lattice QCD correlation functions of the corresponding quark bilinears. This is an explicit construction of the effective theory action in terms of meson fields (baryons can also be included), a very different strategy compared to Ref. [49]. For two-flavor QCD, we can define

$$\begin{aligned} Q_0(x) &= Z_\phi \bar{\psi}(x) \psi(x) \quad \text{and} \\ Q_i(x) &= Z_\phi \bar{\psi}(x) \tau_i \gamma^5 \psi(x) \quad \text{for } i = 1, 2, 3, \end{aligned} \quad (\text{A1})$$

where Z_ϕ is an arbitrary normalization coefficient to match the quark bilinear operator with the desired scalar field. The action of this effective theory can be explicitly constructed as

$$\begin{aligned} e^{-S_{\text{eff}}[\{\phi_i\}]} &= \int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp(-S_{\text{QCD}}[U, \bar{\psi}, \psi] \\ &\quad - \frac{1}{2} \sum_x \sum_{i=0}^3 M_C^2 (\phi_i(x) - Q_i(x))^2). \end{aligned} \quad (\text{A2})$$

Note that the above integral may not always be positive, and so the resulting action $S_{\text{eff}}[\phi_i]$ is not guaranteed to be real. Nevertheless, if we calculate correlation functions $\mathcal{O}[\{\phi_i\}]$ with this action, we obtain

$$\langle \mathcal{O}[\{\phi_i\}] \rangle = \frac{1}{Z} \int \mathcal{D}\phi e^{-S_{\text{eff}}[\{\phi_i\}]} \mathcal{O}[\{\phi_i\}] \quad (\text{A3})$$

$$\begin{aligned} &= \frac{1}{Z} \int \mathcal{D}\phi \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp(-S_{\text{QCD}}[U, \bar{\psi}, \psi] \\ &\quad - \frac{1}{2} \sum_x \sum_{i=0}^3 M_C^2 (\phi_i(x) - Q_i(x))^2) \mathcal{O}[\{\phi_i\}] \end{aligned} \quad (\text{A4})$$

$$= \frac{1}{Z} \int \mathcal{D}\phi' \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left(-S_{\text{QCD}}[U, \bar{\psi}, \psi] - \frac{1}{2} \sum_x \sum_{i=0}^4 M_C^2 \phi_i^2(x) \right) \mathcal{O}[\{Q_i + \phi'_i\}] \quad (\text{A5})$$

$$= \langle \mathcal{O}[\{Q_i + \phi'_i\}] \rangle_{\text{QCD}, \phi'}, \quad (\text{A6})$$

where

$$Z = \int \mathcal{D}\phi e^{-S_{\text{eff}}[\{\phi_i\}]} \quad (\text{A7})$$

$$= \int \mathcal{D}\phi' \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left(-S_{\text{QCD}}[U, \bar{\psi}, \psi] - \frac{1}{2} \sum_x \sum_{i=0}^4 M_C^2 \phi_i^2(x) \right). \quad (\text{A8})$$

Thus, we obtain a relationship between correlation functions in the effective scalar theory and correlation functions in the theory of QCD plus a set of non-propagating fields with distribution $e^{-M_C^2 \phi_i^2/2}$:

$$\langle \mathcal{O}[\{\phi_i\}] \rangle = \langle \mathcal{O}[\{Q_i + \phi'_i\}] \rangle_{\text{QCD}, \phi'}. \quad (\text{A9})$$

The only effect these nonpropagating fields will have on QCD correlation functions is to introduce some additional “contact” terms. For example,

$$\langle \phi_i(x) \phi_j(y) \rangle = \langle Q_i(x) Q_j(y) \rangle_{\text{QCD}} + \langle \phi'_i(x) \phi'_j(y) \rangle_{\phi'}, \quad (\text{A10})$$

where

$$\langle \phi'_i(x) \phi'_j(y) \rangle_{\phi'} = \frac{1}{M_C^2} \delta_{i,j} \delta^{(4)}(x - y). \quad (\text{A11})$$

In the limit of large M_C , even these additional contact terms vanish, and we have

$$\langle \mathcal{O}[\{\phi_i\}] \rangle = \langle \mathcal{O}[\{Q_i\}] \rangle_{\text{QCD}} \quad (\text{when } M_C \rightarrow \infty). \quad (\text{A12})$$

Therefore, the effective theory described by S_{eff} exactly reproduces the underlying QCD dynamics without any approximation. Also, it is straightforward to include additional fields (or exclude some of the existing fields) in the construction.

1. Effective action in the chiral limit

While this explicit construction does not immediately enable us to perform perturbative calculations or numerical simulations, we can prove a very simple relation between the effective action S_{eff} and its form in the chiral limit $S_{\text{eff}}^{m=0}$. We start with the relation of the QCD action:

$$S_{\text{QCD}}[U, \bar{\psi}, \psi] = S_{\text{QCD}}^{m=0}[U, \bar{\psi}, \psi] + \sum_x m \bar{\psi}(x) \psi(x) \quad (\text{A13})$$

$$= S_{\text{QCD}}^{m=0}[U, \bar{\psi}, \psi] + \sum_x \frac{m}{Z_\phi} Q_0(x), \quad (\text{A14})$$

where $S_{\text{QCD}}^{m=0}$ is the QCD action in the chiral limit and m is the mass parameter for the up and down quarks. Note that the $Q_0(x)$ is defined in Eq. (A1). The chiral limit effective action $S_{\text{eff}}^{m=0}$ is constructed with the same approach as S_{eff} in Eq. (A2):

$$e^{-S_{\text{eff}}^{m=0}[\{\phi_i\}]} = \int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left(-S_{\text{QCD}}^{m=0}[U, \bar{\psi}, \psi] - \frac{1}{2} \sum_x \sum_{i=0}^4 M_C^2 (\phi_i(x) - Q_i(x))^2 \right). \quad (\text{A15})$$

Based on Eqs. (A2), (A14), and (A15), we can express the effective action S_{eff} in terms of $S_{\text{eff}}^{m=0}$:

$$e^{-S_{\text{eff}}[\{\phi_i\}]} = \int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left(-S_{\text{QCD}}[U, \bar{\psi}, \psi] - \sum_x \sum_{i=0}^4 \frac{1}{2} M_C^2 (\phi_i(x) - Q_i(x))^2 \right) \quad (\text{A16})$$

$$= \int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left(-S_{\text{QCD}}^{m=0}[U, \bar{\psi}, \psi] - \sum_x \left(\sum_{i=0}^4 \frac{1}{2} M_C^2 (\phi_i(x) - Q_i(x))^2 + \frac{m}{Z_\phi} Q_0(x) \right) \right) \quad (\text{A17})$$

$$= \int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left(-S_{\text{QCD}}^{m=0}[U, \bar{\psi}, \psi] - \sum_x \left(\sum_{i=0}^4 \frac{1}{2} M_C^2 \left(\phi_i(x) - \frac{m}{Z_\phi M_C^2} \delta_{i,0} - Q_i(x) \right)^2 + \frac{m}{Z_\phi} \phi_0(x) - \frac{m^2}{2Z_\phi^2 M_C^2} \right) \right) \quad (\text{A18})$$

$$= \exp \left(-S_{\text{eff}}^{m=0} \left[\left\{ \phi_i - \frac{m}{Z_\phi M_C^2} \delta_{i,0} \right\} \right] - \sum_x \frac{m}{Z_\phi} \phi_0(x) + \sum_x \frac{m^2}{2Z_\phi^2 M_C^2} \right). \quad (\text{A19})$$

Therefore, the general effective action can be expressed in terms of the chiral limit effective action plus a simple linear term:

$$S_{\text{eff}}[\{\phi_i\}] = S_{\text{eff}}^{m=0} \left[\left\{ \phi_i - \frac{m}{Z_\phi M_C^2} \delta_{i,0} \right\} \right] + \sum_x \frac{m}{Z_\phi} \phi_0(x) - \sum_x \frac{m^2}{2Z_\phi^2 M_C^2}. \quad (\text{A20})$$

2. Effective action with baryons

We can include baryons with this style of explicit construction. In the path integral, the fermion fields are represented by the anticommuting Grassmann variables. We start with the following identities:

$$\int dB \int d\eta e^{-\eta(f(\psi)-B)} = 1, \quad (\text{A21})$$

$$\int dB \int d\eta e^{-\eta(f(\psi)-B)} B = f(\psi), \quad (\text{A22})$$

where η , B , and $f(\psi)$ are Grassmann variables or functions of Grassmann variables. They anticommute with themselves and with each other. The identity generalizes to arbitrary functions of B and to the multivariable case:

$$\int dB \int d\eta e^{-\eta(f(\psi)-B)} \mathcal{O}(B) = \mathcal{O}(f(\psi)), \quad (\text{A23})$$

$$\int \mathcal{D}B \int \mathcal{D}\eta \exp \left(- \sum_i \eta_i (f_i(\{\psi_j\}) - B_i) \right) \mathcal{O}(B_i) = \mathcal{O}(f_i(\{\psi_j\})). \quad (\text{A24})$$

We can use these relations to formally construct an effective theory including both baryons and mesons. For example, we can define the proton and neutron operators as

$$P(x) = \epsilon_{a,b,c} u_a(x) (u_b^T(x) C \gamma_5 d_c(x)), \quad (\text{A25})$$

$$N(x) = \epsilon_{a,b,c} d_a(x) (d_b^T(x) C \gamma_5 u_c(x)), \quad (\text{A26})$$

$$\bar{P}(x) = -\epsilon_{a,b,c} \bar{u}_a(x) (\bar{u}_b(x) C \gamma_5 \bar{d}_c^T(x)), \quad (\text{A27})$$

$$\bar{N}(x) = -\epsilon_{a,b,c} \bar{d}_a(x) (\bar{d}_b(x) C \gamma_5 \bar{u}_c^T(x)), \quad (\text{A28})$$

where u , d , $\bar{u}$, $\bar{d}$, and C can be defined as

$$\psi(x) = \begin{pmatrix} u(x) \\ d(x) \end{pmatrix}, \quad (\text{A29})$$

$$\bar{\psi}(x) = (\bar{u}(x) \quad \bar{d}(x)), \quad (\text{A30})$$

$$C = \gamma_i \gamma_y. \quad (\text{A31})$$

The effective action can be constructed as

$$e^{-S_{\text{eff}}[\{\phi_i\}, \bar{p}, p, \bar{n}, n]} = \int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \mathcal{D}\bar{\eta}_p \mathcal{D}\eta_p \mathcal{D}\bar{\eta}_n \mathcal{D}\eta_n \exp \left(-S_{\text{QCD}}[U, \bar{\psi}, \psi] - \frac{1}{2} \sum_x \sum_{i=0}^4 M_C^2 (\phi_i(x) - Q_i(x))^2 - \sum_x (\bar{p}(x) - \bar{P}(x)) \eta_p(x) - \sum_x \bar{\eta}_p(x) (p(x) - P(x)) - \sum_x (\bar{n}(x) - \bar{N}(x)) \eta_n(x) - \sum_x \bar{\eta}_n(x) (n(x) - N(x)) \right). \quad (\text{A32})$$

Based on the previous derivation in Eq. (A24), this construction satisfies the following desired property:

$$\langle \mathcal{O}[\{\phi_i\}, \bar{p}, p, \bar{n}, n] \rangle = \frac{1}{Z} \int \mathcal{D}\phi \mathcal{D}\bar{p} \mathcal{D}p \mathcal{D}\bar{n} \mathcal{D}n e^{-S_{\text{eff}}[\{\phi_i\}, \bar{p}, p, \bar{n}, n]} \mathcal{O}[\{\phi_i\}, \bar{p}, p, \bar{n}, n] \quad (\text{A33})$$

$$= \frac{1}{Z} \int \mathcal{D}\phi' \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left(-S_{\text{QCD}}[U, \bar{\psi}, \psi] - \frac{1}{2} \sum_x \sum_{i=0}^4 M_C^2 \phi_i'^2(x) \right) \mathcal{O}[\{Q_i + \phi_i'\}, \bar{P}, P, \bar{N}, N] \quad (\text{A34})$$

$$= \langle \mathcal{O}[\{Q_i + \phi_i'\}, \bar{P}, P, \bar{N}, N] \rangle_{\text{QCD}, \phi'}, \quad (\text{A35})$$

where

$$Z = \int \mathcal{D}\phi \mathcal{D}\bar{p} \mathcal{D}p \mathcal{D}\bar{n} \mathcal{D}n e^{-S_{\text{eff}}[\{\phi_i\}, \bar{p}, p, \bar{n}, n]} \quad (\text{A36})$$

$$= \int \mathcal{D}\phi' \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left(-S_{\text{QCD}}[U, \bar{\psi}, \psi] - \frac{1}{2} \sum_x \sum_{i=0}^4 M_C^2 \phi_i'^2(x) \right). \quad (\text{A37})$$

This concludes our explicit and exact construction of the effective theory.

APPENDIX B: CORRELATION FUNCTIONS

We use the following correlation functions to define observables:

- (1) To determine the pion mass, we define $\mathcal{O}_\pi(t) \equiv \sum_{i=1}^3 \sum_{\mathbf{x}} \phi_i(\mathbf{x}, t)$ and fit

$$\begin{aligned} & \left\langle T \left[\sum_t \mathcal{O}_\pi(t + \Delta t) \mathcal{O}_\pi(t) \right] \right\rangle \\ &= A \cosh \left[\left(\frac{N_t}{2} - \Delta t \right) m_\pi \right], \end{aligned} \quad (\text{B1})$$

where N_t is the number of lattice sites in the time direction. We use $\cosh[(N_t/2 - t)m_\pi]$ instead of $\exp(-tm_\pi)$ because of the periodic boundary conditions.

- (2) For the effective sigma mass, we define $\mathcal{O}_\sigma(t) \equiv \sum_{\mathbf{x}} \phi_0(\mathbf{x}, t)$ and fit

$$\begin{aligned} & \left\langle T \left\{ \sum_t [\mathcal{O}_\sigma(t + \Delta t) - \langle \mathcal{O}_\sigma \rangle] [\mathcal{O}_\sigma(t) - \langle \mathcal{O}_\sigma \rangle] \right\} \right\rangle \\ &= A \cosh \left[\left(\frac{N_t}{2} - \Delta t \right) m_\sigma^{\text{eff}} \right], \end{aligned} \quad (\text{B2})$$

where $\langle \mathcal{O}_\sigma \rangle$ is the vacuum expectation value of $\mathcal{O}_\sigma$.

- (3) To determine F_π , we define the axial current operator $A_\mu^i(x) = \phi_0(x - \mu) \phi_i(x) - \phi_0(x) \phi_i(x - \mu)$, as discussed in Sec. II C. On a finite lattice, the continuum relation from Eq. (7) becomes

$$\begin{aligned} & \langle T \{ A_0^i(\mathbf{x}, t) \mathcal{O}_\pi(\mathbf{p} = 0, t = 0) \} \rangle \\ &= 2F_\pi m_\pi e^{-m_\pi N_T/2} \sinh \left[\left(\frac{N_T}{2} - t + \frac{1}{2} \right) m_\pi \right]. \end{aligned} \quad (\text{B3})$$

We use $t - 1/2$ instead of t in the above equation because the lattice definition of A_0^i combines fields at t and $t - 1$. To create the pion state, we define the pion interpolating operator

$$\mathcal{O}_\pi^i(t) \equiv \sum_{\mathbf{x}} \phi^i(\mathbf{x}, t). \quad (\text{B4})$$

Taking into account the correct normalization of the pion state, we get

$$\begin{aligned} & \left\langle T \left\{ \left(\sum_{\mathbf{x}} A_0^i(\mathbf{x}, t) \right) \mathcal{O}_\pi^i(0) \right\} \right\rangle \\ & \times \sqrt{2m_\pi L^3} \sqrt{\frac{2e^{-m_\pi N_T/2} \cosh((N_T/2 - t')m_\pi)}{\langle 0 | \mathcal{O}^i(t) \mathcal{O}^i(0) | 0 \rangle}} \\ &= 2F_\pi m_\pi e^{-m_\pi N_T/2} \sinh \left[\left(\frac{N_T}{2} - t + \frac{1}{2} \right) m_\pi \right]. \end{aligned} \quad (\text{B5})$$

We can extract the decay constant using Eq. (B5), but to get a more stable fit, we can instead use Noether's theorem for the lattice to get $\sum_\mu (A_\mu^i(x + \mu) - A_\mu^i(x)) = -a\phi^i(x)$. To get our results, we combined this relationship with Eq. (B5) to get a correlation function we could fit in order to extract F_π .

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