Chiral perturbation theory for the Wilson lattice action

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We extend chiral perturbation theory to include linear dependence on the lattice spacing *a* for the Wilson action. The perturbation theory is written as a double expansion in the small quark mass m_q and lattice spacing *a*. We present formulas for the mass and decay constant of a flavor-nonsinglet meson in this scheme to order *a* and m_q^2 . The extension to the partially quenched theory is also described.

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I. INTRODUCTION

Chiral perturbation theory (χ PT) is an important tool for extracting quantitative information from lattice simulations of QCD. The reason for this is that it is impractical to have dynamical quarks in simulations that are as light as the up and down quarks, and χ PT is needed for a controlled, systematic extrapolation in the quark masses. Since χ PT describes *continuum* QCD at low energies, its application in numerical simulations is possible only after extrapolating lattice data to the continuum limit where the lattice spacing *a* vanishes. In this paper, we study the behavior of the Wilson lattice action close to the continuum by incorporating O(a)effects in a reformulation of χ PT. A similar approach was first taken in Ref. [1] to investigate the phase diagram for Wilson fermions in two-flavor QCD.

The quark mass matrix (considering only the 2 or 3 lightest quarks) has a special role in QCD—it parametrizes the explicit breaking of the axial symmetries. As a result, the light quark masses appear explicitly in the low-energy effective theory. In this paper, we exploit the fact that for the Wilson lattice action there is another independent symmetry breaking parameter, linear in a [1,2]. To O(a) this is the only discretization effect, and thus a generalization of the chiral Lagrangian can be written which includes all terms linear in a.

II. EFFECTIVE LAGRANGIAN

The Wilson action for fermions is given by [3]

$$S_F^{(W)} = \sum_x \left[\bar{\psi}(x) \gamma_\mu \Delta_\mu \psi(x) + \bar{\psi}(x) m_q \psi(x) + ar \bar{\psi}(x) \Delta^2 \psi(x) \right], \qquad (2.1)$$

where

$$\Delta_{\mu}\psi(x) = \frac{1}{2a} [U_{\mu}(x)\psi(x+a\hat{\mu}) - U_{\mu}^{\dagger}(x-a\hat{\mu})\psi(x-a\hat{\mu})].$$
(2.2)

 $U_{\mu}(x)$ is the gauge group valued field defined on the links of the lattice. In typical lattice simulations, r=1 but we will keep it more general for now. Since we are interested in a perturbative study of discretization effects, we follow Ref. [4] and consider an effective action in the continuum which describes the same physics as the discrete lattice action (including the gauge action), well below the cutoff 1/a. The effective action is expanded in powers of a:

$$S_{\rm eff} = S_0 + aS_1 + a^2S_2 + \cdots$$
 (2.3)

By construction, S_0 is the QCD action. Symmetry considerations restrict the number of mass-dimension 5 operators that appear in S_1 . The equations of motion can be used to further reduce the list of operators. One then identifies the operators that already appear in S_0 , which give rise to the renormalization of the quark masses and the coupling constant. Finally, one is left with a single new term at O(a), the Pauli term [2]:

$$aS_1 = ac_{\rm SW}\bar{\psi}\sigma_{\mu\nu}F^{\mu\nu}\psi. \tag{2.4}$$

 c_{SW} is a constant of $\mathcal{O}(1)$ which is a complicated function of the gauge coupling and *r*.

Considering $S_0 + aS_1$ as an underlying theory, it has an $SU(N_f)_L \otimes SU(N_f)_R$ flavor symmetry which is broken down to the vector part by the mass and Pauli terms with coefficients m_q and ac_{SW} respectively. $\bar{\psi}\psi$ and $\bar{\psi}\sigma_{\mu\nu}F^{\mu\nu}\psi$ break the axial symmetry in the same way and therefore, from a spurion analysis point of view, m_q and ac_{SW} are on equal footing, as noted in Ref. [1]. In particular, ac_{SW} is treated as a non-trivial matrix in flavor space, just like m_q . It is possible to give ac_{SW} a flavor structure in simulations by promoting the constant r to a matrix. This can supply extra "knobs" which can aid the continuum extrapolations. The

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squares of the Goldstone boson (GB) masses are linear in the symmetry breaking matrices of parameters [1], conveniently written as

$$\chi \equiv 2B_0 m_a, \quad \rho \equiv 2W_0 a c_{\rm SW}. \tag{2.5}$$

 B_0 and W_0 are unknown dimensionful parameters that appear in the effective Lagrangian at leading order (LO) which is defined below.

The effective Lagrangian is constructed from all operators that respect the symmetries of the underlying action. Each operator appears with an unknown coefficient that cannot be determined from symmetry considerations. It is also necessary to specify a "power counting scheme"—a prescription for selecting terms in the Lagrangian that need to be included in a calculation to achieve a desired accuracy. For QCD (S_0) the result of this procedure is χ PT, which was defined and constructed to next-to-leading order (NLO) by Gasser and Leutwyler [5]. When more terms from S_{eff} in Eq. (2.3) are added, the result is χ PT for the Wilson action ($W\chi$ PT) which contains additional operators involving ρ . This introduces new unknown couplings into the theory.

 $W\chi PT$ is an expansion in the squares of the small momenta *p* and the small pseudo-Goldstone boson masses. We formally consider the expansion to be in two independent small parameters:

$$\epsilon \sim \frac{p^2}{\Lambda_{\chi}^2} \sim \frac{\chi}{\Lambda_{\chi}^2} \text{ and } \delta \sim \frac{\rho}{\Lambda_{\chi}^2}.$$
 (2.6)

 Λ_{χ} is the scale where new high-energy physics enters and the effective field theory (EFT) no longer describes the correct physics. This happens around the mass of the rho meson, or roughly $\Lambda_{\chi} \sim 1$ GeV. From dimensional analysis, and the fact that B_0 and W_0 depend only on the high-energy details, one can check that the expansion is in fact in m_q/Λ_{χ} and in $a\Lambda_{\chi}$.

Since Eq. (2.3) is truncated at $\mathcal{O}(a)$ it makes no sense to go beyond $\mathcal{O}(\delta)$ in W χ PT [we remark on $\mathcal{O}(a^2)$ corrections in the next section]. For *convenience*, we choose to collect terms in the LO and NLO Lagrangians as follows:

LO:
$$\mathcal{L}_2 \sim \mathcal{O}(\epsilon, \delta),$$
 (2.7)

NLO:
$$\mathcal{L}_4 \sim \mathcal{O}(\epsilon^2, \epsilon \delta).$$
 (2.8)

The underlying hierarchy consistent with this ordering is $\{\epsilon, \delta\} \gg \{\epsilon^2, \epsilon\delta\} \gg \delta^2$, and the last inequality also implies $\epsilon \gg \delta$. This choice is somewhat arbitrary. In practice, the perturbative expansion should be organized according to the actual sizes of the expansion parameters, which are determined by the quark masses in the simulation and the size of the lattice spacing. For example, if the simulations are done so close to the continuum that δ is very small, it might make more sense to have the LO Lagrangian be $\mathcal{O}(\epsilon)$, and at NLO $\mathcal{O}(\epsilon^2, \delta)$. With our convention,

$$\mathcal{L}_2 = \frac{f^2}{4} \operatorname{tr}(\partial \Sigma \, \partial \Sigma^{\dagger}) - \frac{f^2}{4} \operatorname{tr}((\chi + \rho)\Sigma^{\dagger} + \Sigma(\chi^{\dagger} + \rho^{\dagger})),$$
(2.9)

is the LO Lagrangian, where $\Sigma = \exp(2i\Pi/f)$ contains the matrix of meson fields, Π . It is useful to note that Eq. (2.9) can be "produced" from the LO Lagrangian of ordinary χ PT by the substitution $\chi \rightarrow \chi + \rho$.

The NLO Lagrangian is

$$\mathcal{L}_{4} = L_{1} \langle \partial \Sigma \partial \Sigma^{\dagger} \rangle^{2} + L_{2} \langle \partial_{\mu} \Sigma \partial_{\nu} \Sigma^{\dagger} \rangle \langle \partial_{\mu} \Sigma \partial_{\nu} \Sigma^{\dagger} \rangle + L_{3} \langle (\partial \Sigma \partial \Sigma^{\dagger})^{2} \rangle + L_{4} \langle \partial \Sigma \partial \Sigma^{\dagger} \rangle \langle \chi^{\dagger} \Sigma + \Sigma^{\dagger} \chi \rangle + W_{4} \langle \partial \Sigma \partial \Sigma^{\dagger} \rangle \langle \rho^{\dagger} \Sigma + \Sigma^{\dagger} \rho \rangle$$

$$+ L_{5} \langle \partial \Sigma \partial \Sigma^{\dagger} (\chi^{\dagger} \Sigma + \Sigma^{\dagger} \chi) \rangle + W_{5} \langle \partial \Sigma \partial \Sigma^{\dagger} (\rho^{\dagger} \Sigma + \Sigma^{\dagger} \rho) \rangle + L_{6} \langle \chi^{\dagger} \Sigma + \Sigma^{\dagger} \chi \rangle^{2} + W_{6} \langle \chi^{\dagger} \Sigma + \Sigma^{\dagger} \chi \rangle \langle \rho^{\dagger} \Sigma + \Sigma^{\dagger} \rho \rangle$$

$$+ L_{7} \langle \chi^{\dagger} \Sigma - \Sigma^{\dagger} \chi \rangle^{2} + W_{7} \langle \chi^{\dagger} \Sigma - \Sigma^{\dagger} \chi \rangle \langle \rho^{\dagger} \Sigma - \Sigma^{\dagger} \rho \rangle + L_{8} \langle \chi^{\dagger} \Sigma \chi^{\dagger} \Sigma + \Sigma^{\dagger} \chi \rangle Z^{\dagger} \chi \rangle + W_{8} \langle \rho^{\dagger} \Sigma \chi^{\dagger} \Sigma + \Sigma^{\dagger} \rho \Sigma^{\dagger} \chi \rangle.$$

$$(2.10)$$

The angled brackets stand for traces over the flavor indices. In the limit $a \rightarrow 0$, Eqs. (2.9), (2.10) become the chiral Lagrangian of Ref. [5]. W χ PT contains ordinary χ PT as it reduces to χ PT in this limit. Since the low-energy constants are independent of *a* (and m_q) by construction, the L_i 's in W χ PT are the GL coefficients of ordinary χ PT.

A word about certain $\log(a\Lambda)$ corrections is appropriate here. In the EFT formulation, the Lagrangian is written in terms of the most general set of operators constructed out of the relevant degrees of freedom that respect the symmetries of the theory. The high-energy physics that was integrated out enters through the unknown couplings that multiply these operators. Thus the low-energy constants or couplings are entirely determined by the high-energy scales. In χ PT, the operators contain only the light meson and photon fields, and the low-energy constants B_0, f, L_i , etc., are functions of the QCD scale $\Lambda_{\rm QCD}$. In particular, the L_i 's are independent of the pion masses $m_{\pi} \sim \sqrt{m_q}$ which are associated with the long-distance physics. All the m_q dependence of χ PT is explicitly written in the operators. This still holds for the m_q dependence of the W χ PT Lagrangian written above, but the same cannot be said about the lattice spacing *a*. It is true that an $\mathcal{O}(a)$ term breaks the chiral symmetry in the same way as m_q , and $a\Lambda^2$ is a soft scale associated with the pseudo GB mass, but 1/a is not a soft scale—it acts as the ultraviolet cutoff for the discrete lattice. Thus, while the low-energy constants of W χ PT are expected to be independent of m_q and ac_{SW} , they could in principal have a complicated dependence on the gauge coupling g, which itself depends on a. However, the running of the coupling constant is determined in simulations by requiring that as one approaches the continuum, some chosen physical quantity remains fixed. Effectively, this means that the coupling g and the cutoff 1/a combine to give the only real scale in the theory— Λ_{QCD} —and the continuum limit is approached smoothly. We therefore expect the L_i 's and W_i 's to depend on Λ_{QCD} , and only weakly on a, the latter dependence coming from higher orders in perturbation theory, or involving higher powers of a which can always be expanded.¹ The parameter c_{SW} in the action S_1 will still depend on $\log(a\Lambda_{QCD})$, and it might be possible to calculate these dependences explicitly in perturbation close to the continuum [6,7].

A related form of implicit *a* dependence exists in the quark masses. The quark masses that appear in the $W_{\chi}PT$ Lagrangian [Eqs. (2.9), (2.10)] are not the same as those that appear in the Wilson action [Eq. (2.1)]. Because of the explicit breaking of chiral symmetry due to the Wilson term, the quark masses are not protected from additive renormalization of the order of the lattice cutoff 1/a. In practice one finds in simulations a "critical" line $m_q^c(a)$ on which the meson masses approximately vanish. The quark mass is then defined as the distance from this line:

$$\widetilde{m}_q = m_q - m_q^c(a), \qquad (2.11)$$

and it is \tilde{m}_q that should be used in Eqs. (2.9), (2.10). \tilde{m}_q compensates for the large $\mathcal{O}(1/a)$ shift in the quark masses, but it also contains positive powers of a. This is not a problem—redefinitions of the mass parameter of this sort only lead to changes in the W_i 's. The GL coefficients L_i 's are not affected because the operators with which they are associated do not contain a. The re-shuffling of the W_i 's does mean, however, that their actual numerical values depend on the prescription that is used to determine $m_q^c(a)$ and to define \tilde{m}_q .

Note that the chiral limit cannot be taken by simply setting $\tilde{m}_q \rightarrow 0$. While m_q^c satisfies $M_{\pi}^2(m_q^c(a),a) = 0$, there is no reason that other quantities will attain their chiral limit for this value of m_q . This is a reflection of the fact that there really are two different operators that break the symmetry.

III. APPLICATIONS

In the following two subsections we calculate the expressions for the mass and decay constant of a flavor-charged meson, with the flavor indices AB ($A \neq B$), having the same quantum numbers as $\overline{\psi}_B \gamma_5 \psi_A$. We take the number of flavors $N_f = 3$. In the calculations that follow we take χ to be a diagonal matrix with entries (χ)_{ii} = χ_i , and use the notation $\chi_{AB} = (\chi_A + \chi_B)/2$. Note that this notation coincides with the standard way of denoting matrix elements only for the diagonal entries. The same convention is used for ρ . It is convenient to define another matrix, $\mu = \chi + \rho$, which is the combination that appears in \mathcal{L}_2 . The subscript notation for μ follows that of χ and ρ , except for the quantities μ_{π} and μ_{η} which are defined below.

A. Masses

The mass of a flavor-charged meson in $W\chi PT$ with three quark flavors is given through NLO by

$$M_{AB}^{2} = (M_{AB}^{2})_{\rm LO} + (M_{AB}^{2})_{\rm NLO, loop} + (M_{AB}^{2})_{\rm NLO, tree},$$
(3.1)

with

$$(M_{AB}^2)_{\rm LO} = \mu_{AB},$$
 (3.2)

$$(M_{AB}^2)_{\rm NLO,loop} = \frac{1}{48f^2\pi^2} \mu_{AB} \sum_{x=\pi,\eta} R_x^{AB} \mu_x \log \mu_x, \qquad (3.3)$$

$$(M_{AB}^{2})_{\rm NLO,tree} = -\frac{24}{f^{2}} L_{4}(\chi_{AB} + \rho_{AB})\bar{\chi} - \frac{24}{f^{2}} W_{4}\chi_{AB}\bar{\rho}$$
$$-\frac{8}{f^{2}} L_{5}(\chi_{AB} + \rho_{AB})\chi_{AB} - \frac{8}{f^{2}} W_{5}\chi_{AB}\rho_{AB}$$
$$+\frac{24}{f^{2}} 2L_{6}\chi_{AB}\bar{\chi} + \frac{24}{f^{2}} W_{6}(\chi_{AB}\bar{\rho} + \rho_{AB}\bar{\chi})$$
$$+\frac{8}{f^{2}} 2L_{8}\chi_{AB}^{2} + \frac{8}{f^{2}} 2W_{8}\chi_{AB}\rho_{AB}, \qquad (3.4)$$

where μ_{π} and μ_{η} are the squares of the LO masses of the two light flavor-neutral mesons, given implicitly by

$$\mu_{\pi} + \mu_{\eta} = 2\bar{\mu}, \qquad (3.5)$$

$$\mu_{\pi}\mu_{\eta} = (\mu_{1}\mu_{2} + \mu_{1}\mu_{3} + \mu_{2}\mu_{3})/3.$$
(3.6)

Here $\bar{\chi} = \text{tr}(\chi)/3$ and similarly for ρ and μ . Also, if we denote by *C* the flavor that is different from both *A* and *B*, we have

$$R_{\pi}^{AB} = \frac{\mu_C - \mu_{\pi}}{\mu_{\eta} - \mu_{\pi}}, \ R_{\eta}^{AB} = \frac{\mu_C - \mu_{\eta}}{\mu_{\pi} - \mu_{\eta}}.$$
 (3.7)

In deriving the expressions for the mass in $W\chi PT$ one could use a very convenient "trick" relating these expressions to the corresponding expressions in ordinary χPT . As mentioned earlier, the LO Wilson chiral Lagrangian \mathcal{L}_2 , Eq. (2.9), can be obtained from χPT LO Lagrangian by the simple substitution $\chi \rightarrow \chi + \rho$ (or $\chi \rightarrow \mu$). Thus any quantity $h(\chi)$ in χPT that depends only on the LO Lagrangian can be trivially reproduced in $W\chi PT$ according to $h(\chi) \rightarrow h(\chi + \rho)$. This is true for the LO and NLO loop diagrams that contribute to the mass. Similar results also hold for the decay constant. We provide the expressions for the mass in ordinary χPT in Appendix A for comparison.

¹We thank Paulo Bedaque and Andrew Cohen for helping us understand this issue.

B. Decay constants

The decay constant is given through NLO by

$$f_{AB} = (f_{AB})_{\text{LO}} + (f_{AB})_{\text{NLO,loop}} + (f_{AB})_{\text{NLO,tree}}, \quad (3.8)$$

with

$$(f_{AB})_{\rm LO} = f, \tag{3.9}$$

$$(f_{AB})_{\rm NLO, loop} = -\frac{1}{64\pi^2 f} \sum_{\substack{i=1,2,3\\j=A,B}} \mu_{ij} \log \mu_{ij} + \frac{1}{192\pi^2 f} (\mu_A - \mu_B) \left\{ \log \left(\frac{\mu_A}{\mu_B} \right) + \sum_{x=\pi,\eta} R_x^{AB} \mu_x \left[\frac{\log(\mu_A/\mu_x)}{\mu_A - \mu_x} - \frac{\log(\mu_B/\mu_x)}{\mu_B - \mu_x} \right] \right\},$$
(3.10)

$$(f_{AB})_{\rm NLO,tree} = \frac{12}{f} (L_4 \bar{\chi} + W_4 \bar{\rho}) + \frac{4}{f} (L_5 \chi_{AB} + W_5 \rho_{AB}).$$
(3.11)

C. W χ PT, $\mathcal{O}(a^2)$, and improvement

In the simplest sense, the expressions for the mass and decay constant in $W\chi PT$ can be used to aid in taking the continuum limit. These forms provide all the linear *a* dependence, as well as non-trivial logarithms that involve *a* and m_q . A test of these formulas would be to check whether they describe the *a* dependence better than naive extrapolations. Perhaps a more useful way to think about it is that with these expressions one can determine the GL coefficients directly from lattice data at finite *a*.

What about higher orders in a? At order a^2 the picture changes qualitatively. There are operators in S_2 , such as $\bar{\psi}D_{\mu}D_{\mu}\psi$, that do not break the chiral symmetry. This means that a can no longer be associated only with symmetry breaking effects, and spurion analysis cannot be used to constrain the a^2 operators. Nevertheless, we might still expand in ϵ and δ simultaneously. The LO, $\mathcal{O}(\epsilon, \delta)$ Lagrangian, and consequently the LO mass and decay constant are unchanged. At NLO, $\mathcal{O}(\epsilon^2, \epsilon \delta, \delta^2)$, there are several $\mathcal{O}(a^2)$ operators that are added to the Lagrangian, but they are all independent of the quark masses and do not contain derivatives. Consequently, the only correction to the meson masses at this order is an additional term of the form ωa^2 , where ω is an unknown constant of mass-dimension 4. The expression for the decay constant does not receive any corrections at this order. This is because tree level contributions to the decay constant can only come from operators that contain derivatives.

Improvement schemes (first suggested by Symanzik in Ref. [4])—using an improved action and improved operators—are another important tool for studying and reducing discretization effects [2,8]. Using improved action in-

volves adding a discretized version of the Pauli term in Eq. (2.4) to the Wilson action in Eq. (2.1) which exactly cancels the S_1 term in the continuum action, Eq. (2.3). This means that up to $\mathcal{O}(a^2)$ the lattice theory is just QCD, and at low energies we expect χ PT to be a good description. From the perspective of $W\chi PT$ this is equivalent to saying that using an improved action sets all $W_i = 0$. This is of course not surprising: the use of improved action is meant to eliminate all $\mathcal{O}(a)$ dependence from observables, and the W_i coefficients parametrize exactly this dependence. One should not conclude from this that improving the action is enough for complete $\mathcal{O}(a)$ improvement. As mentioned above, some dimension-5 operators that are allowed by the symmetries, and can therefore appear in S_1 , are implicitly absorbed in S_0 by replacing the bare parameters of S_0 with renormalized ones. This is a necessary step, and it is compatible with the fact that in improvement schemes, in addition to using an improved action, one must use improved operators.

IV. PARTIALLY QUENCHED THEORIES

 $W\chi PT$ is appropriate for the type of lattice simulations which are called "unquenched." These are simulations in which there are 2 or 3 dynamical fermions (also called "sea quarks"), and expectation values are calculated of operators which are constructed from a different type of fermions ("valence quarks") which have the same masses as the sea quarks. In most lattice simulations, however, the masses of the valence quarks are not taken to be the same as those of the sea quarks. Simulations that are done this way are called partially quenched (PQ). Theoretically this can be described by a QCD-like construction which includes ghosts [9,10]. The low-energy behavior of these theories is described by PQ χ PT [10], which has the same unknown low-energy constants as χ PT for ordinary QCD [11]. Thus, PQ simulations provide additional mass parameters that can be used to probe the theory in a larger parameter space, and gain better statistics in determining the GL coefficients [12,13]. It is of clear practical value to consider the generalization of $W\chi PT$ to the PQ case.

PQ QCD contains three different types of spin-half particles—valence quarks, sea quarks, and ghosts which obey Bose-Einstein statistics. There is a single ghost flavor for every valence quark, and they both have the same mass. The quark mass matrix for a theory with 2 valence quarks, 3 sea quarks, and 2 ghosts is

$$m_q = \operatorname{diag}\left(\underbrace{m_A, m_B}_{\text{valence}}, \underbrace{m_1, m_2, m_3}_{\text{sea}}; \underbrace{m_A, m_B}_{\text{ghost}}\right).$$
(4.1)

 χ PT for PQ QCD is constructed in terms of this matrix, or in terms of χ which is still defined through Eq. (2.5), and the result is a Lagrangian identical to the one for ordinary χ PT, but with an extended flavor structure and with super-traces replacing the traces. Because of the great formal similarity between QCD and PQ QCD, the extension of PQ χ PT to PQ W χ PT is a simple generalization of the discussion in the previous section. In particular, the LO and NLO Lagrangians for PQ W χ PT have forms just like in Eqs. (2.9), (2.10), with traces replaced by super-traces. Further, as in the continuum, the low-energy constants L_i 's and W_i 's are exactly the same in the PQ and unquenched W χ PT. It follows that one can use the Wilson chiral expressions for PQ theories to extract the GL coefficients.

For completeness, we provide the expressions for the mass and decay constant for PQ $W_{\chi}PT$ in Appendix B. Again, as in unquenched theories, the LO and NLO loop results in PQ $W_{\chi}PT$ are trivially related to the corresponding results in PQ χ PT which have been calculated in [12].

V. SUMMARY

We constructed a low-energy EFT, $W\chi PT$, of the Wilson lattice action close to the continuum. The theory extends χPT , and the perturbative framework is described in terms of two small parameters—the quark mass m_q and the lattice spacing *a*. The Gasser-Leutwyler chiral Lagrangian (through $\mathcal{O}(p^4)$ in χPT) was modified to incorporate all linear dependence on *a*. We applied this theory to calculate light meson masses and decay constants. The resulting expressions capture all the linear dependence on *a* as well as non-trivial logarithms that entangle *a* and m_q . A useful application of this theory is the determination of the Gasser-Leutwyler coefficients of ordinary χPT from lattice simulations at small but finite *a*.

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APPENDIX A: χ PT RESULTS

We present the expressions for the mass of a flavorcharged light meson in χ PT for comparison with W χ PT results. As explained in the text, one can see that the LO and NLO loop expressions in W χ PT can be obtained from the corresponding χ PT results with the substitution $\chi \rightarrow \chi + \rho$ ($\chi \rightarrow \mu$). Using the same notation as in Eqs. (3.2)–(3.7), the masses through NLO with three quark flavors are [12]:

$$M_{AB}^{2} = (M_{AB}^{2})_{\rm LO} + (M_{AB}^{2})_{\rm NLO, loop} + (M_{AB}^{2})_{\rm NLO, tree},$$
(A1)

with

$$(M_{AB}^2)_{\rm LO} = \chi_{AB} \,, \tag{A2}$$

$$(M_{AB}^{2})_{\rm NLO,loop} = \frac{1}{48f^{2}\pi^{2}} \chi_{AB} \sum_{x=\pi,\eta} R_{x}^{AB} \chi_{x} \log \chi_{x}, \qquad (A3)$$

$$(M_{AB}^2)_{\rm NLO, tree} = \frac{24}{f^2} (2L_6 - L_4) \chi_{AB} \bar{\chi} + \frac{8}{f^2} (2L_8 - L_5) \chi_{AB}^2,$$
(A4)

where

$$\chi_{\pi} + \chi_{\eta} = 2\bar{\chi}, \tag{A5}$$

$$\chi_{\pi}\chi_{\eta} = (\chi_1\chi_2 + \chi_1\chi_3 + \chi_2\chi_3)/3, \tag{A6}$$

$$R_{\pi}^{AB} = \frac{\chi_C - \chi_{\pi}}{\chi_{\eta} - \chi_{\pi}}, \quad R_{\eta}^{AB} = \frac{\chi_C - \chi_{\eta}}{\chi_{\pi} - \chi_{\eta}}.$$
 (A7)

(Here, again, C is the flavor that is different from both A and B.)

APPENDIX B: PQ W χ PT RESULTS

The forms of the Lagrangians in unquenched and PQ theory are the same, with an implicit difference in the structure of the matrices in flavor space and the replacement of traces with super-traces. Thus all tree contributions in both theories have the same dependence on χ and ρ . In particular, the LO and NLO tree results are still given by Eqs. (3.2), (3.4) and Eqs. (3.9), (3.11) for the mass and the decay constant respectively, with appropriate χ and ρ matrices for PQ simulations. (The structure of ρ in PQ W χ PT is determined by r in the PQ version of the Wilson action. The latter must have a structure similar to m_q , Eq. (4.1), that is needed to guarantee the exact cancellation between valence and ghost loops.) We give here only the NLO loop results, which are different from the unquenched expressions.

$$(M_{AB}^{2})_{\text{NLO,loop}} = \frac{1}{48f^{2}\pi^{2}} \mu_{AB} \sum_{x=A,B,\pi,\eta} R_{x} \mu_{x} \log(\mu_{x}),$$
(B1)

$$(f_{AB})_{\text{NLO,loop}} = -\frac{1}{64\pi^{2}f} \sum_{\substack{i=1,2,3\\ j=A,B}} \mu_{ij} \log \mu_{ij} + \frac{1}{192\pi^{2}f} \\ \times \left\{ -D_{A} - D_{B} + \frac{\log(\mu_{A}/\mu_{B})}{\mu_{A} - \mu_{B}} \right. \\ \left. \times \left[\mu_{A}D_{A} + \mu_{B}D_{B} + (\mu_{A} - \mu_{B})^{2} \right] \\ \left. + \sum_{x=\pi,\eta} R_{x}\mu_{x}(\mu_{A} - \mu_{B}) \left[\frac{\log(\mu_{A}/\mu_{x})}{\mu_{A} - \mu_{x}} \right] \\ \left. - \frac{\log(\mu_{B}/\mu_{x})}{\mu_{B} - \mu_{x}} \right] \right\},$$
(B2)

where

$$R_{x} = \frac{\prod_{i=1,2,3} (\mu_{i} - \mu_{x})}{\prod (\mu_{y} - \mu_{x})}, \quad y = A, B, \pi, \eta, y \neq x$$

$$D_{x} = \frac{\prod_{i=1,2,3} (\mu_{i} - \mu_{x})}{(\mu_{\pi} - \mu_{x})(\mu_{\eta} - \mu_{x})}.$$
 (B3)

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