

**Electromagnetic contribution to  $\Sigma$ - $\Lambda$  mixing using lattice QCD + QED**Z. R. Kordov<sup>1</sup>, R. Horsley<sup>2</sup>, Y. Nakamura<sup>3</sup>, H. Perlt<sup>4</sup>, P. E. L. Rakow<sup>5</sup>, G. Schierholz<sup>6</sup>,  
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Mixing in the  $\Sigma^0$ - $\Lambda^0$  system is a direct consequence of broken isospin symmetry and is a measure of both isospin-symmetry breaking as well as general SU(3)-flavor symmetry breaking. In this work we present a new scheme for calculating the extent of  $\Sigma^0$ - $\Lambda^0$  mixing using simulations in lattice QCD + QED and perform several extrapolations that compare well with various past determinations. Our scheme allows us to easily contrast the QCD-only mixing case with the full QCD + QED mixing.

DOI: [10.1103/PhysRevD.101.034517](https://doi.org/10.1103/PhysRevD.101.034517)**I. INTRODUCTION**

Our best theoretical understanding of the classification and qualities of the low-lying hadron states comes from the theory of SU(3)-flavor symmetry, first summarized by the eightfold way [1]. Since SU(3)-flavor is an approximate symmetry, broken by nondegeneracy in the physical properties of the up, down and strange quarks, it is often only a convenient starting point for precision determinations of hadron properties.

The neutral  $\Sigma$  and  $\Lambda$  states of the spin-1/2 baryon octet, as defined by SU(3) flavor, differ only in isospin (also denoted T spin [2]), which is not an exact symmetry in nature. Consequentially the physical particle states that correspond to these octet baryons are actually mixtures of the idealized isospin states. They are the only two states in the baryon octet that have the same quark content and charge and thus permit mixing under isospin breaking. The neutral members of the pseudoscalar meson nonet present an analogous system of mixing (see e.g., [3,4]).

The amount of mixing that occurs in the physical system depends on the degree of isospin-symmetry breaking, as well as further SU(3)-flavor symmetry breaking by the strange quark, and is driven by both the bare mass parameters and the differences in the quark charges.

One approach in calculating the  $\Sigma^0$ - $\Lambda^0$  mixing, due to Dalitz and Von Hippel (DvH [5]), is based on relationships between the electromagnetic (EM) mass splittings of octet baryons. This was derived by consideration of an effective Lagrangian density exhibiting SU(3)-flavor symmetry plus a perturbation which encodes bare quark mass and QED effects [6], and uses experimental baryon masses as inputs.

Our approach herein is to use simulations in lattice QCD + QED to fit a parametrization of the  $\Sigma^0$ - $\Lambda^0$  mixing angle, which we derive by considering the effects of continuous variations in the quark mass and charge parameters around an SU(3)-symmetric point, and extrapolate to physical values of the quark masses and charges. We find that the inclusion of QED effects in our determination gives us a result comparable to that of DvH, which is the only other determination to explicitly include electromagnetic effects.

Further, when QED is ignored we show that our new extrapolation scheme gives good agreement with previous QCD-only calculations of the mixing, using chiral perturbation theory ( $\chi$ PT) [7,8] and lattice QCD (no QED [9,10]), and gives a magnitude of about half of that found by DvH or this work when QED is incorporated.

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In Sec. II we introduce the practical structure for probing  $\Sigma^0$ - $\Lambda^0$  using lattice QCD + QED and derive a parametrization for use in extrapolating our lattice results to the physical point (physical quark masses and QED coupling). We give details of the lattice simulation parameters used in Sec. III before performing the extrapolation and presenting our results in Sec. IV, and we also observe some traits of the mixing in the cases of QCD only and QCD + QED and contrast these cases. We conclude this work in Sec. V.

## II. SIGMA-LAMBDA MIXING ON THE LATTICE

Hadrons are studied on the lattice by calculation of correlation functions made from operators which are constructed to represent particular hadrons by incorporating their flavor content, symmetries and quantum numbers. The canonical way of doing this is to write down the operators for a particular hadron using the full SU(3)-flavor symmetry with definite isospin, since we know isospin to be a very good approximate symmetry in reality.

In this study we wish to explore other SU(2) symmetries in addition to isospin and hence, to begin with, we do not appeal to the quark flavors up, down and strange, and instead use placeholders  $a$ ,  $b$  and  $c$ .

### A. Standard interpolating operators

Following the notation introduced in [9], we employ standard Euclidean-space interpolating operators for the SU(3)  $\Sigma^0$  and  $\Lambda^0$  octet baryons with flavor content  $a$ ,  $b$ ,  $c$ ,

$$\mathcal{B}_{\Sigma(abc),\alpha}(x) = \frac{1}{\sqrt{2}} \epsilon^{lmn} (b_\alpha^l(x) [a^m(x)^\top C \gamma_5 c^n(x)] + a_\alpha^l(x) [b^m(x)^\top C \gamma_5 c^n(x)]), \quad (1)$$

and

$$\mathcal{B}_{\Lambda(abc),\alpha}(x) = \frac{1}{\sqrt{6}} \epsilon^{lmn} (2c_\alpha^l(x) [a^m(x)^\top C \gamma_5 b^n(x)] + b_\alpha^l(x) [a^m(x)^\top C \gamma_5 c^n(x)] - a_\alpha^l(x) [b^m(x)^\top C \gamma_5 c^n(x)]), \quad (2)$$

where  $C = \gamma_2 \gamma_4$ , the superscript  $\top$  denotes a transpose in Dirac space,  $l$ ,  $m$  and  $n$  are color indices and  $\alpha$  is a Dirac index. These interpolating operators are constructed to create states with definite iso-, U- or V-spin (see [11]) symmetry depending on the choice of Cartan subalgebra [12] used in constructing the octet representation. The  $\Sigma^0$  is symmetric in the flavors  $a$  and  $b$  [which define the SU(2) subalgebra] while the  $\Lambda^0$  is antisymmetric; this ensures that the  $\Sigma^0$  and  $\Lambda^0$  states are orthogonal when the  $a$  and  $b$  quarks are degenerate. From these operators we construct the matrix of correlation functions

$$C_{ij}(t) = \frac{1}{V_s} \text{Tr}_D \Gamma_{unpol} \left\langle \sum_{\vec{y}} \sum_{\vec{x}} \mathcal{B}_i(\vec{y}, t) \bar{\mathcal{B}}_j(\vec{x}, 0) \right\rangle, \quad (3)$$

for  $0 \ll t \ll T/2$ ,  $i, j = \Sigma(abc), \Lambda(abc)$ ,

where  $\Gamma_{unpol} = (1 + \gamma_4)/2$ ,  $V_s$  is the spatial lattice volume and  $T$  is the full temporal extent of the lattice. The correlation matrix is Hermitian and its diagonalization can hence be described by a single parameter which we call the mixing angle,  $\theta_{\Sigma\Lambda}$ .

The labeling of the three distinct quark flavors ( $abc$ ) in the above agrees with the notation used in previous works [9], but for the purpose of this work it is sometimes advantageous to promote these labels to an explicit functional dependence of the correlation matrix elements on the quark masses and charges,

$$C_{ij}(t) \longrightarrow C_{ij}(t, m_a, m_b, m_c, e_a, e_b, e_c) \quad \text{or} \quad C_{ij}(t, \vec{m}_{abc}, \vec{e}_{abc}), \quad i, j = \Sigma, \Lambda, \quad (4)$$

where  $\vec{m}_{abc} = (m_a, m_b, m_c)$  is used for brevity and similar for the quark electric charges. Note that the ordering of the labels, or explicit dependencies, is important, since the  $\Sigma^0$  operator for example has a symmetry in the first two quark flavors,  $a$  and  $b$  in this case. In our notation this is indicated by the ordering of the labels.

### B. Extrapolation scheme

When we have degeneracy in the first two (distinct) quarks (i.e., degenerate masses and charges, and hence numerically identical propagators), by symmetry the correlation matrix is diagonal. Furthermore, if the third quark is also degenerate [SU(3) symmetry], the correlation matrix is proportional to the identity. In general, the diagonal elements of the correlation matrix are symmetric under an interchange of the first two quarks, while the off-diagonal elements are antisymmetric.

For the case of a degeneracy between either the first and third or second and third quarks (these cases are simply related by the symmetry of the correlation matrix under interchange of the first two quarks) we find by explicit manipulations of the correlation functions that we are able to write

$$C_{\Sigma(ab'a)\Sigma(aba')} = \frac{(3C_{\Lambda(aa'b)\Lambda(aa'b)} + C_{\Sigma(aa'b)\Sigma(aa'b)})}{4}, \quad (5)$$

$$C_{\Lambda(ab'a)\Lambda(aba')} = \frac{(3C_{\Sigma(aa'b)\Sigma(aa'b)} + C_{\Lambda(aa'b)\Lambda(aa'b)})}{4}, \quad (6)$$

$$C_{\Sigma(ab'a)\Lambda(aba')} = \frac{\sqrt{3}}{4} (C_{\Lambda(aa'b)\Lambda(aa'b)} - C_{\Sigma(aa'b)\Sigma(aa'b)}). \quad (7)$$

We have primed the second quark label  $a$  to indicate that its flavor is distinct even though it is degenerate in terms of

mass and charge, while the time dependence is left implicit. All correlation function relations in this subsection are assumed to be at equal times.

The relations given in Eqs. (5)–(7) can also be summarized as

$$\begin{bmatrix} C_{\Sigma(aba')\Sigma(aba')} & C_{\Sigma(aba')\Lambda(aba')} \\ C_{\Lambda(aba')\Sigma(aba')} & C_{\Lambda(aba')\Lambda(aba')} \end{bmatrix} = U[C_{i(aa'b)j(aa'b)}]U^T, \quad (8)$$

where the matrix  $U$  is given by

$$U = \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}. \quad (9)$$

These relations can also be reversed to write

$$C_{\Lambda(aa'b)\Lambda(aa'b)} = \frac{(3C_{\Sigma(aba')\Sigma(aba')} - C_{\Lambda(aba')\Lambda(aba')})}{2}, \quad (10)$$

$$C_{\Sigma(aa'b)\Sigma(aa'b)} = \frac{(3C_{\Lambda(aba')\Lambda(aba')} - C_{\Sigma(aba')\Sigma(aba')})}{2}. \quad (11)$$

If for example we associate the degenerate  $a$  and  $a'$  quarks with the up (down) quarks, and the  $b$  quark with the strange, then Eqs. (5)–(7) give the U-spin (V-spin) correlators in terms of the isospin correlators.

In order to construct an SU(3)-flavor breaking expansion in terms of quark masses and charges, we begin by supposing that we have three distinct quark flavors with no electric charge and degenerate mass  $m_0$ . We then give the quarks small charges,  $\epsilon Q_i$ , proportional to the  $uds$  physical charges,  $Q_i$ , but scaled by the small parameter  $\epsilon$  (so as to keep their ratios physical). Since the down and strange quarks are still degenerate (same charge), if we take the ordering of isospin ( $uds$  here; however  $dus$  is also isospin), the first-order Taylor expansion in the quark charge parameter gives

$$\begin{aligned} C(\vec{m}_{uds,0}, \epsilon \vec{Q}_{uds}) &= C(\vec{m}_{uds,0}, 0) + \frac{S}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \epsilon \\ &+ \frac{D_{\text{QED}}}{4} \begin{bmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{bmatrix} \epsilon, \end{aligned} \quad (12)$$

where  $\vec{m}_{uds,0} = (m_0, m_0, m_0)$  and

$$S = \left( \frac{\partial C_{\Sigma\Sigma}(\vec{m}_{dsu,0}, \epsilon \vec{Q}_{dsu})}{\partial \epsilon} + \frac{\partial C_{\Lambda\Lambda}(\vec{m}_{dsu,0}, \epsilon \vec{Q}_{dsu})}{\partial \epsilon} \right) \Big|_{\epsilon=0} \quad (13)$$

$$D_{\text{QED}} = \left( \frac{\partial C_{\Sigma\Sigma}(\vec{m}_{dsu,0}, \epsilon \vec{Q}_{dsu})}{\partial \epsilon} - \frac{\partial C_{\Lambda\Lambda}(\vec{m}_{dsu,0}, \epsilon \vec{Q}_{dsu})}{\partial \epsilon} \right) \Big|_{\epsilon=0}. \quad (14)$$

This form follows from realizing that with constant and equal mass parameters for the three quarks, the correlation matrix elements obey the relations in Eqs. (5)–(7) for all values of  $\epsilon$ , and hence the first derivatives of each isospin element can be written in terms of the diagonal U-spin elements.

Since the term  $C(m_{i,0}, 0)$  is proportional to the identity and has no effect on the eigenvectors, we make the definition

$$C(\vec{m}_{uds,0}, 0) + \frac{S}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \epsilon \equiv A\mathbb{I}_2, \quad (15)$$

and also absorb a factor of  $\epsilon$  into  $D_{\text{QED}}$ :  $D_{\text{QED}} \rightarrow \epsilon D_{\text{QED}}$ . We have now, to first order, described the breaking of SU(3) symmetry down to SU(2) U-spin symmetry in the  $\Sigma^0$ – $\Lambda^0$  correlation matrix by introducing electromagnetism. Next we seek to break the remaining SU(2) symmetry by expanding the correlation matrix in powers of  $\delta m_i = m_i - m_0$ , the deviations in the masses from the SU(3) symmetric point (QED aside) where all three flavors of quark have mass  $m_i = m_0$ . To do this we make use of Eqs. (5)–(7) to notice that, for example,

$$\frac{\partial C_{ij}(\vec{m}_{uds}, 0)}{\partial m_d} \Big|_{(\vec{m}_{uds}, 0)} = U_{ik} \frac{\partial C_{kl}(\vec{m}_{uds}, 0)}{\partial m_s} \Big|_{(\vec{m}_{uds}, 0)} U_{lj}^T, \quad (16)$$

for the matrix  $U$  from Eq. (9). We find that if we also enforce the constraint that the average quark mass is held fixed as we move away from the SU(3) symmetric point [13],

$$\bar{m} \equiv \frac{1}{3}(m_u + m_d + m_s) = m_0 \quad (17)$$

$$\Rightarrow \delta m_u + \delta m_d + \delta m_s = 0 \quad (18)$$

$$\text{for } \delta m_i = m_i - \bar{m}, \quad (19)$$

then the first-order expansion in the masses reduces to (see the Appendix for a more detailed calculation)

$$\begin{aligned} C(\vec{m}_{uds}, \epsilon \vec{Q}_{uds}) &= A\mathbb{I}_2 + \frac{D_{\text{QED}}}{4} \begin{bmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{bmatrix} \\ &+ \frac{D_{\text{QCD}}}{4} \begin{bmatrix} -3(\delta m_u + \delta m_d) & \sqrt{3}(\delta m_u - \delta m_d) \\ \sqrt{3}(\delta m_u - \delta m_d) & 3(\delta m_u + \delta m_d) \end{bmatrix}, \end{aligned} \quad (20)$$

where

$$D_{\text{QCD}} = \left( \frac{\partial C_{\Sigma\Sigma}(\vec{m}_{uds}, 0)}{\partial m_s} - \frac{\partial C_{\Lambda\Lambda}(\vec{m}_{uds}, 0)}{\partial m_s} \right) \Big|_{\vec{m}_{uds,0}}. \quad (21)$$

This first-order expression is diagonalized to yield

$$\tan 2\theta_{\Sigma\Lambda, \text{isospin}} = -\sqrt{3} \left( \frac{D_{\text{QCD}}(\delta m_u - \delta m_d) + D_{\text{QED}}}{3D_{\text{QCD}}(\delta m_u + \delta m_d) + D_{\text{QED}}} \right). \quad (22)$$

Repeating this process with the starting point of U- and V-spin correlation matrices gives

$$\tan 2\theta_{\Sigma\Lambda, \text{V-spin}} = \sqrt{3} \left( \frac{D_{\text{QCD}}(\delta m_u - \delta m_s) + D_{\text{QED}}}{3D_{\text{QCD}}(\delta m_u + \delta m_s) + D_{\text{QED}}} \right), \quad (23)$$

$$\tan 2\theta_{\Sigma\Lambda, \text{U-spin}} = \frac{\sqrt{3}D_{\text{QCD}}(\delta m_d - \delta m_s)}{3D_{\text{QCD}}(\delta m_d + \delta m_s) + 4D_{\text{QED}}^{\text{U-spin}}}, \quad (24)$$

where  $D_{\text{QED}}^{\text{U-spin}}$  parallels  $D_{\text{QED}}$  but with derivatives of correlation functions of definite isospin instead of U spin.

Notice that if we set  $D_{\text{QED}} = 0$ , the parameter  $D_{\text{QCD}}$  cancels and the isospin expression reduces to exactly that presented in leading order (LO)  $\chi$ PT [8], as well as the leading order term presented in our previous work [9] based on a more group-theoretic approach. It is interesting to note that the method used in [9] was to diagonalize the octet mass matrix to find the mixing angle before expanding the  $\Sigma^0/\Lambda^0$  masses in terms of quark masses, while we have herein expanded the correlation matrix in terms of quark masses and then diagonalized.

At this point it is necessary for us to recall that our parameters  $D_i$  still carry an implicit time dependence, and unlike in the QCD-only limit, for full QCD + QED our mixing angle depends explicitly on these parameters. We can take the usual route of diagonalizing at large times in our lattice simulations where the ground state dominates the signal. As we see in the results of Sec. IV, the time dependence of the mixing angle appears to be much weaker than that of the effective masses of the baryons themselves.

### C. Running quark masses

Since we are operating with QED, we must also consider that variation in the input bare quark masses will no longer result in the same mass differences for quarks of different charges, due to renormalization. This leads us to include one further parameter in our fit function, which comes from taking

$$\begin{aligned} & \delta m_u + \delta m_d + \delta m_s \\ & = 0 \rightarrow \frac{1}{Z_{2/3}} \delta m_u + \frac{1}{Z_{-1/3}} (\delta m_d + \delta m_s) = 0, \end{aligned} \quad (25)$$

where the  $Z_i$  factors correct for the running of the masses due to QED, specifically to account for the resultant difference in the  $u$  and  $d/s$  quark propagators from an equal change in their respective quark mass parameters, analogous to the Dashen scheme presented in [14].

Upon updating our fit functions and making the definitions

$$D_{\text{QED}} \rightarrow Z_{2/3} D_{\text{QED}} \quad \text{and} \quad Z \equiv \frac{Z_{2/3}}{Z_{-1/3}}, \quad (26)$$

we are left with

$$\tan 2\theta_{\Sigma\Lambda, \text{isospin}} = \sqrt{3} \left( \frac{(\delta m_u - Z\delta m_d) + D_{\text{QED}}/D_{\text{QCD}}}{3(\delta m_u + Z\delta m_d) + D_{\text{QED}}/D_{\text{QCD}}} \right), \quad (27)$$

and similar for V spin, while for U spin no extra factor is needed explicitly, although in keeping with the formalism a factor  $Z_{-1/3}$  can be thought to have been absorbed by  $D_{\text{QED}}^{\text{U-spin}}$ .

In practice, the mixing angle can be determined on the lattice by numerical diagonalization of the correlation matrix. By performing calculations at a range of quark mass parameters and constant electric charge parameters we are able to fit the parameters  $D_{\text{QED}}/D_{\text{QCD}}$  and  $Z$ . Assuming the functional form of Eq. (27) we are able to use these parameters to extrapolate to the physical point—the details for which are given in the following sections.

Finally, considering terms beyond leading order, we can incorporate some higher order terms by replacing

$$D_{\text{QED}} \rightarrow \left[ \sum_{n=0}^{\infty} \frac{1}{(n+1)!} \left( \epsilon \frac{\partial}{\partial \epsilon} \right)^n \right] D_{\text{QED}}, \quad (28)$$

and absorbing all higher order QED terms (however not mixed QED-QCD terms) into the existing parameter without changing our established functional form. This is possible because we do not wish to vary  $\epsilon$  in our extrapolation to the physical point, and the correlation matrix exhibits U-spin symmetry for all values of  $\epsilon$ . We can therefore think of our parametrization as including all orders of pure-QED terms automatically, in theory. In practice however, as is discussed in Sec. IV, we scale our QED parameter linearly to match the physical electromagnetic coupling and hence negate the inclusion of these higher order terms in the present study.

We have found that at second order in the quark masses two additional parameters must appear in the correlation

matrix expansion, and further parameters for mixed QCD-QED terms. Given the relatively few number of lattice ensembles available in the current analysis we therefore forgo inclusion of higher order QCD terms.

### III. LATTICE SCHEME

We extract the  $\Sigma^0$ - $\Lambda^0$  mixing angles from a combination of  $24^3 \times 48$  and  $48^3 \times 96$ ,  $N_f = 1 + 1 + 1$ , dynamical QCD + QED lattice simulations around the U-spin symmetric point [approximate SU(3)-symmetric point] defined in [14]. The gauge actions used are the tree-level Symanzik improved SU(3) gauge action and the noncompact U(1) QED gauge action (further details in [14,15]). The fermions are described by an  $\mathcal{O}(a)$ -improved stout link nonperturbative clover (SLiNC) action [16]. The couplings used and lattice spacing are

$$\beta_{\text{QCD}} = 5.5, \quad \beta_{\text{QED}} = 0.8, \quad a^{-1}/\text{GeV} = 2.91(3), \quad (29)$$

which gives a QED coupling  $\alpha_{\text{QED}} \simeq 0.1$ , roughly  $10\times$  larger than the physical value.

We presently neglect electromagnetic modifications to the clover term. This leaves us with corrections of  $\mathcal{O}(\alpha_{\text{QED}}e^2a)$ , which turn out to be no larger than the  $\mathcal{O}(a^2)$  corrections from QCD (see [17] for numerical evidence of this). Adding an electromagnetic clover term with  $c_{em} = 1$  would leave us with corrections of  $\mathcal{O}(\alpha_{\text{QED}}e^2g^2a)$  (to this order in  $\alpha_{\text{QED}}$ ), which is not a significant improvement, if at all. Furthermore, since the current manuscript is concerned with isospin-breaking effects, these discretization effects are further suppressed by a power of  $m_d - m_u$  for QCD effects and  $e_u^2 - e_d^2$  for QED effects.

The lattice ensembles used for this study have been selected to focus on the region near an approximate

SU(3)-flavor symmetry. Given the difference in charges, this symmetry cannot be exact, and our approach is to tune the neutral (connected) pseudoscalar mesons to be degenerate (see [14]). Starting from this point, the approximate symmetry is further broken along a trajectory that leaves no residual invariant (or approximate invariant) SU(2) subgroup. In particular, we introduce a breaking  $m_u - m_s$ , while holding fixed both  $m_d$  and the average quark mass. In this way we preserve the physical mass hierarchy,  $m_u < m_d < m_s$ . To further improve the constraint on our expansion parameters we also consider partially quenched (PQ) propagators, where the valence masses are allowed to vary independently of the simulated sea quarks. The simulation parameters used in this study are listed in Table I.

### IV. RESULTS

From the expressions presented in Eqs. (22)–(24), in the absence of QED, it is clear that the mixing angle depends only on the relative quark mass splitting at first order,

$$\tan 2\theta_{\Sigma\Lambda, \text{isospin, QCD-only}} = \frac{\delta m_d - \delta m_u}{\sqrt{3}(\delta m_u + \delta m_d)}, \quad (30)$$

provided that the average quark mass  $\bar{m}$  is held constant. As a consequence, given a set of quark mass parameters, we can directly predict the QCD-only mixing angle.

In a recent QCD-only lattice study of the  $\Sigma^0$ - $\Lambda^0$  mixing [9], the quark masses at the physical point were determined to be

$$a\delta m_u = -0.01140(3), \quad a\delta m_d = -0.01067(3), \quad (31)$$

giving

TABLE I. The lattice volumes,  $\kappa$  values used in the generation of the lattice configurations, valence  $\kappa$  values of the hadron operators and the fitted isospin mixing angles. Physical electric charges were associated with the  $\kappa$ 's for each flavor of quark (although the coupling is nonphysical; see Sec. IV) and we also present the lightest neutral flavor-singlet meson  $M_{u\bar{u}}$  on each ensemble for reference. The mixing angle result for the first ensemble follows theoretically from Eqs. (5)–(7).

Volume	Lattice ensembles						$\theta_{\Sigma\Lambda, \text{isospin}}$	$M_{u\bar{u}}$ (MeV)
	$\kappa_u, \kappa_d, \kappa_s$	(sea)		$\kappa_u, \kappa_d, \kappa_s$	(valence)			
$24^3 \times 48$	0.124362	0.121713	0.121713	0.124362	0.121713	0.121713	$-30^\circ$ (theory)	442(9)
$24^3 \times 48$	0.124374	0.121713	0.121701	0.124374	0.121713	0.121701	$-21.8(1.1)^\circ$	423(9)
				0.124387	0.121713	0.121689	$-19.5(1.2)^\circ$	423(10)
				0.124400	0.121740	0.121649	$-6(1)^\circ$	378(28)
$24^3 \times 48$	0.124400	0.121713	0.121677	0.124400	0.121713	0.121677	$-17.8(7)^\circ$	405(8)
				0.124420	0.121713	0.121657	$-16.7(7)^\circ$	387(8)
				0.124430	0.121760	0.121601	$-4.8(7)^\circ$	377(8)
$48^3 \times 96$	0.124508	0.121821	0.121466	0.124508	0.121821	0.121466	$-3.5(4)^\circ$	284(4)
				0.124400	0.121713	0.121677	$-18.5(9)^\circ$	389(5)

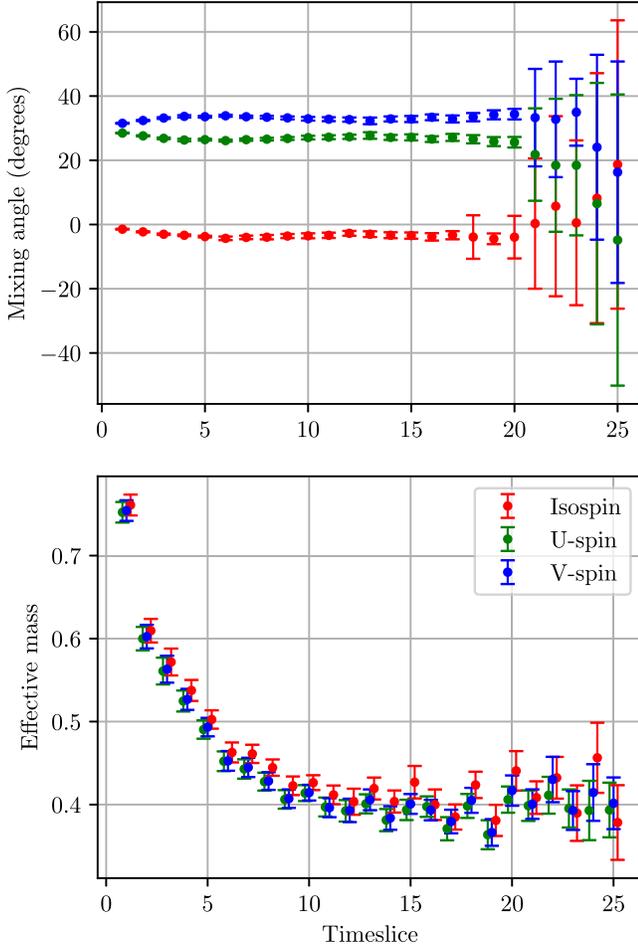


FIG. 1. An example of the mixing angle from diagonalization and corresponding effective mass, in this case on the largest-volume lattice used (unitary). The effective mass shows the  $\Sigma^0$ - $\Sigma^0$  component of the correlation matrix for each SU(2)-subgroup with a slight offset in time applied for clarity.

$$\Rightarrow \theta_{\Sigma\Lambda, \text{isospin, QCD-only}} = -0.55(3)^\circ. \quad (32)$$

Note that we are using a sign convention that followed from our choice of ordering for isospin ( $uds$  vs  $dus$ ) as well as the ordering of the  $\Sigma^0$  and  $\Lambda^0$  along the diagonal of the correlation matrix, and differs from that used in [9].

We also note that using the mass ratios of the latest FLAG review [18], the QCD-only mixing angle is predicted to be  $\theta_{\Sigma\Lambda, \text{isospin, QCD-only}} = -0.65(3)^\circ$ .

In the present work we directly determine the lattice mixing angle for each of the QCD + QED ensembles listed in Table I. This is done by calculating all four elements of the  $\Sigma^0$ - $\Lambda^0$  correlation matrix [Eq. (3)] on an ensemble, for each site in the time dimension of the lattice, and numerically diagonalizing the matrix  $C(t)$ . A constant is fitted to the observed plateau region. We perform this direct diagonalization in favor of the more typical generalized eigenvalue problem (GEVP, first introduced in [19]) as it is more

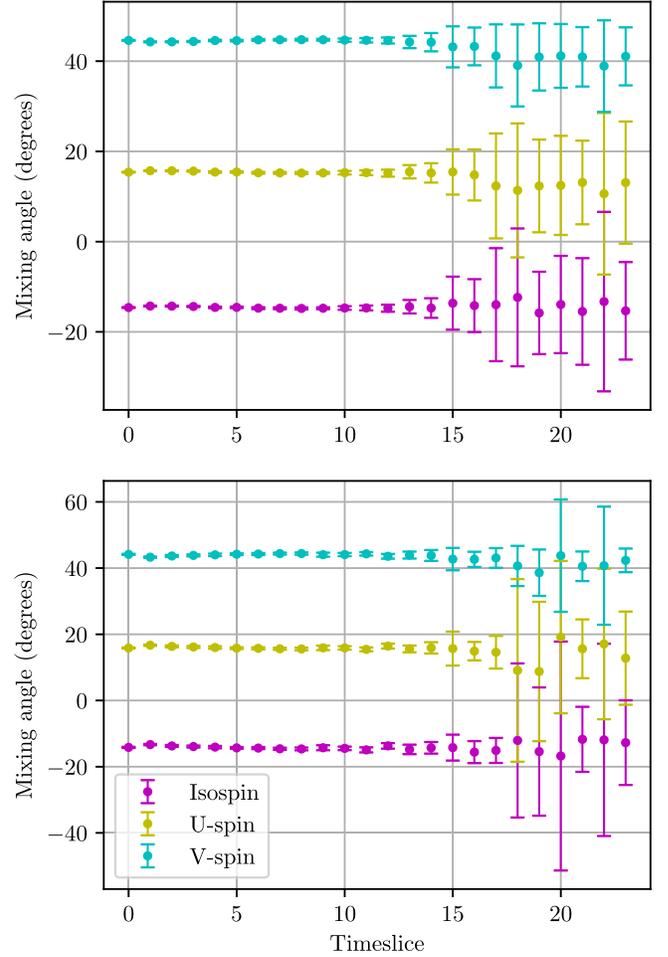


FIG. 2. This figure shows the T-, U- and V-spin mixing angles for the two PQ calculations we performed with the constituent quark charges set to 0. The top plot has  $(\kappa_u, \kappa_d, \kappa_s) = (0.12092, 0.1209, 0.12088)$  and the bottom plot has  $(\kappa_u, \kappa_d, \kappa_s) = (0.12094, 0.1209, 0.12086)$ . The QCD-only mixing angle formula we have derived predicts that the mixing angles are time independent at first order when QED is absent.

consistent with our extrapolation formalism, and the advantages of the GEVP are in extracting eigenvalues of  $C(t)$ , while we are herein only interested in the eigenvectors.

Upon including QED, the resulting mixing angles are displayed in Table I. These results are used to fit Eq. (27).

It is a feature of our method for determining the mixing angle that we avoid fitting effective masses and instead fit the mixing angle directly. As it can be seen in Fig. 1, the signal quality and ability to resolve the T-, U- and V-spin signals is much greater for the mixing angle, since it generally exhibits a much weaker time dependence than the effective masses of the baryons themselves. Theoretically, we have shown that when QED is absent there is no time dependence in the mixing angle at first order, while this is no longer true for QCD + QED mixing, but as the QCD contribution to the mixing angle is much larger than the contribution of QED for most of our mass splittings, the mixing angle appears roughly time independent.

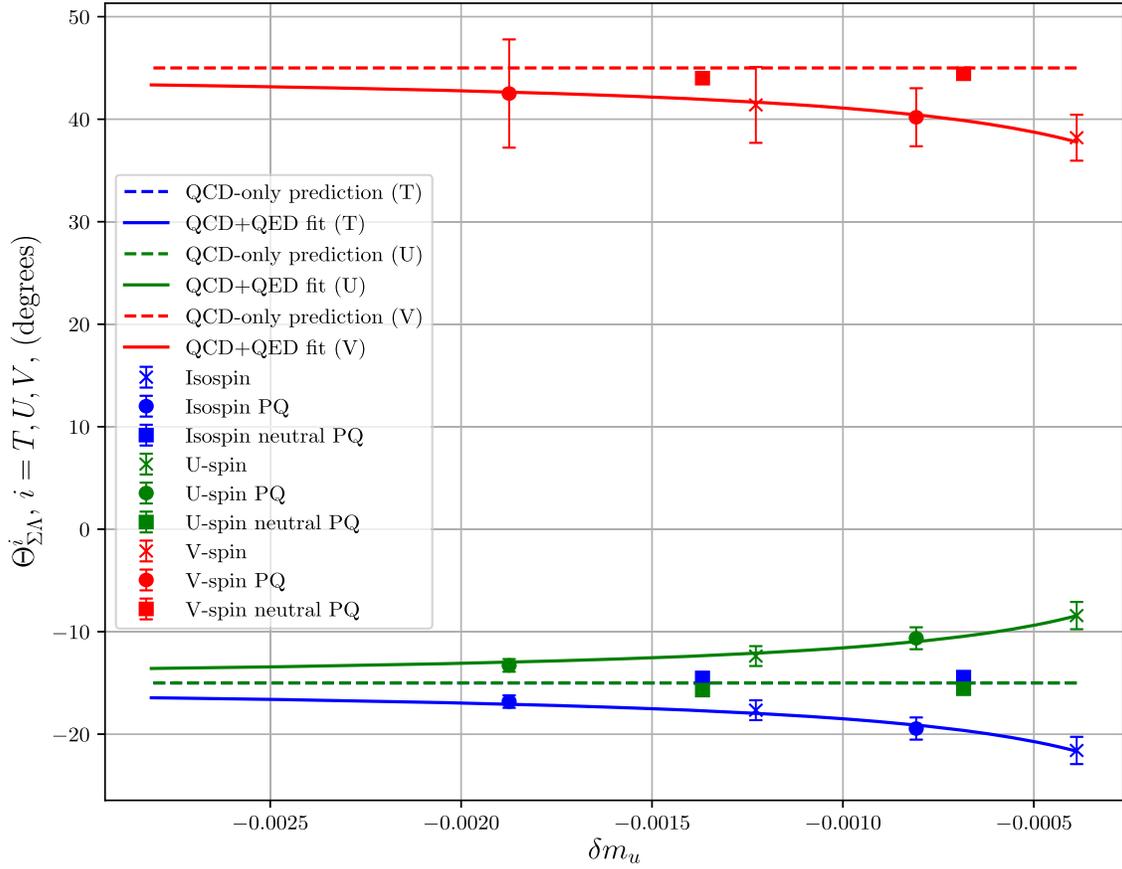


FIG. 3. This plot shows our simulation results for the mixing angles at the quark  $\kappa$  values with  $\delta m_d = 0$ . In this scenario the QCD-only mixing angle is a constant (dotted lines) and we can see the QED-inclusive mixing angle asymptoting to that of only QCD as the T-, U- or V-spin symmetry becomes more broken by the mass parameters. The squares are mixing results from PQ calculations performed with all charges set to 0 to approximate the QCD-only scenario while the circles are PQ with physical charges (unphysical coupling; see Sec. III) and the crosses are unitary.

We have performed mixing angle calculations at two additional partially quenched points with the up, down and strange quark electric charges set to 0 which are presented in Fig. 2, where we see our first-order prediction of time independence of the QCD-only mixing angle (for constant  $\bar{m}$ ) to be manifest.

In Fig. 3 we show a comparison of the QCD-only and QCD + QED mixing angle fit functions [Eqs. (22)–(24) with  $D_{\text{QED}} \equiv 0$  for QCD-only mixing] for lattice simulations with  $\delta m_d = 0$ , for which the QCD-only mixing angle function is constant. In addition to the relevant points from Table I, we have included the two neutral partially quenched diagonalizations of Fig. 2, which can be seen to agree well with the theoretical prediction of QCD-only mixing.

It can be seen in Fig. 3 and from Eqs. (22)–(24) that in the absence of QED ( $D_{\text{QED}} \rightarrow 0$ ), the differences between any two of the mixing angles is a constant (magnitude  $\pi/3$  or  $\pi/6$ ), while with QED instated, only the isospin-V difference remains constant. This is because the isospin and V-spin doublets have the same combination of charges. Another feature of Fig. 3 is that as we move to the left, and

the SU(3)-flavor symmetry becomes more broken, the mixing angle for QCD + QED is asymptoting to that of QCD only, which is a result of the bare quark mass differences becoming dominant in their mixing contribution over the electric charge differences (which do not change).

As can be observed from Table I, we have determined the mixing angle on both  $24^3 \times 48$  and  $48^3 \times 96$  volumes. The mixing angles on the larger volume are consistent with the  $24^3 \times 48$  result and hence we do not attempt to correct for finite-volume effects in this work. We have investigated the results of excluding the  $48^3 \times 96$  result from our fits but given the small number of total simulations, it has proven to reduce the uncertainty by about 25% to include it, despite the possibility of finite-volume differences.

To extrapolate our result to the physical point, we use the physical quark mass parameters determined in [14],

$$a\delta m_u = -0.00834(8), \quad a\delta m_d = -0.00776(7),$$

and

TABLE II. The best-fit parameter values ( $\chi^2/\text{DOF} = 0.84$ ) from the fit of the QCD + QED isospin mixing angles with  $D_{\text{QED}}$  scaled to the physical EM coupling. The correlation coefficient for the two parameters is  $-0.45$ .

Fit parameters		
Parameter	$D_{\text{QED}}/D_{\text{QCD}}$	$Z$
Central value	$-3.8(7) \times 10^{-5}$	0.96(4)

$$a\delta m_u = -0.00791(4), \quad a\delta m_d = -0.00740(4),$$

using  $32^3 \times 64$  and  $48^3 \times 96$  volume lattices, respectively. No  $24^3 \times 48$  physical point is available; however our mixing angles seem consistent between  $24^3 \times 48$  and  $48^3 \times 96$  volumes within uncertainty, and it is interesting to observe the variation in the result due to systematic differences. Using the best-fit parameters displayed in Table II, where the parameter  $D_{\text{QED}}$  has been scaled down by the proportionality factor  $\alpha_{\text{QED}}^*/\alpha_{\text{QED}} = 0.07338$  that relates our simulated EM coupling  $\alpha_{\text{QED}}$  to that of the real world,  $\alpha_{\text{QED}}^*$ , we find

$$\theta_{\Sigma\Lambda, \text{isospin}}|_{\text{QCD+QED}} = -1.00(32)^\circ,$$

and

$$\theta_{\Sigma\Lambda, \text{isospin}}|_{\text{QCD+QED}} = -0.96(31)^\circ,$$

for the physical quark masses determined on  $32^3 \times 64$  and  $48^3 \times 96$  volumes, respectively. These first-order results compare well with the widely used DvH formula result [5,20],  $-0.86(6)^\circ$ , which also incorporates QED effects implicitly, in the sense that it cannot separate QCD from QED effects on the mixing angle.

While a direct confirmation of the validity of the assumed linear-in- $\alpha_{\text{QED}}$  scaling of the QED parameter has not yet been performed, it was shown in [16] that  $1/\kappa_q^c$ ,  $1/\bar{\kappa}_q$  and the bare quark mass at the symmetric point,  $1/2\bar{\kappa}_q - 1/2\kappa_q^c$ , all displayed linear behavior with scaling of the quark charge squared.

We note that our renormalization parameter  $Z$  is consistent with that presented in [14] of 0.93 using the Dashen scheme, which is defined by the running of connected neutral pseudoscalar meson masses. As was found in [9], the magnitude of the next-to-leading order QCD term was roughly one third that of the LO QCD term, and hence we approximate the contributions from higher order QCD terms as a systematic uncertainty of 20%. The effects of higher order QED terms remain to be investigated.

## V. CONCLUSION

In this work we have used the symmetry properties of the pure baryon-octet wave functions (and hence, interpolating operators) to simplify an expansion in QCD and QED parameters about the SU(3)-symmetric point, and consequently derived a scheme for extrapolating the  $\Sigma^0-\Lambda^0$  mixing angle to the physical point along a path where the average quark mass is held constant.

We have observed that our extrapolation scheme accommodates past determinations of the mixing angle in the cases of both QCD-only mixing and physical QCD + QED mixing, and offers new insight into the interplay between QCD and QED effects on the mixing. We find that the QED contribution to the mixing angle at first order is of comparable magnitude to that of the quark mass differences and acts to effectively double the mixing.

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## APPENDIX: EXPLICIT CALCULATION OF QCD TERM

We present here a more detailed derivation of the QCD term in Eq. (20) and note that the QED term is derived in an analogous manner. The starting point is the Taylor expansion in quark masses about the nominated SU(3)-symmetric point,  $m_i = \bar{m}$ . In the following we ignore the correlation matrix dependence on the electric charges of the quarks, since they are identically set to 0 throughout. We find, dropping  $\mathcal{O}(\delta m^2)$  terms,

$$\begin{aligned}
C_{ij}(\vec{m}_{uds}) &\simeq C_{ij}(\vec{m}_{uds,0}) + \left( \frac{\partial C_{ij}(\vec{m}_{uds})}{\partial m_u} \Big|_{\vec{m}_{uds,0}} \right) \delta m_u + \left( \frac{\partial C_{ij}(\vec{m}_{uds})}{\partial m_d} \Big|_{\vec{m}_{uds,0}} \right) \delta m_d + \left( \frac{\partial C_{ij}(\vec{m}_{uds})}{\partial m_s} \Big|_{\vec{m}_{uds,0}} \right) \delta m_s \\
&= C_{ij}(\vec{m}_{uds,0}) + \left( U_{ik}^T \frac{\partial C_{kl}(\vec{m}_{uds})}{\partial m_s} \Big|_{\vec{m}_{uds,0}} U_{lj} \right) \delta m_u + \left( U_{ik} \frac{\partial C_{kl}(\vec{m}_{uds})}{\partial m_s} \Big|_{\vec{m}_{uds,0}} U_{lj}^T \right) \delta m_d + \left( \frac{\partial C_{ij}(\vec{m}_{uds})}{\partial m_s} \Big|_{\vec{m}_{uds,0}} \right) \delta m_s,
\end{aligned}$$

or written as a matrix equation,

$$\left[ \begin{array}{c} C_{\Sigma\Sigma}(\vec{m}_{uds,0}) + \frac{3}{4} \frac{\partial C_{\Lambda\Lambda}(\vec{m}_{uds})}{\partial m_s} \Big|_{\vec{m}_{uds,0}} (\delta m_u + \delta m_d) + \frac{\partial C_{\Sigma\Sigma}(\vec{m}_{uds})}{\partial m_s} \Big|_{\vec{m}_{uds,0}} \left( \frac{1}{4} \delta m_u + \frac{1}{4} \delta m_d + \delta m_s \right) \\ \frac{\sqrt{3}}{4} \left( \frac{\partial C_{\Sigma\Sigma}(\vec{m}_{uds})}{\partial m_s} - \frac{\partial C_{\Lambda\Lambda}(\vec{m}_{uds})}{\partial m_s} \right) \Big|_{\vec{m}_{uds,0}} (\delta m_u - \delta m_d) \\ \frac{\sqrt{3}}{4} \left( \frac{\partial C_{\Sigma\Sigma}(\vec{m}_{uds})}{\partial m_s} - \frac{\partial C_{\Lambda\Lambda}(\vec{m}_{uds})}{\partial m_s} \right) \Big|_{\vec{m}_{uds,0}} (\delta m_u - \delta m_d) \\ C_{\Sigma\Sigma}(\vec{m}_{uds,0}) + \frac{3}{4} \frac{\partial C_{\Sigma\Sigma}(\vec{m}_{uds})}{\partial m_s} \Big|_{\vec{m}_{uds,0}} (\delta m_u + \delta m_d) + \frac{\partial C_{\Lambda\Lambda}(\vec{m}_{uds})}{\partial m_s} \Big|_{\vec{m}_{uds,0}} \left( \frac{1}{4} \delta m_u + \frac{1}{4} \delta m_d + \delta m_s \right) \end{array} \right],$$

and this, upon making the constant- $\vec{m}$  substitution  $\delta m_s = -\delta m_u - \delta m_d$ , reduces to

$$C(\vec{m}_{uds}) \simeq C(\vec{m}_{uds,0}) + \frac{1}{4} \left[ \begin{array}{cc} -3(\delta m_u + \delta m_d) & \sqrt{3}(\delta m_u - \delta m_d) \\ \sqrt{3}(\delta m_u - \delta m_d) & 3(\delta m_u + \delta m_d) \end{array} \right] \left( \frac{\partial C_{\Sigma\Sigma}(\vec{m}_{uds})}{\partial m_s} - \frac{\partial C_{\Lambda\Lambda}(\vec{m}_{uds})}{\partial m_s} \right) \Big|_{\vec{m}_{uds,0}},$$

and we can now see the connection to Eq. (20), with the term in parentheses being the previously defined  $D_{\text{QCD}}$ . The above expression can be directly diagonalized to yield the QCD-only mixing formula familiar from  $\chi\text{PT}$  (for constant  $\vec{m}$ ) and the matching first-order term presented in [9]. Furthermore we can make the connection to our previous work that for the expansion parameter  $A_2$  in [9], at large times we must have  $D_{\text{QCD}}(t) = 2A_2$ .

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