Neutral kaon mixing from new physics: Matrix elements in $N_f = 2 + 1$ lattice QCD

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We present results for matrix elements of $\Delta S = 2$ four-fermion operators arising generically in models of new physics. These are needed to constrain such models using the measured values of ε_K and ΔM_K . We use lattice QCD with 2 + 1 flavors of improved staggered fermions on lattices generated by the MILC Collaboration. We extrapolate to the continuum from three lattice spacings ranging down to $a \approx 0.045$ fm. Total errors are ~5%-6%, arising primarily from our use of one-loop matching between lattice and continuum operators. For two of the matrix elements, our results disagree significantly from those obtained using different fermion discretizations.

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Processes that are highly suppressed in the standard model (SM) provide a window into beyond-the-standard model (BSM) physics complementary to that from direct searches. Indeed, in a given model, such processes can set lower limits on the scale of BSM physics which are beyond the reach of present accelerators (see, e.g., Refs. [1-3]). Here we focus on kaon mixing, which provides some of the most powerful constraints. For both the CP-conserving mass difference ΔM_K and the *CP*-violating part parametrized by ε_K , the sum of contributions from SM and BSM physics must add to the observed values. BSM contributions involve heavy particles and are thus short-distance dominated. In order to determine the contributions in a given model, one needs to calculate, in OCD, the matrix elements of local $\Delta S = 2$ four-fermion operators. A generic BSM model introduces four operators (listed below) having Dirac structures different from those that arise in the SM. Lattice QCD is the only available quantitative tool for calculating such matrix elements from first principles, and we present here such a calculation.

In a generic BSM model (be it supersymmetry, extra dimensions, little Higgs, etc.) $\Delta S = 2$ processes involve loops of heavy particles, that, when integrated out, lead to the effective Hamiltonian

$$H_{\Delta S=2}^{\text{BSM}} = \sum_{i} C_i(\mu) Q_i, \qquad (1)$$

$$Q_{1} = [\bar{s}^{a} \gamma_{\mu} (1 - \gamma_{5}) d^{a}] [\bar{s}^{b} \gamma_{\mu} (1 - \gamma_{5}) d^{b}], \qquad (2)$$

$$Q_2 = [\bar{s}^a (1 - \gamma_5) d^a] [\bar{s}^b (1 - \gamma_5) d^b], \qquad (3)$$

$$Q_3 = [\bar{s}^a \sigma_{\mu\nu} (1 - \gamma_5) d^a] [\bar{s}^b \sigma_{\mu\nu} (1 - \gamma_5) d^b], \quad (4)$$

$$Q_4 = [\bar{s}^a (1 - \gamma_5) d^a] [\bar{s}^b (1 + \gamma_5) d^b], \tag{5}$$

$$Q_5 = [\bar{s}^a \gamma_\mu (1 - \gamma_5) d^a] [\bar{s}^b \gamma_\mu (1 + \gamma_5) d^b].$$
(6)

Here C_i are Wilson coefficients that can be calculated in a given theory (with μ the renormalization scale); *a*, *b* are color indices; $\sigma_{\mu\nu} = [\gamma_{\mu}, \gamma_{\nu}]/2$; and repeated indices are summed. The local $\Delta S = 2$ operators Q_i are in the chiral basis of Ref. [4].¹ Q_1 is the "left-left" operator arising in the SM contribution to ε_K , while Q_{2-5} are the BSM operators. In previous lattice calculations, a different basis (the "SUSY basis") for the operators has been used. We prefer the chiral basis as it has been used to calculate the two-loop anomalous dimensions which we use to run the results between different renormalization scales [4]. Results can be easily converted to the SUSY basis at the end—see below.

In our lattice setup (described below) we obtain directly ratios of matrix elements. Specifically, we calculate the following B parameters for the BSM operators:

$$B_{i}(\mu) = \frac{\langle \bar{K}_{0} | Q_{i}(\mu) | K_{0} \rangle}{N_{i} \langle \bar{K}_{0} | \bar{s} \gamma_{5} d(\mu) | 0 \rangle \langle 0 | \bar{s} \gamma_{5} d(\mu) | K_{0} \rangle}$$
(7)

$$(N_2, N_3, N_4, N_5) = (5/3, 4, -2, 4/3).$$
 (8)

The operators in both numerator and denominator are renormalized in the \overline{MS} scheme using naive dimensional

¹Our normalization differs from Ref. [4], but this has no impact on the associated B parameters.

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regularization for γ_5 and other conventions described in Ref. [4]. The matrix elements of Q_i can be obtained from the *B* parameters since the denominators can be expressed in terms of known quantities $(M_K, f_K, m_s + m_d)$.² We also calculate B_K .

There have been two previous calculations of the BSM matrix elements using dynamical quarks, one using domain-wall fermions [5] and the other twisted-mass fermions [6].³ The former uses the physical complement of 2 + 1 light sea quarks, but has results only at a single lattice spacing. The latter uses 2 dynamical flavors, with the strange quark being quenched. Our calculation uses 2 + 1 flavors of dynamical staggered quarks, with multiple lattice spacings. It is thus the first to control all sources of error. We have previously used similar methodology to calculate B_K [11], with results that are consistent with those from other types of fermion.

An important advantage of staggered fermions is that they are computationally cheap, allowing calculations at multiple lattice spacings, quark masses and volumes.⁴ Their main disadvantage is that each flavor comes in four copies ("tastes"), with the associated SU(4) symmetry broken at nonzero lattice spacing *a*. Removing the extra tastes requires rooting the fermion determinant, but we assume that the artifacts this introduces vanish in the continuum limit $a \rightarrow 0$.

We use ensembles generated with the improved "asqtad" staggered action by the MILC Collaboration [12]. Those used here are listed in Table I, with m_{ℓ} the average up/down sea-quark mass and m_s the strange sea-quark mass (which lies close to the physical value on all ensembles). For valence quarks, we use HYP-smeared staggered fermions [13]. These are known to substantially reduce both artifacts due to taste symmetry breaking and perturbative corrections to matching factors [13,14].

Our mixed action setup is identical to that we used previously to calculate B_K , and the detailed lattice methodology is also very similar [11,15]. On each lattice, we place two wall sources separated by a fixed interval Δt . These create kaons having taste ξ_5 and zero spatial momenta. Lattice versions of the BSM operators are placed between the two wall sources, as are the pseudoscalar operators needed for the denominators of the B_i [see Eq. (7)]. We choose Δt such that the contamination from excited states and from kaons "propagating around the

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TABLE I. MILC ensembles used in this work, with "ens" the number of gauge configurations and "meas" the number of measurements per configuration. ID identifies the ensemble, with F = fine, S = superfine and U = ultrafine.

| a (fm) | am_{ℓ}/am_s | Size | $Ens \times meas$ | ID |
|--------|------------------|---------------------|-------------------|------------|
| 0.09 | 0.0062/0.031 | $28^3 \times 96$ | 995×9 | F1 |
| 0.09 | 0.0093/0.031 | $28^{3} \times 96$ | 949 	imes 9 | F2 |
| 0.09 | 0.0031/0.031 | $40^{3} \times 96$ | 959 	imes 9 | F3 |
| 0.09 | 0.0124/0.031 | $28^{3} \times 96$ | 1995 	imes 9 | F4 |
| 0.09 | 0.00465/0.031 | $32^{3} \times 96$ | 651×9 | F5 |
| 0.06 | 0.0036/0.018 | $48^{3} \times 144$ | 749 	imes 9 | S 1 |
| 0.06 | 0.0072/0.018 | $48^{3} \times 144$ | 593 	imes 9 | S2 |
| 0.06 | 0.0025/0.018 | $56^{3} \times 144$ | 799 	imes 9 | S 3 |
| 0.06 | 0.0054/0.018 | $48^{3} \times 144$ | 582×9 | S 4 |
| 0.045 | 0.0028/0.014 | $64^{3} \times 192$ | 747×1 | U1 |

world" can be ignored. We use the same values as in our B_K calculation, the justification for which has been discussed in Ref. [15]. Multiple measurements with random time translations are carried out on each lattice (see Table I). After averaging over configurations, we form the ratios needed for the B_i . The overlap of the wall sources with the kaon states cancels in these ratios, as well as some of the statistical error. Away from the sources, these ratios should be independent of t. We find this to be the case within errors, and we fit them to a constant over a central "plateau" region.

Our lattice operators are matched to those in the continuum scheme of Ref. [4] using 1-loop, mean-field improved perturbation theory. Previous one-loop matching calculations matched the lattice operators to those in a different continuum scheme [16], but we have now determined the matching between the two continuum schemes [17]. At each lattice spacing, we match to the continuum scheme at scale $\mu = 1/a$. The one-loop corrections are typically 10%–20%, with the largest being 30%. This is in line with the expectation that the coefficient of α should be of $\mathcal{O}(1)$ or smaller.

We use a partially quenched setup with ten different valence quark masses: $am_{x,y} = am_s \times (n/10)$ and n = 1, 2, ..., 10. Here x and y refer to valence d and s quarks, respectively. Our lightest valence pions have $M_{x\bar{x}} \approx 200$ MeV. For our valence kaons, we use the lightest four values of am_x and the heaviest three of am_y . These combinations satisfy $m_x \ll m_y \sim m_s^{\text{phys}}$, so that our result lies in the regime in which heavy-kaon SU(2) chiral perturbation theory (ChPT) is applicable [18,19].

For our chiral extrapolations, we use B_K (whose behavior is well understood from prior work) as well as the four "golden" combinations

$$G_{23} = \frac{B_2}{B_3}, \qquad G_{45} = \frac{B_4}{B_5}, \qquad G_{24} = B_2 B_4, \qquad G_{21} = \frac{B_2}{B_K}.$$
(9)

²In other calculations of the BSM matrix elements [5,6], different ratios have been used so as to avoid the need to use quark masses. However, quark masses are now quite well determined [7], with the ~6% error in $(m_s + m_d)^2$ being comparable to those we obtain for the B_i .

³There have also been earlier quenched calculations, which established the basic methodology [8-10].

⁴Staggered fermions also preserve part of the continuum chiral symmetry, although this is less important for the BSM matrix elements than for B_K , as the former are not constrained by chiral symmetry to vanish in the SU(3) chiral limit.

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These have no chiral logarithms at next-to-leading order (NLO) [20], and thus have simpler chiral extrapolations than the B_i and reduced sensitivity to taste-breaking lattice artifacts. At the end, we invert these relations to determine the B_i . We have checked that extrapolating the B_i directly leads to compatible results [21].

We extrapolate to physical quark masses and a = 0 in three steps. The first two are done on each ensemble separately: we extrapolate m_x to m_d^{phys} ("X-fit") and then m_y to m_s^{phys} ("Y-fit"). For B_K the fitting is as described in Refs. [11,15]. For the G_i we fit to

$$c_1 + c_2 X + c_3 X^2 + c_4 X^2 \ln^2 X + c_5 X^2 \ln X + c_6 X^3, \quad (10)$$

where $X \equiv X_P / \Lambda_{\chi}^2$, with $X_P = M_{\chi\bar{\chi}}^2$ and $\Lambda_{\chi} = 1$ GeV. This incorporates the absence of the NLO logarithm. The NNLO chiral logarithms are not known, so we use the generic form of such terms. We also include a single analytic NNNLO term, which is required for good fits. Our X-fits include the full correlation matrix, and constrain the coefficients c_{3-6} with Bayesian priors: $c_i = 0 \pm 1$. Examples of X-fits for G_{23} are shown in Fig. 1. We see that the chiral extrapolations are short and the dependence mild. This holds also for the other G_i . Systematic errors are estimated by doubling the widths of the Bayesian priors, and also by comparing with fits using the eigenmode shift method [22]. These two estimates are then combined in quadrature.

The m_y dependence is close to linear, so we use a linear extrapolation for our central value and a quadratic fit to estimate a systematic error. After these Y-fits, we evolve results from all lattices to a common renormalization scale, either $\mu = 2$ or 3 GeV, using the two-loop anomalous dimensions given in Ref. [4]. It turns out that the standard form of the solution is singular, but this can be removed by the analytic continuation method proposed in Ref. [23]. Details will be given in Ref. [17].



FIG. 1 (color online). G_{23} (NDR, 1/a GeV) vs X_P on the F1, S1, and U1 ensembles. Data points are shown by circles, while the triangle, pentagon, and diamond show the extrapolated results.

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In our final extrapolation we simultaneously extrapolate sea-quark masses to their physical values and $a \rightarrow 0$. As for B_K , we use only the three finest lattice spacings. For our central values we fit to

$$f_1 = d_1 + d_2 (a\Lambda_Q)^2 + d_3 L_P / \Lambda_\chi^2 + d_4 S_P / \Lambda_\chi^2, \quad (11)$$

with L_P (S_P) the squared masses of the taste ξ_5 pseudoscalars composed of light (strange) sea quarks. We set $\Lambda_Q = 0.3$ GeV and expect $d_2 \sim \mathcal{O}(1)$. In fact, for the G_i we find $|d_2| \sim 2-7$, indicating enhanced discretization errors. We also find that $d_3 \neq d_4$, indicating substantial SU(3) breaking, although both coefficients are of the expected size $|d_{3,4}| \ll 1$. Examples of fits are shown in Figs. 2 and 3, for B_K and G_{23} respectively. These fits have $\chi^2/d.o.f. = 1.9$ and 2.7 respectively. Those for the other G_i are slightly better, with $\chi^2/d.o.f. = 1.6-1.7$.

We also consider more elaborate fits, using

$$f_2 = f_1 + d_5 (a\Lambda_Q)^2 \alpha_s + d_6 \alpha_s^2 + d_7 (a\Lambda_Q)^4, \quad (12)$$

with $\alpha_s = \alpha_s(\overline{\text{MS}}, 1/a)$. This form includes all terms expected at NLO in staggered ChPT [20] plus one NNNLO term. We impose Bayesian constraints, $d_{2-7} = 0 \pm 2$, and find improved fits with $\chi^2/\text{d.o.f.} = 0.8-1.5$. We take the



FIG. 2 (color online). Chiral-continuum extrapolation of B_K (NDR, 2 GeV). The red circle shows the extrapolated result.



FIG. 3 (color online). As for Fig. 2 but for G_{23} .

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TABLE II. Final results for the B_i and G_i at two renormalization scales. Errors are respectively statistical and systematic.

| | $\mu = 2 \text{ GeV}$ | $\mu = 3 \text{ GeV}$ |
|-----------------------|-----------------------|-----------------------|
| B _K | 0.537 (7)(24) | 0.519 (7)(23) |
| B_2 | 0.620 (4)(31) | 0.549 (3)(28) |
| <i>B</i> ₃ | 0.433 (3)(19) | 0.390 (2)(17) |
| B_4 | 1.081 (6)(48) | 1.033 (6)(46) |
| B_5 | 0.853 (6)(49) | 0.855 (6)(43) |
| G ₂₃ | 1.430 (3)(63) | 1.405 (2)(62) |
| G ₄₅ | 1.267 (2)(72) | 1.209 (1)(60) |
| G_{24} | 0.670 (4)(30) | 0.567 (4)(27) |
| G_{21}^{21} | 1.155 (12)(66) | 1.058 (11)(62) |
| G ₂₁ | 1.155 (12)(66) | 1.058 (11)(62 |

difference between f_2 and f_1 fits as the systematic error in the chiral-continuum extrapolation.

We present our final results and error budgets in Tables II and III respectively. Statistical errors are estimated by bootstrap and are at the percent-level or smaller. Of the errors not discussed above, the dominant one comes from our use of one-loop matching. We estimate this as $\delta B/B = \alpha_s^2$, with α_s evaluated on our finest lattice [15]. Support for this estimate comes from a recent comparison of perturbative and nonperturbative renormalization using staggered bilinears [24]. Since this error is also accounted for by the d_6 term when fitting to Eq. (12), to avoid double counting we take the largest of " $f_2 - f_1$ error" and the " α^2 error" for our combined chiral-continuum-matching error. Finite volume errors are estimated by comparing fits using ChPT with and without finite-volume corrections. Since the chiral logarithms in all BSM *B* parameters have the same relative magnitude as that in B_K , we take this estimate from our earlier work on B_K [11]. Specifically, the largest error estimate is from the F1 ensemble (see Table I of Ref. [25]).

We close by comparing our results to those of Ref. [5].⁵ As noted above, the results for B_K agree. For the BSM *B* parameters, Ref. [5] finds, at $\mu = 3$ GeV, $B_{i=2-5}^{SUSY} =$ 0.43(5), 0.75(9), 0.69(7), 0.47(6). Only B_3 differs between

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TABLE III. Error budgets (in percent) for the B_i (2 GeV).

| Source of error | B_K | B_2 | <i>B</i> ₃ | B_4 | <i>B</i> ₅ |
|---|-------|-------|-----------------------|-------|-----------------------|
| Statistics | 1.37 | 0.64 | 0.63 | 0.60 | 0.66 |
| { Matching Cont – extrap. } | 4.40 | 4.95 | 4.40 | 4.40 | 5.69 |
| X-fit (F1) | 0.10 | 0.10 | 0.10 | 0.12 | 0.12 |
| Y-fit (F1) | 0.62 | 0.12 | 0.19 | 0.22 | 0.16 |
| Finite volume | 0.50 | 0.50 | 0.50 | 0.50 | 0.50 |
| $r_1 = 0.3117(22) \text{ fm}$ | 0.34 | 0.18 | 0.17 | 0.05 | 0.02 |
| $f_{\pi} = 132 \text{ vs } 124 \text{ MeV} (\text{F1})$ | 0.46 | 0.46 | 0.46 | 0.46 | 0.46 |

SUSY and chiral bases, with $B_3^{\text{SUSY}} = (5B_2^{\text{chiral}} - 3B_3^{\text{chiral}})/2$. Our results convert to $B_3^{\text{SUSY}}(3 \text{ GeV}) = 0.79(3)$. Using this result and Table II, we find that B_2 and B_3^{SUSY} are consistent with Ref. [5] (the former only at 2σ), while B_4 and B_5 differ significantly (by 4σ and 5σ , respectively). Our B_4 and B_5 are larger than those of Ref. [5] by 50% and 80%, respectively.

Given this difference, we have cross-checked the components of our calculation in several ways e.g. comparing our renormalization group running matrices with those in Refs. [1,5]. Clearly, further investigation is needed to resolve the disagreement with Refs. [5,6]. One possibility that we are investigating is that the true truncation errors in perturbative matching are larger than our estimate, which can be checked by renormalizing our operators nonperturbatively. Another useful test would be for the other calculations to calculate directly the golden combinations, so as to pinpoint the source of the disagreement.

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⁵We use this work rather than Ref. [6], since the latter quenches the strange quark. This choice is not quantitatively important, however, since the results from these two works are consistent.

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