Neutral-Kaon Mixing from (2 + 1)-Flavor Domain-Wall QCD

D. J. Antonio,[1] P. A. Boyle,[1] T. Blum,[8,2] N. H. Christ,[3] S. D. Cohen,[3] C. Dawson,[2] T. Izubuchi,[2,6] R. D. Kenway,[1] C. Jung,[4] S. Li,[3] M. F. Lin,[3] R. D. Mawhinney,[3] J. Noaki,[7,9] S. Ohta,[9,2,10] B. J. Pendleton,[1] E. E. Scholz,[4] A. Soni,[4] R. J. Tweedie,[1] and A. Yamaguchi[5]

(RBC and UKQCD Collaborations)

[1]*SUPA, School of Physics, The University of Edinburgh, Edinburgh EH9 3JZ, United Kingdom*
[2]*RIKEN-BNL Research Center, Brookhaven National Laboratory, Upton, New York 11973, USA*
[3]*Physics Department, Columbia University, New York, New York 10027, USA*
[4]*Brookhaven National Laboratory, Upton, New York 11973, USA*
[5]*SUPA, Department of Physics & Astronomy, University of Glasgow, Glasgow G12 8QQ, United Kingdom*
[6]*Institute for Theoretical Physics, Kanazawa University, Kanazawa 920-1192, Japan*
[7]*School of Physics and Astronomy, University of Southampton, Southampton SO17 1BJ, United Kingdom*
[8]*Physics Department, University of Connecticut, Storrs, Connecticut 06269-3046, USA*
[9]*Institute of Particle and Nuclear Studies, KEK, Tsukuba, Ibaraki 305-0801, Japan*
[10]*Physics Department, SOKENDAI, Tsukuba, Ibaraki 305-0801, Japan*
(Received 9 February 2007; revised manuscript received 6 September 2007; published 22 January 2008)

We present the first results for neutral-kaon mixing using (2 + 1)-flavors of domain-wall fermions. A new approach is used to extrapolate to the physical up and down quark masses from our numerical studies with pion masses in the range 240–420 MeV; only $SU(2)_L \times SU(2)_R$ chiral symmetry is assumed and the kaon is not assumed to be light. Our main result is $B_K^{\overline{\rm MS}}(2\ {\rm GeV}) = 0.524(10)(28)$ where the first error is statistical and the second incorporates estimates for all systematic errors.

DOI: 10.1103/PhysRevLett.100.032001 PACS numbers: 12.38.Gc, 11.15.Ha, 11.30.Rd, 12.38.Aw

The phenomena of *CP* violation is a central component of the standard model, in which *CP* violation is only possible when all three of the quark doublets present in nature interact. The Cabibbo-Kobayashi-Maskawa (CKM) flavor mixing matrix contains a single, physically meaningful phase which must describe all *CP* violating phenomena. For bottom mesons, it is possible to make a direct connection between the measured *CP* violation in *B* decays and this CKM phase. However, for *K* mesons, the system in which *CP* violation was originally observed, this connection is far more challenging.

One begins with the measure of indirect *CP* violation $\epsilon_K = 2.232 \pm 0.007 \times 10^{-3}$ [1], determined experimentally from the mixing between K^0 and $\bar{K}^0$ mesons. The operator product expansion relates ϵ_K to the QCD matrix element of a four quark operator $\mathcal{O}_{VV+AA} = (\bar{s}\gamma_\mu d) \times (\bar{s}\gamma_\mu d) + (\bar{s}\gamma_5\gamma_\mu d)(\bar{s}\gamma_5\gamma_\mu d)$ between kaon states via a well known perturbative expression [2] involving this CKM phase. This matrix element is parameterized by the renormalization scheme dependent parameter

$$B_K = \frac{\langle K^0|\mathcal{O}_{VV+AA}|\bar{K}^0\rangle}{\frac{8}{3} f_K^2 M_K^2}. \tag{1}$$

Lattice QCD offers the only first-principles determination of B_K, which is essential to determine if the *CP* violations observed in the *B* and *K* systems have a common, standard model origin. We describe a lattice QCD calculation of B_K in which the most important errors present in earlier lattice results have been substantially reduced. We exploit the domain-wall fermion (DWF) formulation with 2 + 1 dynamical flavors. This suppresses $O(a)$ errors, both on and off shell, and also chiral symmetry breaking (measured by a (small) additive "residual mass" $m_{\rm res}$). This allows us to renormalize $\mathcal{O}_{VV+AA}$ multiplicatively via a nonperturbative matching [3–5]. Thus, we simultaneously avoid the complexity of lattice operator mixing, avoid poorly convergent lattice perturbation theory and include the correct light flavor content.

Alternative lattice approaches to B_K must treat either a chirality or taste mixing matrix and result in larger errors. For Wilson fermions a chirality mixing matrix can be determined using nonperturbative off-shell renormalization, but large cancellations leave results imprecise. While staggered fermion simulations successfully treat simpler quantities, current staggered results have a 10%–20% error for B_K due to large taste mixing [6].

By using large lattice volumes and meson masses as light as 243 MeV, we can determine the light quark limit with substantially improved accuracy. Instead of using a chiral perturbation theory (ChPT) which treats the *K* meson as light compared to the chiral scale, we evaluate the chiral limit using $SU(2)_L \times SU(2)_R$ ChPT and assume that only our pions are light.

Simulation.—Our calculation is performed with a fixed lattice spacing and two space-time volumes, $16^3 \times 32$ and $24^3 \times 64$, using the Iwasaki gauge action [7] with $\beta = 2.13$ and the DWF action with a fifth dimension of size 16.

Each ensemble uses the same dynamical strange quark mass $am_s^{\rm sea} = 0.04$ in lattice units. We use three 16^3 ensembles with degenerate up and down quarks of mass $am_l^{\rm sea} \in \{0.01, 0.02, 0.03\}$ and two 24^3 ensembles with $am_l^{\rm sea} \in \{0.005, 0.01\}$. The ensembles, described in [8,9], were generated using the RHMC algorithm [10] with trajectories of unit length. The 16^3 ensembles each contain 4000 trajectories, from which we omit 1000 trajectories for thermalization. We perform measurements on 150 configurations separated by 20 trajectories for each ensemble, calculating matrix elements of all possible pseudoscalar states with valence quark masses $am^{\rm val} \in \{0.01, 0.02, 0.03, 0.04, 0.05\}$. We bin the data using up to 80 trajectories per bin to reduce the correlations between our samples. The $am_l^{\rm sea} = 0.005$ and 0.01, 24^3 ensembles are composed of 4460 and 5020 trajectories, respectively, with measurements performed on the final 90 configurations separated by 40 trajectories. These data are binned into blocks of 2 configurations representing 80 trajectories. All possible pseudoscalar states are studied, composed of valence quark masses $am^{\rm val} \in \{0.001, 0.005, 0.01, 0.02, 0.03, 0.04\}$.

We use the mass of the Ω^- baryon, linearly extrapolated to $m_l = (m_u + m_d)/2$, and m_K and m_π treated in $SU_L(2) \times SU_R(2)$ ChPT to determine $1/a = 1.73(3)$ GeV, and unrenormalized masses $am_s + am_{\rm res} = 0.0375(16)$ and $am_l + am_{\rm res} = 0.00130(6)$. Since in our simulation, $am_s = 0.04$ and $am_{\rm res} = 0.00315(2)$, we must take into account our 15% too large input value of m_s. We obtained the pseudoscalar decay constant $af_\pi = 0.0718(18)$ using $Z_A\langle P|A_0|0\rangle = -iM_P f_P$, and the axial-vector current renormalization constant $Z_A = 0.7162(2)$ [8]. (Note, the above errors are all statistical.)

We use an established method [4,11,12] for evaluating the lattice matrix elements. Zero-momentum kaon states are created and annihilated using Coulomb-gauge–fixed wall sources at times 5 and 27 for the 16^3 volume and 5 and 59 for 24^3, with $\mathcal{O}_{VV+AA}$ inserted at each intervening point. Use of a combination of periodic and antiperiodic boundary conditions in time removes unwanted propagation around the boundary, resulting in a good plateau for the ratio of matrix elements

$$B_K^{\rm lat} = \frac{\langle K^0(t_1)|\mathcal{O}_{VV+AA}(t)|\bar{K}^0(t_2)\rangle}{\frac{8}{3}\langle K^0(t_1)|A_0(t)\rangle\langle A_0(t)|\bar{K}^0(t_2)\rangle}. \qquad (2)$$

A sample fit is displayed in Fig. 1. For each ensemble the pseudoscalar mass, M_P, decay constant, f_P, and B-parameter, B_P, are computed for each combination $(m_x^{\rm val}, m_y^{\rm val})$. We tabulate a portion of the 16^3 and 24^3 results for B_P and M_P in Tables I and II.

Our lightest dynamical pion masses are 331 MeV. We must extrapolate our result for B_P to the physical value of $m_l = (m_u + m_d)/2$, and we treat only the up and down quarks as light by using the $SU(2)_L \times SU(2)_R$ partially quenched ChPT (PQChPT) formula [13]

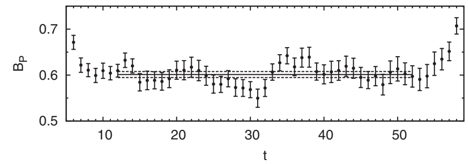

FIG. 1. Typical plateau for the lattice B parameter for the pseudoscalar state made up from quarks of mass $am_x^{\rm val} = 0.001$, $am_y^{\rm val} = 0.04$, on the $am_l^{\rm sea} = 0.005$, $am_s^{\rm sea} = 0.04$, 24^3 ensemble.

$$B_P(m_x, m_l) = B_P(0)\left\{1 + c_0 m_l + c_1 m_x - k \ln\frac{2B_0 m_x}{\Lambda_{\rm ch}^2}\right\}.$$

Here m_x is the light valence quark mass, m_l the light sea quark mass, $\Lambda_{\rm ch}$ the chiral scale, $B_P(0)$, c_0 and c_1 are m_s-dependent low energy constants, $k = B_0 m_l/(4\pi f_\pi)^2$, B_0 is the constant in the expression $m_\pi^2 = 2B_0 m_x$, and we include $m_{\rm res}$ in all masses entering these formulas. m_K is now the lowest scale that can dimensionally balance higher order terms in the chiral expansion, and m_π^2/m_K^2 will determine the suppression of successive orders. This is a better expansion parameter than the $m_K^2/\Lambda_{\rm ch}^2$ of $SU(3)$ ChPT. We should note that the pseudoscalar masses and decay constants are also well described by a $SU(2)_L \times SU(2)_R$ PQChPT analysis.

Figure 2 shows B_P versus m_x together with the $SU(2)_L \times SU(2)_R$ partially quenched ChPT fit to the 24^3 data. The fit does not include correlations so the resulting $\chi^2/{\rm dof} = 0.14$ is not a meaningful indication of goodness of fit. The 16^3 unitary data, also shown in Fig. 2, are well described by a straight line which, if simply extrapolated to the physical limit gives a result about 6% larger than the more accurate chiral extrapolation that is possible if the smaller masses in the 24^3 simulation are used [14]. This $SU(2)_L \times SU(2)_R$ chiral extrapolation gives $B_K^{\rm lat} = 0.565(10)$ for physical m_l. (B_K is determined at the correct valence value of $am_s = 0.0343$ by linearly interpolating between $am_y = 0.03$ and 0.04.)

We have previously demonstrated [11,15,16] that the wrong-chirality mixing in our simulation is sufficiently suppressed that we may ignore it. Thus, we consider only

TABLE I. Bare pseudoscalar B parameter B_P, and mass M_P, for the 16^3 volume. The fit range is 12–20 for B_P and 15–27 for M_P. In the first column, e.g., 1,2 denotes a meson composed of quarks with lattice masses $(am_x^{\rm val}, am_y^{\rm val}) = (0.01, 0.02)$.

$am^{\rm val}$	$am_l^{\rm sea} = 0.01$ B_P	$am_l^{\rm sea} = 0.01$ aM_P	$am_l^{\rm sea} = 0.02$ B_P	$am_l^{\rm sea} = 0.02$ aM_P	$am_l^{\rm sea} = 0.03$ B_P	$am_l^{\rm sea} = 0.03$ aM_P
1,1	0.546(8)	0.247(3)	0.539(8)	0.250(3)	0.527(7)	0.251(3)
1,2	0.577(6)	0.290(3)	0.569(6)	0.292(3)	0.556(6)	0.289(3)
2,2	0.598(5)	0.323(3)	0.589(5)	0.325(3)	0.580(5)	0.325(3)
1,4	0.620(5)	0.356(3)	0.616(6)	0.359(3)	0.599(5)	0.356(3)
2,4	0.633(4)	0.387(3)	0.627(4)	0.388(3)	0.618(4)	0.385(3)
3,4	0.647(4)	0.414(3)	0.641(4)	0.415(3)	0.634(3)	0.412(3)
4,4	0.659(3)	0.438(3)	0.655(3)	0.440(3)	0.648(3)	0.442(3)

TABLE II. Bare pseudoscalar B parameter B_P, and mass M_P, results for the 24^3 configurations. The fit range is 12–52 for the B parameter and 15–59 for the mass.

$am_x^{\rm val}$, $am_y^{\rm val}$	$am_l^{\rm sea} = 0.005$		$am_l^{\rm sea} = 0.01$	
	B_P	aM_P	B_P	aM_P
0.001, 0.001	0.469(8)	0.1402(9)	0.470(5)	0.1434(10)
0.001, 0.005	0.491(7)	0.1681(8)	0.495(4)	0.1707(9)
0.005, 0.005	0.508(5)	0.1916(8)	0.512(3)	0.1938(8)
0.001, 0.01	0.514(6)	0.1971(8)	0.521(4)	0.1995(9)
0.005, 0.01	0.527(4)	0.2172(8)	0.531(3)	0.2194(8)
0.01, 0.01	0.542(3)	0.2400(7)	0.546(3)	0.2421(8)
0.001, 0.04	0.601(6)	0.3204(11)	0.613(7)	0.3234(11)
0.005, 0.04	0.607(4)	0.3329(8)	0.611(3)	0.3358(8)
0.01, 0.04	0.614(3)	0.3482(7)	0.616(2)	0.3509(7)

multiplicative renormalization of $\mathcal{O}_{VV+AA}$, and use the RI-MOM nonperturbative renormalization technique to match our lattice scheme to the $\overline{\rm MS}$ scheme via $B_K^{\overline{\rm MS}} = (Z_{\mathcal{O}_{VV+AA}}^{\overline{\rm MS}}/Z_A^2)B_K^{\rm lat} \equiv Z_{B_K}^{\overline{\rm MS}} B_K^{\rm lat}$.

The technique performs well since domain-wall fermions are off-shell improved. We evaluate the amputated, four-leg and two-leg vertex functions $\Lambda_{\mathcal{O}_{VV+AA}}$, Λ_A, and Λ_V in Landau gauge. Because of the relatively low lattice cutoff, Λ_A and Λ_V differ by 2%. We use their average and add their difference to the systematic error.

We both quote lattice results in the RI-MOM scheme without perturbative error and convert to other schemes using the continuum NLO result [17,18]. We obtain $Z_{B_K}^{\rm RI}(2\ {\rm GeV}) = 0.910(5)(13)$. The first error in parenthesis is statistical and the second systematic. As shown in Fig. 3, we use the RGI scheme as a scale invariant intermediate step to reveal and remove possible $(ap)^2$ errors. Only weak scale dependence is seen in the window $1.0 \le (ap)^2 \le 2.5$, implying artefact-free perturbative behavior. We obtain $Z_{B_K}^{\rm RGI} = 1.275(10)(25)$ by linearly extrapolating to $(ap)^2 = 0$ to remove $O(a^2)$ effects.

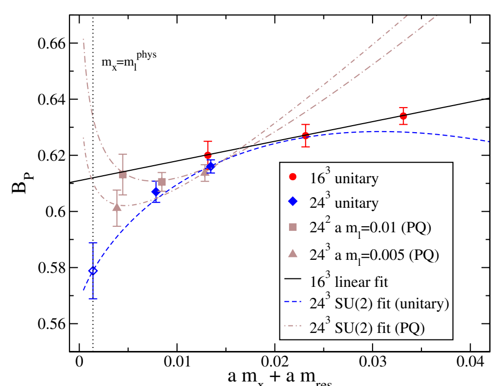

FIG. 2 (color online). Results for B_P together with the NLO partially quenched $SU(2)_L \times SU(2)_R$ ChPT fit to the 24^3 data plotted versus the light valence quark lattice mass am_x. From top to bottom on the left-hand side, the three curves are $am_l = 0.01$, 0.005 and am_x respectively. The valence strange quark mass is fixed at its unitary value $am_y = am_s = 0.04$. While the statistical errors are large, the growing upward curvature in m_x as the sea quark mass is increased from 0.005 to 0.01 predicted by ChPT is visible. Some m_x values are slightly shifted for clarity.

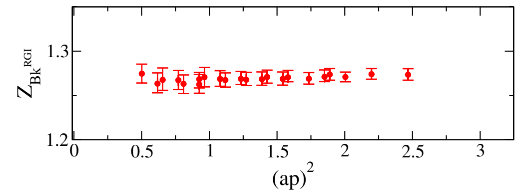

FIG. 3 (color online). A plot of $Z_{B_K}^{\rm RGI}(p^2)$ showing that the perturbative running, removed from $Z_{B_K}^{\rm RGI}$, accounts for most p^2 dependence.

Conversion to $\overline{\rm MS}$ is a 2% effect at NLO, consistent with $O(1) \times \alpha_s/4\pi$. While the error estimate could be as low as $O({\rm few}) \times (\alpha_s/4\pi)^2$, we add in quadrature the size of the NLO correction itself as a perturbative systematic, giving $Z_{B_K}^{\overline{\rm MS}}(2\ {\rm GeV}) = 0.928(5)(23)$. For comparison, 1-loop lattice perturbation theory [19] gives $Z_{B_K}^{\overline{\rm MS}}(2{\rm GeV}) = 1.007$ with the difference likely due to slow convergence of lattice perturbation theory.

Results and conclusions.—We combine the bare B_K given above with these Z factors to obtain physically normalized results from (2 + 1)-flavor DWF at $a^{-1} = 1.73(3)$ GeV on a $24^3 \times 64$ volume, where the second error is the renormalization systematic: $B_K^{\rm RI}(2\ {\rm GeV}) = 0.514(10)(7)$, and $B_K^{\overline{\rm MS}}(2\ {\rm GeV}) = 0.524(10)(13)$. The RI result involves no use of perturbation theory and has a reduced systematic error.

We plot the $\overline{\rm MS}$ result in relation to those quenched [11,20] and two flavor [12] DWF results that could allow dependence on flavor content to be seen. (Of course differences arising from different lattice spacing and gauge action are also to be expected.) In addition, we include the (2 + 1)-flavor staggered fermion result [6] in Fig. 4.

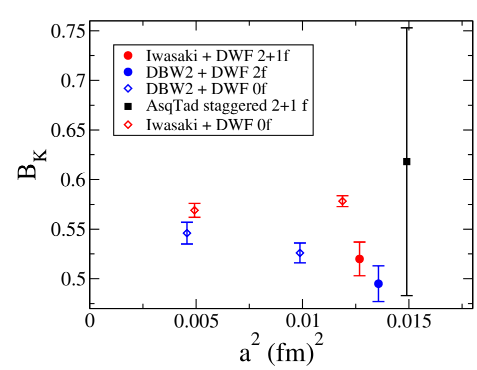

FIG. 4 (color online). We compare our (2 + 1)-flavor results with earlier quenched [20] and 2 flavor DWF [12] as well as (2 + 1)-flavor staggered calculations [6]. The quenched Iwasaki points show statistical errors only while our point and the staggered point include renormalization systematics. While our point lies below these Iwasaki results due to our improved chiral limit and flavor content, we expect similar a^2 dependence.

Finite volume chiral perturbation theory [21] suggests that finite volume effects are negligible for all masses and volumes in our simulation except for $am_x = 0.001$ where the effect may be 2%. However, since our fit is insensitive to this point, we adopt our 1%, 16^3–24^3, $am_l = 0.01$ difference as an estimate of the finite volume error.

Finite lattice spacing errors are likely larger, but also difficult for us to estimate. We can make use of the quenched, perturbatively renormalized results of CP-PACS [20] also obtained for the Iwasaki and DWF lattice action which suggest a (poorly determined) scaling violation of size 3.5% at our coarser lattice spacing. We choose a 4% systematic error as the most likely estimate for $O(a^2)$ effects in our $(2 + 1)$-flavor result. A second approach to estimating discretization errors is to compare a variety of presumably reliable quantities computed from our $1/a = 1.73(3)$ GeV ensembles with experiment. For example, we find f_π and f_K about 4% below experiment, a discrepancy consistent with our 4% error estimate.

While we have interpolated to the physical valence strange quark mass, we have results for only one strange sea quark mass. We estimate the error resulting from our 15% too large m_s by observing that for fixed valence masses (0.01, 0.04) B_P increases by 3% when the light sea quark mass is changed from 0.03 to 0.02. Scaling this to the 0.0057 change needed for a single flavor of sea quark implies a 1% error. Finally, we add a 2% chiral extrapolation error by estimating the effects of NNLO ChPT as the 6% difference between the linear and NLO chiral limits in Fig. 2 scaled by $m_l/m_s = 0.4$ for $am_l = 0.01$.

Thus, we take our central value, which removes all quenching systematics, and add the 1% finite volume, 4% scaling, 1% m_s extrapolation, 2% ChPT and renormalization error estimates in quadrature and obtain

$$B_K^{\mathrm{RI}}(2\ \mathrm{GeV}) = 0.514(10)(25), \tag{3}$$

$$B_K^{\overline{\mathrm{MS}}}(2\ \mathrm{GeV}) = 0.524(10)(28), \tag{4}$$

$$\hat{B}_K = 0.720(13)(37), \tag{5}$$

where the first error is statistical and the second is the estimated systematic. A recent review, including all lattice data then available, quoted a continuum limit value of $B_K^{\overline{\mathrm{MS}}}(2\ \mathrm{GeV}) = 0.58(3)(6)$ [22]. Our result is consistent with this and reduces both types of error substantially. This improvement arises because, using QCDOC computers, we have for the first time combined the correct dynamical flavor content with a lattice formulation with good chiral symmetry, $O(a)$ improvement, control over operator mixing, nonperturbative renormalization and a new use of $SU(2)_L \times SU(2)_R$ ChPT for kaons.

In order to reduce the significant discretization systematic error in our result for B_K, the RBC and UKQCD collaborations are now doing simulations at a smaller lattice spacing, which will give quantitative control of this effect. A continuum NNLO perturbative calculation is required to convert lattice results to $\overline{\mathrm{MS}}$ with better precision.

We thank Dong Chen, Mike Clark, Calin Cristian, Zhihua Dong, Alan Gara, Andrew Jackson, Changhoan Kim, Ludmila Levkova, Xiaodong Liao, Guofeng Liu, Konstantin Petrov, and Tilo Wettig for developing with us the QCDOC machine and its software. This development and the computers used in this calculation were funded by the U.S. DOE Grant No. DE-FG02-92ER40699, PPARC JIF Grant No. PPA/J/S/1998/00756 and by RIKEN. This work was supported by DOE Grant No. DE-FG02-92ER40699 and PPARC Grants No. PPA/G/O/2002/00465 and No. PP/D000238/1. We thank the University of Edinburgh, PPARC, RIKEN, BNL, and the U. S. DOE for providing these facilities. C. J., E. S., T. B., and A. S. were supported by the U. S. Department of Energy under Contracts No. DE-AC02-98CH10886, and No. DE-FG02-92ER40716. J. N. was partially supported by the Japan Society for the Promotion of Science. We thank Chris Sachrajda, and Steve Sharpe for useful discussions and the referee for questioning our original treatment of the chiral limit.

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