

$K \rightarrow (\pi\pi)_{I=2}$ Decay Amplitude from Lattice QCD

T. Blum,¹ P. A. Boyle,² N. H. Christ,³ N. Garron,² E. Goode,⁴ T. Izubuchi,^{5,6} C. Jung,⁵ C. Kelly,³ C. Lehner,⁶
M. Lightman,^{3,7} Q. Liu,³ A. T. Lytle,⁴ R. D. Mawhinney,³ C. T. Sachrajda,⁴ A. Soni,⁵ and C. Sturm⁸

(RBC and UKQCD Collaborations)

¹Physics Department, University of Connecticut, Storrs, Connecticut 06269-3046, USA

²SUPA, School of Physics, The University of Edinburgh, Edinburgh EH9 3JZ, United Kingdom

³Physics Department, Columbia University, New York, New York 10027, USA

⁴School of Physics and Astronomy, University of Southampton, Southampton SO17 1BJ, United Kingdom

⁵Brookhaven National Laboratory, Upton, New York 11973, USA

⁶RIKEN-BNL Research Center, Brookhaven National Laboratory, Upton, New York 11973, USA

⁷Physics Department, Washington University, 1 Brookings Drive, St. Louis, Missouri 63130-4899, USA

⁸Max-Planck-Institut für Physik, Föhringer Ring 6, 80805 München, Germany

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We report on the first realistic *ab initio* calculation of a hadronic weak decay, that of the amplitude A_2 for a kaon to decay into two π mesons with isospin 2. We find $\text{Re}A_2 = (1.436 \pm 0.063_{\text{stat}} \pm 0.258_{\text{syst}})10^{-8}$ GeV in good agreement with the experimental result and for the hitherto unknown imaginary part we find $\text{Im}A_2 = -(6.83 \pm 0.51_{\text{stat}} \pm 1.30_{\text{syst}})10^{-13}$ GeV. Moreover combining our result for $\text{Im}A_2$ with experimental values of $\text{Re}A_2$, $\text{Re}A_0$, and ϵ'/ϵ , we obtain the following value for the unknown ratio $\text{Im}A_0/\text{Re}A_0$ within the standard model: $\text{Im}A_0/\text{Re}A_0 = -1.63(19)_{\text{stat}}(20)_{\text{syst}} \times 10^{-4}$. One consequence of these results is that the contribution from $\text{Im}A_2$ to the direct CP violation parameter ϵ' (the so-called Electroweak Penguin contribution) is $\text{Re}(\epsilon'/\epsilon)_{\text{EWP}} = -(6.52 \pm 0.49_{\text{stat}} \pm 1.24_{\text{syst}}) \times 10^{-4}$. We explain why this calculation of A_2 represents a major milestone for lattice QCD and discuss the exciting prospects for a full quantitative understanding of CP violation in kaon decays.

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Introduction.— CP violation is a necessary ingredient for the generation of the matter-antimatter asymmetry in the Universe and understanding its origin, both within and beyond the standard model, is one of the primary goals of particle physics research. It was first discovered in the decays of kaons into two pions, and in this Letter we report on a calculation of the amplitude A_2 for $K \rightarrow (\pi\pi)_{I=2}$ decays from first principles. (Bose symmetry implies that the two-pion eigenstates have isospin 0 or 2 and we denote the corresponding complex amplitudes by A_0 and A_2 .) A_2 is obtained by combining our lattice results for matrix elements of the four-quark operators in the effective Hamiltonian [the matrix elements are given in Eqs. (7)–(9)] with Wilson coefficients and Cabibbo-Kobayashi-Maskawa (CKM) matrix elements. For $\text{Re}A_2$ we find good agreement with the known experimental value [see Eq. (10)] and, more importantly, we are also able to determine the previously unknown quantity $\text{Im}A_2$ [Eq. (11)]. In addition, within the standard model we can combine our result for $\text{Im}A_2$ with the experimental values of $\text{Re}A_0$, $\text{Re}A_2$, and ϵ'/ϵ to determine the remaining unknown quantity $\text{Im}A_0$, so that both the complex amplitudes A_0 and A_2 are now known.

This is the first quantitative determination of an amplitude for a realistic hadronic weak decay and extends the

framework of lattice QCD into the important domain of nonleptonic weak decays. It has taken several decades for a realistic lattice QCD calculation of $K \rightarrow (\pi\pi)_{I=2}$ decay amplitudes to become possible because very significant theoretical developments and technical progress were required. These are briefly discussed below and explained in more detail in [1], where a full description of our calculation can be found. Among the key issues is the fact that performing the simulations in Euclidean space makes the evaluation of $\pi\pi$ rescattering effects nontrivial. The presence of two pions interacting strongly in a finite box leads to finite-volume effects which must be controlled [2]. In fact the effects of finite volume can be exploited to ensure the equality of the energies of the initial kaon and final two-pion states by the imposition of carefully devised boundary conditions. Finally, it is only relatively recently, with the improvement of algorithms and access to teraflops-scale computing resources, that it has become possible to perform simulations at physical u and d -quark masses.

The calculation of A_2 is also important in that it determines the $O(5\%)$ contribution of direct CP violation to ϵ [3,4], a level of precision which has become relevant due to the major recent improvements in the evaluation of the B_K parameter with an uncertainty of less than 3%, see e.g., [5] (for a recent review see [6]). Of course, a complete

understanding of CP violation in $K \rightarrow \pi\pi$ decays, including the evaluation of ϵ'/ϵ and an understanding of the $\Delta I = 1/2$ rule, requires the ability to compute both A_0 and A_2 directly. The present calculation is an important milestone on the road to achieving this. For A_0 however, the two pions have vacuum quantum numbers and the correlation functions are dominated by the vacuum intermediate state. We report on our exploratory work in developing techniques for the efficient subtraction of the vacuum contributions in [7] and look forward to presenting results of a realistic computation of A_0 in the future.

Details of the simulation.—The simulations were performed using domain wall fermions (DWFs) with a gauge action which we call IDSDR. This is the Iwasaki action modified by a weighting factor, called the dislocation suppressing determinant ratio (DSDR) [8–10], which allows us to suppress configurations with large numbers of modes of the 5-dimensional DWF transfer matrix with near unit eigenvalue while retaining adequate topological change. This modification is necessary since we have a relatively large lattice spacing a which increases the frequency of dislocations which break the chiral symmetry.

We have generated two ensembles of $2 + 1$ flavor DWFs with the IDSDR gauge action at $\beta = 1.75$ and a lattice size of $32^3 \times 64 \times 32$, where the final number is the length of the fifth dimension. We determine the residual mass to be $m_{\text{res}} = 0.00184(1)$ [11]. (Masses written without units are to be understood as being in lattice units.) The ensembles are generated with a simulated strange-quark mass of $m_h = 0.045$ and light-quark masses of $m_l = 0.001$ and $m_l = 0.0042$, with corresponding unitary pion masses of approximately 170 MeV and 250 MeV, respectively. Quark propagators are generated for a range of valence masses. The analysis presented in this Letter is performed using 63 configurations from the 0.001 ensemble, each separated by 8 molecular dynamics time units, and quark propagators with $m_h = 0.049$ and $m_l = 0.0001$. The (partially quenched) pion has a near-physical mass of approximately 140 MeV. A subsequent detailed analysis with greater statistics and improved procedures has yielded a slightly lower value for the bare physical strange-quark mass [0.0464(7)] [11].

We obtain the lattice spacing and the two physical quark masses m_{ud} and m_s using a combined analysis of these IDSDR ensembles and our $\beta = 2.25$, $32^3 \times 64 \times 16$ and $\beta = 2.13$, $24^3 \times 64 \times 16$ domain wall fermion configurations with the Iwasaki gauge action [12,13]. This involves a combined fit of pion and kaon masses and decay constants and the mass of the Ω baryon as functions of the quark masses and lattice spacing. We extrapolate to the continuum limit along a family of scaling trajectories defined by constant values of m_π , m_K , and m_Ω [13]. In our fits we take the lattice artifacts to be $O(a^2)$ as expected and note that the coefficients of the a^2 terms are not equal for the two different lattice actions. From the combined chiral

and continuum fits we obtain for the IDSDR ensembles $a^{-1} = 1.375(9)$ GeV and physical quark masses of $\tilde{m}_l = 0.00174(3)$ and $\tilde{m}_s = 0.0483(7)$ in lattice units, which correspond to $m_{ud}^{\overline{\text{MS}}}(2 \text{ GeV}) = 3.43(13)$ MeV and $m_s^{\overline{\text{MS}}}(2 \text{ GeV}) = 95.1(3.0)$ MeV. (Here $\tilde{m} = m + m_{\text{res}}$.) In this single fit to all three ensembles, the lighter quark masses in the IDSDR ensemble better determine the common ChPT parameters that are less well constrained by the more massive Iwasaki ensembles. Similarly, the two lattice spacings of the Iwasaki ensembles determine a continuum limit which then yields the a^2 correction terms present in the IDSDR results.

In order to ensure that the energy of the two-pion final state (in the rest frame of the kaon) is (almost) equal to m_K , we have carefully chosen both the volume of the lattice and the boundary conditions on the quark fields. With periodic boundary conditions, the two-pion ground state corresponds to each pion being at rest (up to finite-volume corrections) so for the physical decay we would need to consider an excited state [2]. Instead we introduce antiperiodic spatial boundary conditions for some components of the d quark's momentum, so that the corresponding components of the momentum of a π^+ meson are odd-integer multiples of π/L ($L = 32$ is the spatial extent of the lattice). There is now no state with both pions at rest. This is not sufficient however, since the physical decay $K^+ \rightarrow \pi^+ \pi^0$ involves a π^0 which, even with antiperiodic boundary conditions on the d quark, has momentum components which are integer multiples of $2\pi/L$. It is therefore not possible to construct the $\pi^+ \pi^0$ state at rest. These problems are overcome by using isospin symmetry and the Wigner-Eckart theorem to relate the matrix elements for the decay $K^+ \rightarrow \pi^+ \pi^0$ to those for the unphysical process $K^+ \rightarrow \pi^+ \pi^+$:

$$\langle \pi^+ \pi^0 | Q_{\Delta I_z=1/2}^{\Delta I=3/2} | K^+ \rangle = \frac{\sqrt{3}}{2} \langle \pi^+ \pi^+ | Q_{\Delta I_z=3/2}^{\Delta I=3/2} | K^+ \rangle, \quad (1)$$

an approach proposed and first explored in [14,15]. The superscripts and subscripts on the operators Q denote how the total isospin I and the z component I_z change between initial and final state. Neglecting violations of isospin symmetry, (1) is exact and so we can use the two- π^+ state to calculate the physical $\Delta I = 3/2$ decay amplitudes. In this way we are able to avoid the need to consider an excited state and at the same time we reduce the required size of the lattice.

The kaon and pion masses and the energy of the two-pion state in the simulation, together with the corresponding physical values are presented in Table I.

TABLE I. m_{K^+} , m_{π^+} , and $E_{\pi\pi}$ in the simulation and the corresponding physical values. The results are given in MeV.

	m_{K^+}	m_{π^+}	$E_{\pi\pi}$	$m_K - E_{\pi\pi}$
Simulated	511.3(3.9)	142.9(1.1)	492.6(5.5)	18.7(4.8)
Physical	493.677(0.016)	139.57018(0.00035)	m_{K^+}	0

Evaluation of A_2 .—The generic form of the effective Hamiltonian for $K \rightarrow \pi\pi$ decays is

$$H_{\text{eff}} = \frac{G_F}{\sqrt{2}} \sum_i (V_{\text{CKM}})_i C_i Q_i, \quad (2)$$

where G_F is the Fermi constant, $(V_{\text{CKM}})_i$ are the appropriate CKM matrix elements, (specifically we use $V_{us} = 0.2253$, $V_{ud} = 0.97429$ and $\tau = -V_{ts}^* V_{td} / V_{us}^* V_{ud} = 0.0014606 - 0.00060408i$), Q_i are four-quark operators, and C_i are the Wilson coefficients. The calculation of A_2 requires the evaluation of the matrix elements of three operators, classified by their transformations under $\text{SU}(3)_L \times \text{SU}(3)_R$ chiral symmetry:

$$\begin{aligned} Q_{(27,1)} &= (\bar{s}^i d^i)_L (\bar{u}^j d^j)_L, \\ Q_{(8,8)} &= (\bar{s}^i d^i)_L (\bar{u}^j d^j)_R, \\ Q_{(8,8)_{\text{mix}}} &= (\bar{s}^i d^j)_L (\bar{u}^j d^i)_R, \end{aligned} \quad (3)$$

where i, j are color labels which run from 1 to 3. ($Q_{(8,8)}$ and $Q_{(8,8)_{\text{mix}}}$ are the electroweak penguin (EWP) operators contributing mainly to $\text{Im}A_2$.) The main achievement being reported here is the successful determination of the matrix elements ${}_{I=2}\langle \pi\pi | Q_i | K \rangle$. This starts with the evaluation of the correlation function

$$\begin{aligned} C_{K\pi\pi}^i(t_K, t_Q, t_{\pi\pi}) &= \langle 0 | J_{\pi\pi}(t_{\pi\pi}) Q_i(t_Q) J_K^\dagger(t_K) | 0 \rangle \\ &= e^{-m_K(t_Q - t_K)} e^{-E_{\pi\pi}(t_{\pi\pi} - t_Q)} \langle 0 | J_{\pi\pi}(0) | \pi\pi \rangle \\ &\quad \times \langle \pi\pi | Q_i(0) | K \rangle \langle K | J_K^\dagger(0) | 0 \rangle + \dots \quad (4) \end{aligned}$$

where J_K^\dagger and $J_{\pi\pi}$ are interpolating operators for the kaon and two-pion states, which are summed over space and hence have zero momentum. The energy of the two-pion state, $E_{\pi\pi}$, is a little larger than $2\sqrt{m_\pi^2 + n(\pi/L)^2}$ because of finite-volume effects (in the isospin 2 state the two-pion potential is repulsive). Here n is the number of spatial directions in which antiperiodic boundary conditions have been imposed on the d quark. The ellipsis represents the

contributions of heavier states, which are suppressed if $t_Q - t_K$ and $t_{\pi\pi} - t_Q$ are sufficiently large. The sources for the kaon and two pions are placed at fixed times, t_K and $t_{\pi\pi}$ (in lattice units), and we vary the position of the operator t_Q .

The required $\langle \pi\pi | Q_i | K \rangle$ matrix element is one of the factors in Eq. (4) and we need to remove the remaining factors. This is achieved by evaluating two-point correlation functions $C_K(t) = \langle 0 | J_K(t) J_K^\dagger(0) | 0 \rangle$ and $C_{\pi\pi}(t) = \langle 0 | J_{\pi\pi}(t) J_{\pi\pi}^\dagger(0) | 0 \rangle$, and calculating the ratio

$$R(t_Q) \equiv \frac{C_{K\pi\pi}(t_K, t_Q, t_{\pi\pi})}{C_K(t_Q - t_K) C_{\pi\pi}(t_{\pi\pi} - t_Q)} \quad (5)$$

$$\simeq \frac{\langle \pi\pi | Q_i | K \rangle}{\langle 0 | J_{\pi\pi}(0) | \pi\pi \rangle \langle K | J_K^\dagger(0) | 0 \rangle}, \quad (6)$$

where the factors in the denominator of Eq. (6) are determined by fitting the correlation functions C_K and $C_{\pi\pi}$. $R(t_Q)$ is independent of t_Q if all the time intervals are sufficiently large. For illustration of the plateaus we present in Fig. 1 the t_Q behavior for the 3 operators for $t_{\pi\pi} - t_K = 24$. (We also have results for $t_{\pi\pi} = 20, 28$ and 32 .)

Having obtained the matrix elements of the bare lattice operators $\langle \pi\pi | Q_i^{\text{att}} | K \rangle$, in order to obtain A_2 we must renormalize the operators and apply finite-volume corrections. The latter are given by the Lellouch-Lüscher factor in terms of the s -wave $\pi\pi$ -phase shift [2] (the phase-shift can be obtained from $E_{\pi\pi}$ [16]). In order to combine our results with the Wilson coefficients calculated in the $\overline{\text{MS}}$ -NDR scheme [17–19], we perform the renormalization in 3 steps. We start by obtaining the renormalization constants in four RI-SMOM schemes using the procedures described in [5]. Because the lattice is coarse the renormalization scale is chosen to be low, 1.145 GeV, to avoid lattice artifacts. We determine the universal, nonperturbative continuum step-scaling function required to evolve the operators to 3 GeV using our Iwasaki lattices

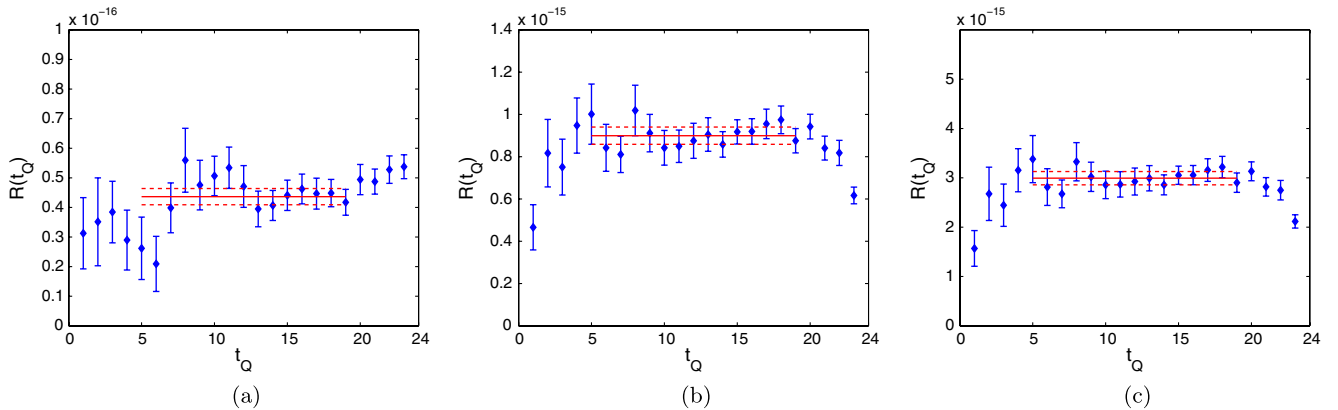


FIG. 1 (color online). $R(t_Q)$ for the 3 operators which contribute to $K \rightarrow (\pi\pi)_{I=2}$ decay amplitudes: (a) $(\bar{s}d)_L(\bar{u}d)_L$, (b) $(\bar{s}d)_L(\bar{u}d)_R$, and (c) $(\bar{s}^i d^j)_L(\bar{u}^j d^i)_R$, where $(\bar{s}d)_L(\bar{u}d)_{L,R} = (\bar{s}^i \gamma^\mu (1 - \gamma^5) d^i)(\bar{u}^j \gamma_\mu (1 \mp \gamma^5) d^j)$. i, j are color labels and t_K and $t_{\pi\pi}$ are 0 and 24.

[20,21]. Finally at 3 GeV we convert the results to the $\overline{\text{MS}}$ -NDR scheme using one-loop perturbation theory.

Our final results for the matrix elements in the $\overline{\text{MS}}$ -NDR scheme at a renormalization scale of 3 GeV are:

$$M_{(27,1)} = (3.20 \pm 0.13_{\text{stat}} \pm 0.58_{\text{syst}}) \times 10^{-2} \text{ GeV}^3, \quad (7)$$

$$M_{(8,8)} = (5.85 \pm 0.89_{\text{stat}} \pm 1.11_{\text{syst}}) \times 10^{-1} \text{ GeV}^3, \quad (8)$$

$$M_{(8,8)_{\text{mix}}} = (2.75 \pm 0.12_{\text{stat}} \pm 0.52_{\text{syst}}) \text{ GeV}^3, \quad (9)$$

where for each operator Q_i , $M_i = \langle \pi^+ \pi^+ | Q_i | K^+ \rangle$. In terms of these matrix elements, $A_2 e^{i\delta_2} = \sqrt{3}/2 (G_F/\sqrt{2}) \sum_i (V_{\text{CKM}})_i C_i M_i$, where the Wilson coefficients correspond to operators for the physical $K^+ \rightarrow \pi^+ \pi^0$ decays with the normalization $(\bar{s}d)_L [(\bar{u}u)_L - (\bar{d}d)_L] + (\bar{s}u)_L (\bar{u}d)_L$ for the (27, 1) operator and similarly for the EWP operators.

Combining the results in Eqs. (7)–(9) with the Wilson coefficients, CKM matrix elements, and G_F we find:

$$\text{Re} A_2 = (1.436 \pm 0.062_{\text{stat}} \pm 0.258_{\text{syst}}) \times 10^{-8} \text{ GeV} \quad (10)$$

$$\text{Im} A_2 = -(6.83 \pm 0.51_{\text{stat}} \pm 1.30_{\text{syst}}) \times 10^{-13} \text{ GeV}. \quad (11)$$

The result for $\text{Re} A_2$ agrees well with the experimental value of $1.479(4) \times 10^{-8} \text{ GeV}$ obtained from K^+ decays and $1.573(57) \times 10^{-8} \text{ GeV}$ obtained from K_S decays (the small difference arises from the unequal u and d quark masses and from electromagnetism, two small effects not included in our calculation). $\text{Im} A_2$ is unknown so that the result in Eq. (11) provides its first direct determination. For the phase of A_2 we find $\text{Im} A_2 / \text{Re} A_2 = -4.76(37)_{\text{stat}} \times (81)_{\text{syst}} \times 10^{-5}$.

The various sources of systematic error are analyzed in detail in [1] and our conclusions are summarized in Table II. The dominant source of uncertainty is due to lattice artifacts, and since we have a relatively coarse lattice and the matrix elements are proportional to a^{-3} , these errors are substantial. The estimate of 15% is obtained in two ways. First, in order to determine A_2 in physical units we must divide by a^3 , a quantity which varies by 12% when a is determined in physical units

TABLE II. Systematic error budget for $\text{Re} A_2$ and $\text{Im} A_2$.

	$\text{Re} A_2$	$\text{Im} A_2$
Lattice artifacts	15%	15%
Finite-volume corrections	6.2%	6.8%
Partial quenching	3.5%	1.7%
Renormalization	1.7%	4.7%
Unphysical kinematics	3.0%	0.22%
Derivative of the phase-shift	0.32%	0.32%
Wilson coefficients	7.1%	8.1%
Total	18%	19%

from a lattice determination of m_Ω , f_π , f_K , and r_0 . Second, we use the global fit described earlier to determine the a^2 correction in the similar matrix element $\langle K^0 | Q_{(27,1)}^{\Delta S=2} | \bar{K}^0 \rangle$. This correction is found to be 14%. The finite-volume uncertainties are estimated from the differences of infinite- and finite-volume one-loop chiral perturbation theory. The uncertainties in the Wilson coefficients are conservatively taken as the difference between the leading and next-to-leading order terms as defined in [22]. We estimate the truncation errors in the perturbative factors converting the operators to the $\overline{\text{MS}}$ -NDR scheme from the variation of the results obtained using different RI-SMOM intermediate schemes. We note also, that in contrast to $\Delta I = 1/2$ decays, all the quarks participating directly in $\Delta I = 3/2$ decays are valence quarks and in such cases the effect of using partially quenched or partially twisted boundary conditions is small [23]. For more details and for a discussion of the remaining uncertainties, due to the small difference from physical kinematics, and in the evaluation of the Lellouch-Lüscher factor and the step-scaling functions, we refer the reader to [1].

Using Eqs. (31), (32), and (40) of [24], our result for $\text{Im} A_2$ can be combined with the experimental results for $\text{Re} A_2$, $\text{Re} A_0 = 3.3201(18) \times 10^{-7} \text{ GeV}$, and ϵ'/ϵ to obtain the unknown ratio:

$$\frac{\text{Im} A_0}{\text{Re} A_0} = -1.63(19)_{\text{stat}}(20)_{\text{syst}} \times 10^{-4}. \quad (12)$$

This ratio allows us to determine in full QCD the effect of direct CP violation in $K_L \rightarrow \pi\pi$ on ϵ , customarily denoted by κ_ϵ [3], $(\kappa_\epsilon)_{\text{abs}} = 0.923 \pm 0.006$, where the subscript “abs” denotes that at present only the absorptive long-distance contribution ($\text{Im} \Gamma_{12}$) is included [4]. (The error is now dominated by the experimental uncertainty in ϵ'/ϵ .) The analogous contribution from the dispersive part ($\text{Im} M_{12}$) [4] is yet to be determined in lattice QCD, but we describe progress towards being able to do this in [25]. The continuum result $(\kappa_\epsilon)_{\text{abs}} = 0.92(2)$ in [3] was updated to $\kappa_\epsilon = 0.94(2)$ after the long-distance contributions to $\text{Im} M_{12}$ were included [4]. For a recent review of continuum determinations of A_0 and A_2 see [26].

Using our value of $\text{Im} A_2$ in Eq. (11) and taking the experimental value given above for $\text{Re} A_2$ from K^+ decays we obtain the EWP contribution to ϵ'/ϵ , $\text{Re}(\epsilon'/\epsilon)_{\text{EWP}} = -(6.52 \pm 0.49_{\text{stat}} \pm 1.24_{\text{syst}}) \times 10^{-4}$.

Conclusions and outlook. The *ab initio* calculation of the complex $K \rightarrow (\pi\pi)_{I=2}$ decay amplitude A_2 described above builds upon substantial theoretical advances, achieved over many years as outlined in the introduction. It is encouraging that the value we find for $\text{Re} A_2$ is in good agreement with experiment and we are also able to determine $\text{Im} A_2$ for the first time. It will be important to repeat this calculation using a second lattice spacing so that a continuum extrapolation can be performed thus eliminating the dominant contribution to the error, reducing the

total uncertainty to about 5%. We expect that the dominant remaining errors in A_2 will then come from the omission of electromagnetic and other isospin breaking mixing between the large amplitude A_0 and A_2 .

Much more challenging but of even greater interest is the application of these methods to the evaluation of A_0 allowing for a calculation of ϵ'/ϵ and an understanding of the $\Delta I = 1/2$ rule. Although the framework presented here will also support the calculation of A_0 , serious obstacles must be overcome. Much larger Monte Carlo samples will be required to remove the large fluctuations remaining after the contribution of the vacuum state has been removed. The antiperiodic boundary conditions for the d -quark field used in this Letter cannot be applied to the $I = 0 \pi\pi$ state. Instead more sophisticated boundary conditions, mixing quarks and antiquarks, and an isospin rotation, (G -parity boundary conditions) [14], must be used for both the valence and the sea quarks. Exploratory studies [7] suggest that obtaining adequate statistics will be practical with the next generation of machines which will become available to our collaboration within the next few months.

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