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A Virtual Tribute to Quark Confinement and the Hadron Spectrum (vConf21)

Direct CP violation and the $\Delta I = 1/2$ rule in $K \to \pi\pi$ decay in the Standard Model

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Abstract. We discuss the RBC & UKQCD collaborations' recent [1] lattice calculation of ϵ', the measure of direct CP-violation in kaon decays. This result significantly improves on our previous 2015 calculation, with nearly 4× the statistics and more reliable systematic error estimates. We discuss how our results demonstrate the Standard Model origin of the $\Delta I = 1/2$ rule, and present our plans for future calculations.

1 Introduction

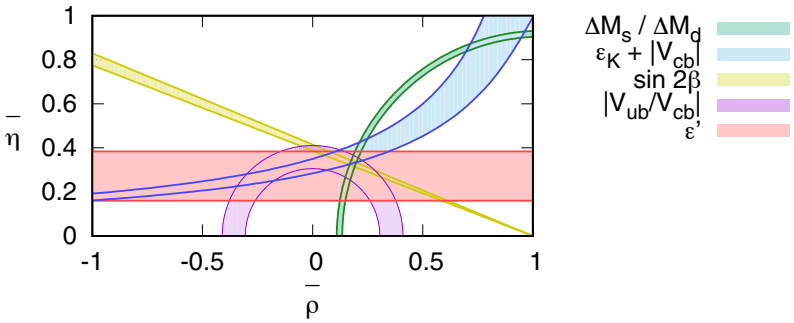

Figure 1. The CKM matrix unitarity triangle in the $\rho - \eta$ plane. The horizontal band is the constraint imposed by our calculation of ϵ'.

Direct CP-violation (CPV) in the decays of neutral kaons into two pions is highly suppressed in the Standard Model, making it an ideal probe for new sources of CPV. Beyond the Standard Model CPV processes appear necessary to explain the predominance of matter over antimatter in the observable Universe assuming that baryogeneses is responsible for this phenomenon. Measurements of these processes also provide a new, horizontal band constraint on the CKM matrix unitarity triangle in the $\rho - \eta$ plane, as illustrated in Fig. 1 where we compare the constraint from our calculation versus those of other sources.

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Direct CPV in kaon decays was first observed by the NA48 [2] and KTeV [3] experiments in the late 1990s, and the current world average of the measure of this phenomenon, ϵ', is [4]

$$\mathrm{Re}(\epsilon'/\epsilon) = 16.6(2.3) \times 10^{-4} \tag{1}$$

where ϵ is the measure of indirect CP-violation, itself heavily suppressed: $|\epsilon| = 2.228(11) \times 10^{-3}$. Unfortunately a correspondingly precise Standard Model prediction for this quantity has remained out of reach until recently, due to the fact that the underlying high-energy weak decay processes receive substantial corrections from low-energy hadronic physics that cannot be treated reliably with perturbation theory.

The first *ab initio* calculation of ϵ' in the Standard Model [5] was performed by the RBC & UKQCD collaborations in 2015 using lattice QCD, the only known systematically improvable (i.e. for which all systematic errors can be identified and reduced/eliminated with sufficient computational effort) technique for treating non-perturbative hadronic physics. The calculation was performed in three-flavor, isospin-symmetric QCD where ϵ' emerges from the difference between the complex phases of the decay amplitudes of neutral kaons into two-pions in the $I = 0$ (with amplitude A_0) and $I = 2$ (with amplitude A_2) isospin representations,

$$\epsilon' = \frac{i\omega e^{i(\delta_2 - \delta_0)}}{\sqrt{2}} \left(\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0} \right), \tag{2}$$

where $\omega = \mathrm{Re}A_2/\mathrm{Re}A_0$ and δ_I are the $\pi\pi$ scattering phase shifts. We obtained the following result,

$$\mathrm{Re}(\epsilon'/\epsilon) = 1.38(5.15)(4.59) \times 10^{-4} \tag{3}$$

where the errors are statistical and systematic respectively. This result exhibits a 2.1σ tension with the experimental number, providing strong motivation for an improved calculation. The calculation also exhibited an unexplained tension of a similar size in the $I = 0$ $\pi\pi$ scattering phase shift that we determine as a necessary component of the $K \to \pi\pi$ measurement, further spurring the desire for a follow-up work. In this document we present the results of an updated calculation [1] published in 2020, where we have reduced our statistical error by a factor of two and dramatically improved our understanding and confidence in the systematic error resulting from the contribution of excited $\pi\pi$ states – thus resolving the phase-shift discrepancy – alongside several other important systematic error sources. We also discuss our ongoing efforts to further refine our calculation over the coming years.

2 Summary of the calculations

We perform an isospin symmetric three-flavor calculation with degenerate light quarks, and a physical strange quark mass. The weak interaction is treated using first order weak effective theory, which for three-flavors is expressed as a Hamiltonian comprising ten four-quark operators Q_i with Wilson coefficients z_i and y_i that encapsulate the high-energy contributions and are computed using perturbation theory:

$$H_W = \frac{G_F}{\sqrt{2}} V_{ud}^* V_{us} \sum_{i=0}^{10} [z_i(\mu) + \tau y_i(\mu)] Q_i(\mu) \tag{4}$$

where $\tau = -\frac{V_{ts}^* V_{td}}{V_{us}^* V_{ud}}$. The $K \to \pi\pi$ amplitudes are then defined as

$$A^I = \langle (\pi\pi)_I | H_W | K^0 \rangle . \tag{5}$$

Both the Wilson coefficients and the operators require renormalization as indicated by the renormalization scale μ in Eq. (4), while their product is renormalization scheme independent. The renormalization is conventionally performed in the $\overline{\text{MS}}$ scheme which is not amenable to a lattice treatment as it involves fractional dimensions. Therefore, for the lattice calculation we first renormalize in an intermediate non-perturbative renormalization (NPR) scheme – the so-called RI-SMOM schemes – at a high energy at which the conversion factors relating the result to $\overline{\text{MS}}$ can be computed perturbatively. Note that the energy at which we perform this matching is bounded by the lattice cutoff and we must stay sufficiently below this scale to avoid discretization errors. This often leads to larger systematic errors arising from the truncation of the perturbative series used for the matching.

The $K \to \pi\pi$ matrix elements are obtained by fitting to three-point functions of the form

$$C_i(t, t_{\text{sep}}^{K\to\text{snk}}) = \langle 0|O_{\text{snk}}^{\dagger}(t_{\text{sep}}^{K\to\text{snk}})Q_i(t)O_K(0)|0\rangle \tag{6}$$

where O_K is the kaon operator, O_{snk} creates the $\pi\pi$ state and Q_i are the four-quark operators discussed above. The kaon and $\pi\pi$ operators actually generate *all* states with the corresponding quantum numbers, but due to the Euclidean time direction the contribution of each state dies away exponentially in lattice time according to their energy such that at large times only the lowest energy states have significant contributions. A key challenge of the lattice calculation is that with the typical periodic spatial boundary conditions, the O_{snk} operator also generates a state comprising two-pions at rest, hence the unphysical energy-nonconserving amplitude of a kaon of mass ∼500 MeV decaying into two pions of total energy ∼260 MeV dominates the signal at large times. Multi-state fits to extract the subdominant physical contribution are possible but it is often very difficult to reliably isolate the excited-state terms, particularly with noisy data. Therefore, for these calculations we instead take advantage of the ability to manipulate the spatial boundary conditions (BCs) while incurring only exponentially-suppressed finite-volume errors: In the $I = 2$ case an isospin rotation relates the amplitude of interest to $K^+ \to \pi^+\pi^+$. By replacing the periodic BCs of the down-quark with antiperiodic BCs, the charged pions in the final state also become antiperiodic and as a result their lattice momenta become discretized in odd-integer multiples of π/L where L is the lattice size. We are then able to tune L such that the lowest-energy state comprises two pions with a total energy that matches the kaon mass. Note that this operation explicitly breaks the isospin symmetry, but fortunately any mixing of the final state is prevented by virtue of it being the only allowed doubly-charged state. In the $I = 0$ case this isospin breaking cannot be avoided, therefore we instead utilize G-parity BCs, where a charge-conjugation and isospin rotation are performed at the lattice boundary. Both charged and neutral pions are negative eigenstates of G-parity hence we achieve the effect of imposing antiperiodic BCs on all pions without breaking isospin, at the cost of significantly increasing the computational expense of the lattice calculation[6].

2.1 2015 calculations

The $\Delta I = 3/2$ amplitude A_2 arises from three linear combinations of Q_i that are labeled by their representation under chiral $\text{SU}(3)_L \times \text{SU}(3)_R$. The dominant contribution to $\text{Re}A_2$ arises from the $(27, 1)$ combination, and $\text{Im}A_2$ is dominated by the remaining two $(8, 8)$ operators. The most recent calculation of A_2 [7] was performed in 2015 using physical light and strange quark masses, a large volume to reduce finite-volume systematic errors, and two lattice spacings allowing a continuum limit to be taken. We obtained the following results,

$$\text{Re}A_2 = 1.50(4)(14) \times 10^{-8}\ \text{GeV} \tag{7a}$$
$$\text{Im}A_2 = -6.99(20)(84) \times 10^{-14}\ \text{GeV} \tag{7b}$$

where the errors are statistical and systematic, respectively. A significant achievement of this calculation is obtaining a result with $< 1\%$ statistical errors despite having performed a continuum extrapolation. The systematic error is considerably larger and arises mainly from the truncation of the perturbative series used in the matching of our NPR scheme to $\overline{\text{MS}}$ (8%) and in the Wilson coefficients (12%). The value obtained for the real part agrees well with the experimental value of $\text{Re}A_2 = 1.4787(31) \times 10^{-8}$ GeV from charged kaon decays and $1.570(53) \times 10^{-8}$ GeV from neutral kaon decays.

The $\Delta I = 1/2$ amplitude A_0 receives contributions from all ten effective four-quark operators, with Q_2 the dominant contribution to the real part and Q_6, and to a lesser extent Q_4, dominating the imaginary part. In 2015 we performed the first calculation [5] of this amplitude. This calculation is much more expensive than that of A_2, not just due to the G-parity BCs but also because the $\pi\pi$ final state has vacuum quantum numbers and hence the calculation involves evaluating disconnected diagrams where the two pions are connected to the four-quark operator only through background gluons; these types of diagram are typically much more noisy and require larger statistics, along with more sophisticated methods, to adequately resolve. As a result we performed the calculation on only a single, somewhat coarse lattice spacing which allows us to simulate with a large physical volume, and thus have better control over finite-volume errors, at the cost of incurring larger discretization errors. We used a single $\pi\pi$ operator in which the two constituent pions are generated moving back-to-back with momentum $(\pm 1, \pm 1, \pm 1)\pi/L$. We label this operator $\pi\pi(111)$. For the A_0 amplitude we obtained

$$\text{Re}A_0 = 4.66(1.00)(1.26) \times 10^{-7} \text{ GeV} \tag{8a}$$

$$\text{Im}A_0 = -1.90(1.23)(1.08) \times 10^{-11} \text{ GeV}\,, \tag{8b}$$

where the relative error on the imaginary part is much larger than for the real part primarily due to a large cancelation between the dominant Q_4 and Q_6 contributions. Despite the coarse lattice spacing, the systematic error is again dominated by perturbative truncation errors. The real part agrees with the experimental result of $\text{Re}A_0 = 3.3201(18) \times 10^{-7}$ GeV.

Combining the above results for A_0 and A_2 using Eq. (2), we found

$$\text{Re}(\epsilon'/\epsilon) = 1.38(5.15)(4.59) \times 10^{-4}\,, \tag{9}$$

which is 2.1σ below the experimental value. While the errors on the calculation are large, roughly 3× those of the experiment, this result clearly demonstrates that ϵ' is now accessible to lattice calculation.

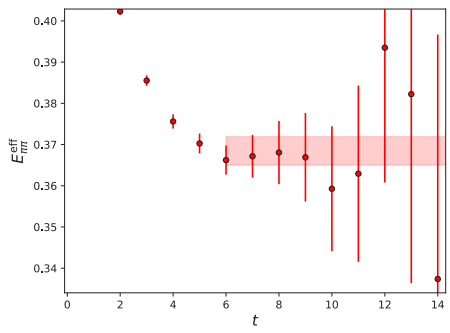

Figure 2. The $\pi\pi$ effective energy obtained using 1438 configurations with the $\pi\pi(111)$ operator.

A puzzle that arose from the $I = 0$ calculation is a $\sim 3\sigma$ disagreement between the value obtained for the $I = 0$ $\pi\pi$ scattering phase shift, $\delta_0(E_{\pi\pi} \approx m_K) = 23.8(4.9)(1.2)^\circ$, and the prediction of $\sim 39^\circ$ obtained by combining the dispersive Roy equations with experimental input [8]. This phase-shift, and the $\pi\pi$ energy from which it is derived, are necessary inputs to the $K \to \pi\pi$ calculation, hence it is vital that a reliable result is obtained. In order to address this issue, following the 2015 calculation we increased the statistics on the $\pi\pi$ measurement by almost $7\times$ but instead found that the disagreement became worse, with a value obtained of $19.1(2.5)^\circ$ [9]. The corresponding effective mass plot, the plateau value of which indicates the ground-state energy, is shown in Fig. 2. While the plateau appears clear, the rapid reduction of the signal-to-noise ratio makes the most likely explanation for this disagreement the existence of an excited state with an energy close to that of the ground-state, whose contribution is masked by the growth of the error bars.

2.2 Updated calculation of A_0 [1]

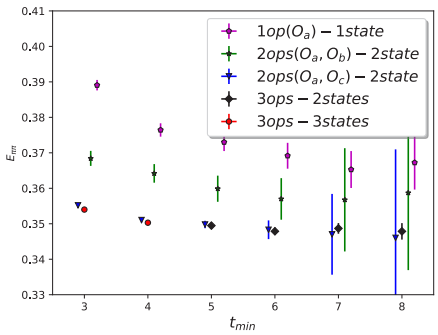

Figure 3. The $I = 0$ $\pi\pi$ energy obtained by varying the lower bound on the fit range $t_{\rm min}$, the number of operators and number of states. In the legend O_a, O_b, O_c correspond to the $\pi\pi(111)$, $\pi\pi(311)$ and σ operators, respectively. Our best fit is the 3-operator, 2-state result with $t_{\rm min} = 6$.

In order to address the possibility of excited-state contamination we introduced two additional $\pi\pi$ operators, the $\pi\pi(311)$ operator for which the two pions again move back-to-back but with momenta $(\pm 3, \pm 1, \pm 1)\pi/L$ and permutations thereof, and the $\sigma = (\bar{u}u + \bar{d}d)/\sqrt{2}$ operator, which also has vacuum quantum numbers and hence projects onto the $I = 0$ $\pi\pi$ state. This allows us to perform simultaneous fits to the matrix of $\pi\pi$ correlation functions obtained by varying the source and sink $\pi\pi$ operator to extract the energies and amplitudes of multiple $\pi\pi$ states with considerably higher precision and control. The power of this method is illustrated in Fig. 3 where we show the fitted $\pi\pi$ energy as we vary the number of operators used and the number of states to which we fit. Clearly a significant advantage is gained in both the statistical error and the quality of the plateau. This calculation was performed on $3.4\times$ statistics of our original 2015 calculation. We found [9]

$$\delta_0(471\ \text{MeV}) = 32.3(1.0)(1.4)^\circ\,, \tag{10}$$

which is in much better agreement with the dispersive prediction at this energy of 35.9°. We therefore conclude that excited state contamination was indeed responsible for the disagreement and that it has now been resolved.

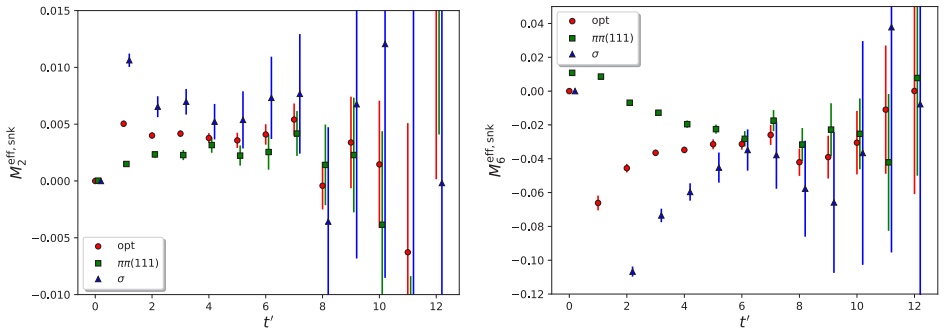

Figure 4. The effective matrix elements of the Q_2 and Q_6 operators for the $\pi\pi(111)$, σ and optimal operators as a function of the time separation t' between the four-quark operator and the $\pi\pi$ sink operator.

The additional operators also had a significant effect on the fits to the $K \to \pi\pi$ matrix elements. In Fig 4 we plot the effective matrix elements defined as,

$$\begin{aligned} M_i^{\text{eff,snk}}(t') &= C_i(t, t_{\text{sep}}^{K\to\text{snk}})\left(\frac{1}{\sqrt{2}} A_K A_{\text{snk}}^0 e^{-m_K t} e^{-E_0(t_{\text{sep}}^{K\to\text{snk}}-t)}\right)^{-1} \\ &= M_i^0 + \sum_j \frac{A_{\text{snk}}^j}{A_{\text{snk}}^0} M_i^j e^{-(E_j-E_0)t'} \,. \end{aligned} \tag{11}$$

where $t' = t_{\text{sep}}^{K\to\text{snk}} - t$ and C_i are defined in Eq. 6. Here A_K and m_K are the ground-state kaon operator-overlap coefficient and mass, respectively, A_{snk}^j and E_j are the operator-overlap and energy of the $\pi\pi$ ground and excited states, for which the results are obtained from their respective two-point function fits. We apply a uniform cut of $t_{\text{min}} = 6$ to ensure that only the kaon ground state contributes. These effective matrix elements converge to the desired matrix elements M_i^0 at large t'. In the figure we compare the $\pi\pi(111)$ and σ effective matrix elements against the optimal combination of those two operators that best projects onto the ground state. As in the case of the $\pi\pi$ fits, we observe that the additional operators have a significant impact on both the statistical error and the length and quality of the plateau.

In Fig. 5 we plot the fit results for the Q_2 and Q_6 operators as we vary the number of operators, states and the temporal cuts. For Q_2, the dominant contribution to $\text{Re}A_0$, we find good agreement between all of the fits for $t'_{\text{min}} \geq 4$, although we see improved statistical errors with the additional operators. However for Q_6, the dominant contribution to $\text{Im}A_0$, we see a clear pattern of excited state contamination in the one and two-operator fit results, the latter converging later than the former as we would expect. The final best fit for all operators was obtained with three operators and two states with $t'_{\text{min}} = 5$ and $t_{\text{min}} = 6$. The best fit from the 2015 calculation would correspond here to the "1×1 $t_{\text{min}} = 6$" point with $t'_{\text{min}} = 4$, which we see is very different from our new best fit; unfortunately this implies that our $\leq 5\%$ estimate for the excited state contamination in our 2015 calculation was significantly underestimated.

Another notable improvement in this updated calculation is the use of the "step-scaling" technique [10] in the non-perturbative renormalization. Due to the rather coarse lattice spacing, the errors resulting from the truncation of the perturbative series in the RI-SMOM$\to \overline{\text{MS}}$ matching were estimated to be 15% for the 2015 calculation of A_0. Step-scaling is a procedure whereby the matrix parameterizing the non-perturbative running between a low and high

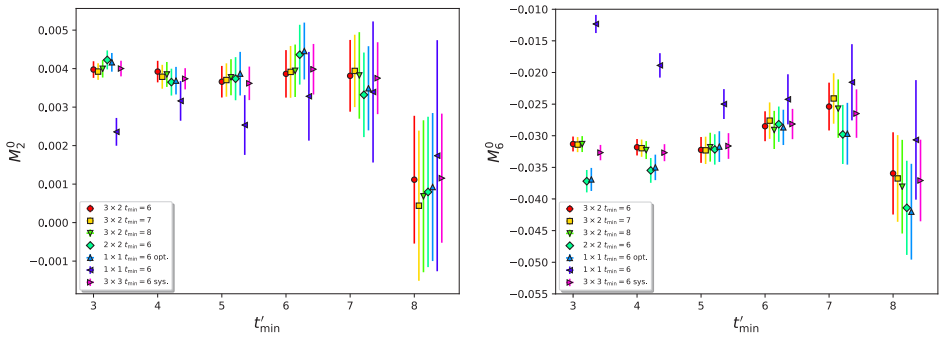

Figure 5. The fitted ground-state matrix elements of the Q_2 and Q_6 operators for various choices of the number of operators, number of states and the cut t_{min} between the kaon and four-quark operators, as a function of the cut t'_{min} between the four-quark operator and the $\pi\pi$ sink. In the legend "$a \times b$" indicates the fit was performed with a operators and b states, and "opt." indicates the optimal operator was used. In the two-operator case we drop the $\pi\pi(311)$ operator and in the one-operator case we further drop the σ. The "sys." results are obtained using three operators and three states for both the $\pi\pi$ and $K \to \pi\pi$ fits and is used in the systematic error estimation. The values are shifted for clarity.

energy scale is computed a fine lattice. The low scale is one that is accessible to the coarse lattice calculation and the high scale is only accessible to the fine lattice. As this running is universal it can be used to run the matrix of renormalization factors determined on the coarse lattice at the low scale to a scale much higher than the lattice cutoff. For the updated calculation we used this procedure to raise the renormalization scale from 1.53 GeV to 4 GeV, which reduced the corresponding systematic error by a factor of 3×. Unfortunately we did not observe a corresponding decrease in the systematic error arising from the use of perturbation theory to compute the Wilson coefficients, which are also evaluated at this 4 GeV scale, due to the fact that perturbation theory is still being applied to match between the 4- and 3-flavor theories at the charm mass scale $m_c \approx 1.3$ GeV.

3 Results of the updated calculation

3.1 The $\Delta I = 1/2$ rule

A longstanding puzzle in $K \to \pi\pi$ physics relates to the experimental observation that the $\Delta I = 1/2$ decay is ∼500 more common than the $\Delta I = 3/2$ decay. This $\Delta I = 1/2$ rule is reflected in the ratio

$$\frac{1}{\omega} = \frac{\text{Re}A_0}{\text{Re}A_2} = 22.45(6)\,, \tag{12}$$

the inverse of which appears as a coefficient in the equation for ϵ', Eq. (2). The perturbative running from the weak to the charm scale can be shown to give rise to a factor of two difference in the amplitudes, but there has been no widely accepted explanation as to the origin of the remaining factor of 10. With our lattice calculation we are now able to answer this question: in computing $\text{Re}A_2$ we found a strong, 70%-level cancelation between the two dominant diagrams C_1 and C_2 of the $(27, 1)$ operator amplitude as illustrated in Fig. 6. This is very different from the behavior predicted by naïve color counting which suggests these terms should have the same sign and differ by a factor of three in magnitude. From our lattice

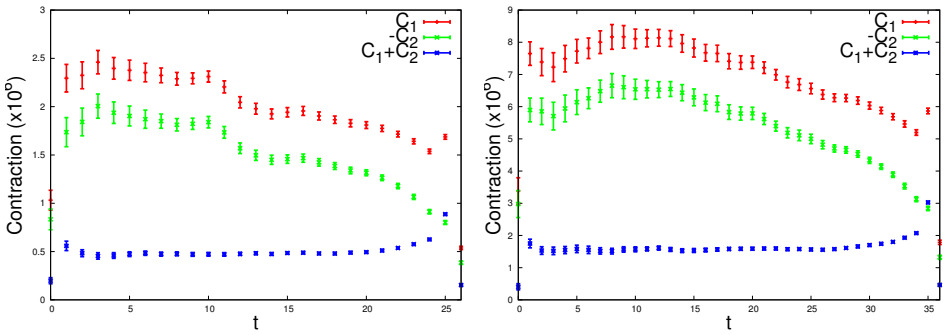

Figure 6. The two dominant contributions C_1 and C_2 to $\mathrm{Re}A_2$ and their sum on the 48I (left) and 64I (right) ensembles, reproduced from Fig. 11 of Ref. [7].

calculation we obtain

$$\frac{1}{\omega} = \frac{\mathrm{Re}A_0}{\mathrm{Re}A_2} = 19.9(5.0) \tag{13}$$

which is completely consistent with the experimental number. We therefore conclude that the $\Delta I = 1/2$ rule is a consequence of low-energy QCD.

3.2 A_0 and ϵ'

For the updated calculation we obtain

$$\mathrm{Re}A_0 = 2.99(0.32)(0.59) \times 10^{-7} \text{ GeV} \tag{14a}$$

$$\mathrm{Im}A_0 = -6.98(0.62)(1.44) \times 10^{-11} \text{ GeV} \tag{14b}$$

The former agrees well with the experimental result $\mathrm{Re}A_0 = 3.3201(18) \times 10^{-7}$ GeV and with our previous result. The value for $\mathrm{Im}A_0$ differs substantially from our previous result however, which gives rise to a similarly large change in ϵ':

$$\mathrm{Re}(\epsilon'/\epsilon) = 21.7(2.6)(6.2)(5.0) \times 10^{-4}\,. \tag{15}$$

Here the first set of parentheses gives the statistical error. The systematic error has been broken into two contributions: the third set of parentheses corresponds to an estimate (23%) of the effects of isospin breaking (IB) and electromagnetism (EM) obtained through next-to-leading order chiral perturbation theory with input from the $1/N_c$ expansion [11]. These effects were not formerly included in the budget as the result was considered a pure-QCD calculation. EM+IB effects typically enter at the percent scale in hadronic quantities, but for $K \to \pi\pi$ their relative effects are enhanced due to the 20× suppression of A_2 by the mechanics of the $\Delta I = 1/2$ rule. The remaining systematic error is given by the second set of parentheses and is dominated by the discretization error (12%) and the perturbative truncation error in the Wilson coefficients (12%). The excited state systematic error is treated as negligible compared to the other sources of error given the control over such effects provided by the multi-operator method demonstrated in the previous section.

This result for $\mathrm{Re}(\epsilon'/\epsilon)$ is now in good agreement with the experimental number.

4 Conclusions and outlook

The RBC & UKQCD collaborations have completed an update [1] to our 2015 calculation [5] of A_0. Among the notable changes are a 3.4× increase in the number of measurements; the addition of two more $\pi\pi$ operators to the data which vastly improves the statistical resolution and the quality of the fit plateaus, and also resolves a discrepancy previously observed between the lattice and dispersive predictions of the $I = 0$ $\pi\pi$ scattering phase shift at the kaon mass scale; and the use of step-scaling to raise the renormalization scale from 1.53 GeV to 4 GeV resulting in a 3× improvement in the formerly-dominant error resulting from the $\overline{\text{MS}}$ matching. By combining the results with our earlier calculation of A_2 we obtain an *ab initio* determination of $\text{Re}A_0/\text{Re}A_2$ that is consistent with experiment and thus demonstrate that the $\Delta I = 1/2$ rule mainly arises from non-perturbative QCD effects. We also obtain a result for $\text{Re}(\epsilon'/\epsilon)$ that is now consistent with the experimental value and has a total error that is ∼3.6× that of the experiment.

We believe that ϵ' remains a promising avenue in which to search for new physics, and since the recent publication have commenced work towards further improving our result. The most significant single source of error is due to the missing contributions of isospin breaking and electromagnetism. Unfortunately the lattice treatment of electromagnetism is complicated by the long-range nature of its interactions and so significant theoretical hurdles must be overcome before a first principles calculation is possible. We are presently exploring a novel technique for treating the interactions using a truncated potential in Coulomb gauge where the truncation range is set to confine the interaction within the finite box resulting in finite-volume errors that can be treated analytically using infinite-volume perturbation theory [12].

A second significant source of error arises from the use of perturbation theory to match between the four- and three-flavor effective theories in the Wilson coefficients. While a four-flavor lattice calculation with physical charm quarks is possible, the requirement of large statistics, a fine lattice spacing to control charm discretization effects and a large volume to control finite-volume effects puts this outside of the reach of present and near-future supercomputers. In the interim we are investigating the possibility of computing the $4 \to 3$f matching non-perturbatively [13, 14].

The dramatic improvement in control over excited state effects that we discussed in this document has reopened the question as to whether we can perform multi-state fits to extract the physical $\Delta I = 1/2$ matrix element from a calculation with periodic boundary conditions, forgoing the use of the computationally-expensive G-parity boundary conditions to remove the dominant contribution of the unphysical decay of the kaon to a stationary $\pi\pi$ state. We are presently conducting a preliminary calculation on two different coarse lattices to evaluate this approach [15].

Finally, the largest pure-lattice systematic error is due to the fact that A_0 has only been computed at a single, somewhat coarse lattice spacing. We are presently generating two additional ensembles with G-parity boundary conditions which will allow for the controlled continuum extrapolation of our result for A_0 [16], eliminating this source of error.

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