PROCEEDINGS OF SCIENCE

Progress towards an improved lattice calculation of Standard Model direct CP-violation in kaon decays

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We discuss progress towards the RBC & UKQCD collaborations' next generation of measurements of Standard Model direct CP-violation in kaon decays with G-parity boundary conditions, for which we aim to leverage the power of the upcoming exascale computers to perform the continuum limit and thus eliminate this dominant lattice systematic error.

The 39th International Symposium on Lattice Field Theory,
8th-13th August, 2022,
Rheinische Friedrich-Wilhelms-Universität Bonn, Bonn, Germany

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PoS(LATTICE2022)415

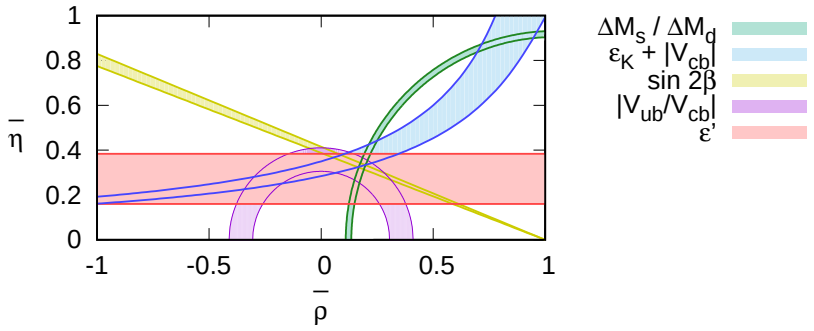

Figure 1: A comparison of the constraints imposed by several quantities on the apex of the CKM unitarity triangle in the $\rho - \eta$ plane.

Direct CP violation – the form of CP violation occuring in particle decays – was first discovered in the late 1990s by the NA31/NA48 experiments at CERN and the KTeV experiment at FermiLab in the decays of neutral kaons into two pions. It is conventionally expressed as $\mathrm{Re}(\epsilon'/\epsilon)$ where ϵ' and ϵ are the measures of direct and indirect CP violation, respectively. This quantity can be obtained by measuring the ratios of amplitudes of the long and short-lived neutral kaon species decaying into pairs of neutral and charged pions:

$$\eta_{00} = \frac{A(K_L \to \pi^0\pi^0)}{A(K_S \to \pi^0\pi^0)} \qquad \eta_{+-} = \frac{A(K_L \to \pi^+\pi^-)}{A(K_S \to \pi^+\pi^-)} \tag{1}$$

from which

$$\mathrm{Re}(\epsilon'/\epsilon) \approx \frac{1}{6}\left(1 - \left|\frac{\eta_{00}}{\eta_{+-}}\right|^2\right) = 16.3(2.3) \times 10^{-4} \tag{2}$$

where the value provided is the current world average [2].

Given that ϵ itself is small ($|\epsilon| = 2.228(11) \times 10^{-3}$), ϵ' is very small indeed, which makes it an ideal probe for new sources of CP violation that are expected to arise through Beyond the Standard Model physics. This search touches on one of the most important open questions in cosmology: the origin of the matter/antimatter asymmetry in the observable Universe, for which CP violation is a necessary condition for baryogenesis and the amount of CP violation in the Standard Model does not appear sufficient.

ϵ' also provides a new horizontal-band constraint on the apex of the CKM unitarity matrix in the $\rho - \eta$ plane. In Fig. 1 we compare the constraint imposed by our calculation of ϵ' to several others. While the errors are somewhat large at present, our continuing work on improving the calculation might be expected to yield a competitive constraint within the timescale of a decade.

While the underlying physics of the decay is governed by second-order Weak interactions occuring at the electroweak energy scale $O(80\ \mathrm{GeV})$, the process receives large corrections from non-perturbative QCD effects occuring at low energy scales $O(\Lambda_{\mathrm{QCD}} \approx 250\ \mathrm{MeV})$, a regime in which first-principles perturbative methods are inapplicable. As a result, despite the experiments being performed over 20 years ago, it is only recently that reliable Standard Model determinations of ϵ' have become possible through a combination of fundamental theoretical and algorithmic advances in the field of lattice QCD – which offers the only known systematically-improvable

technique for studying low-energy strong dynamics – and the development of sufficiently capable computational hardware.

In these proceedings we provide an overview of the lattice approach and the most recent results, followed by a discussion of our ongoing work to further improve the calculation.

1. Lattice approach

For CP-violation to occur it is necessary for the decay or mixing process to occur via two channels with different strong and weak phases such that an imbalance between the process and its CP conjugate can appear through interference. In the neutral kaon decays these different pathways arise from the nearly-conserved isospin symmetry, where the decay can occur into two pions in either the $I = 2$ or $I = 0$ isospin representations:

$$A(K^0 \to (\pi\pi)_{I=0}) = A_0 e^{i\delta_0} \qquad A(K^0 \to (\pi\pi)_{I=2}) = A_2 e^{i\delta_2} \tag{3}$$

where A_I are the (complex) isospin amplitudes and δ_I are the strong phases, which arise due to interations between the final state pions and correspond to the $\pi\pi$ scattering phase shifts. We perform our lattice calculation with equal up and down quark masses, hence it is convenient to continue to express ϵ' purely in terms of these isospin amplitudes:

$$\epsilon' = \frac{i\omega e^{\delta_2-\delta_0}}{\sqrt{2}}\left(\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}\right) \tag{4}$$

where $\omega = \mathrm{Re}A_2/\mathrm{Re}A_0$. Due to the difference in energy scales, the isospin amplitudes can be very accurately expressed in terms of first-order weak effective theory, $A_I = \langle(\pi\pi)_I|H_W|K^0\rangle$, where H_W is the $\Delta S = 1$ weak Hamiltonian. We use the three-flavor effective theory as the lattice spacings used for our calculations are not yet fine enough to reliably include a dynamical charm quark. In this theory,

$$H_W = \frac{G_F}{\sqrt{2}} V_{us}^* V_{ud} \sum_{i=1}^{10} [z_i(\mu) + \tau y_i(\mu)] Q_i(\mu), \tag{5}$$

where Q_i are effective four-quark operators describing the low-energy interactions and z_i, y_i are Wilson coefficients encapsulating the high-energy physics that are computed perturbatively and are available at NLO in the $\overline{\mathrm{MS}}$ scheme [3]. Both the Wilson coefficients and four-quark operators are renormalization scheme dependent and so care must be taken to ensure that their schemes match. In the above, $\tau = -\frac{V_{ts}^* V_{td}}{V_{us}^* V_{ud}} = 0.0014606 + 0.00060408i$, for which the imaginary part is responsible for the CP violation. On the lattice we must compute

$$\mathcal{M}_i = F\langle(\pi\pi)_I|Q_i(\mu)|K^0\rangle \tag{6}$$

where F is the Lellouch-Lüscher finite volume correction. We also compute the $\pi\pi$-scattering phase shifts on the lattice. As the $\overline{\mathrm{MS}}$ scheme involves fractional dimensions, it is not directly accessible to a lattice calculation. Instead we renormalize into an intermediate non-perturbative scheme, the regularization-independent momentum scheme with symmetric kinematics (RI-SMOM), in which we run to a sufficiently high scale at which the conversion between this scheme and $\overline{\mathrm{MS}}$ can be performed reliably in (continuum) perturbation theory. Note that the scale at which the non-perturbative renormalization (NPR) can be applied is limited by the inverse lattice spacing of the calculation.

2. $I = 2$ calculation

The $I = 2$ amplitude can be measured very precisely using mostly conventional lattice techniques. The primary difficulty arises from the fact that the lightest $\pi\pi$ state, which will dominate the lattice matrix element at large times, comprises two pions at rest with energy ~ 260 MeV and therefore corresponds to an unphysical, energy non-conserving decay from a stationary kaon of mass ~ 500 MeV.

While one could attempt to directly extract the desired matrix element as an excited-state contribution, reliably isolating such subdominant terms can be very challenging. Instead, for our existing lattice calculations we exploit the finite volume and modify the spatial boundary conditions (BCs) for the down-quark propagator such that the charged pions become antisymmetric in the boundary and thus have momenta discretized in odd-integer multiples of π/L where L is the lattice size. By then tuning L we can raise the ground-state energy of the $\pi\pi$ system to match that of the kaon. This technique explicitly breaks isospin and applies only to the charged pions (for neutral pions the quark momenta cancel), however a Wick rotation allows the amplitude to be expressed in terms of the decay $K^+ \to \pi^+\pi^+$ which involves only charged pions and avoids the mixing of isospin representations induced by breaking the symmetry by virtue of being the only doubly-charged state.

For our most recent calculation [4] we obtained

$$\mathrm{Re}A_2 = 1.50(4)(14) \times 10^{-8}\ \ \mathrm{GeV} \tag{7}$$

$$\mathrm{Im}A_2 = -6.99(20)(84) \times 10^{-14}\ \ \mathrm{GeV} \tag{8}$$

where the errors are statistical and systematic, respectively. Here the value for $\mathrm{Re}A_2$ agrees well with the experimental value of $\mathrm{Re}A_2 = 1.4787(31) \times 10^{-8}$ GeV.

The calculation was performed with physical quark masses and large physical volumes of $(5.5\ \mathrm{fm})^3$ to control finite-volume effects. It achieved a very high statistical precision of $O(1\%)$ despite incorporating a full continuum limit extrapolation over two lattice spacings. The systematic error of $O(10\%)$ is dominated by perturbative truncation errors in the Wilson coefficients and in the RI-SMOM$\to \overline{\mathrm{MS}}$ matching coefficients. We discuss these systematic errors and potential avenues to reduce them later in this document.

An interesting result of this calculation is an explanation for the "$\Delta I = 1/2$ rule", a name given to the previously mysterious experimental observation of a factor of 20 difference in $\mathrm{Re}A_0$ vs $\mathrm{Re}A_2$:

$$\frac{1}{\omega} = \frac{\mathrm{Re}A_0}{\mathrm{Re}A_2} = 22.45(6)\,. \tag{9}$$

The quantity ω above enters in the expression for ϵ' and is part of the explanation for its small magnitude. A factor of 2 can be explained by the perturbative running from the weak scale to the hadronic scale. A conclusive demonstration of the origin of the remaining factor of 10 was obtained by our lattice calculation, in which we noted a 70%-level cancelation of the two dominant non-perturbative contributions [4] to $\mathrm{Re}A_2$ that is not prediced by naïve factorization. Combined with our lattice calculation of $\mathrm{Re}A_0$ we obtain

$$\frac{\mathrm{Re}A_0}{\mathrm{Re}A_2} = 19.9(5.0)\,, \tag{10}$$

in good agreement with the experimental number.

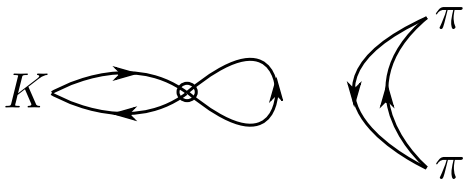

Figure 2: The *type4* disconnected diagrams contributing to the $I = 0$ amplitude. Here the two halves of the diagram are coupled only by sea gluons and as such are very statistically noisy.

3. $I = 0$ calculation and ϵ'

The $I = 0$ calculation is considerably more challenging than the $I = 2$ for two reasons: Due to its vacuum quantum numbers, the $I = 0$ calculation necessarily involves disconnected contributions of the form illustrated in Fig. 2 which are very difficult to compute precisely on the lattice. Secondly, the isospin symmetry breaking induced by imposing antiperiodic BCs on the down quark propagator cannot be avoided and alternative approaches must be explored. We address the first challenge by measuring with very high statistics and by utilizing the all-to-all propagator techniques of Ref. [5] to carefully tune the spatial shape of the two-pion source to maximize the overlap with the state of interest and minimize the overlap with the vacuum. For the second we employ a different form of spatial boundary condition, G-parity BCs [6], under which both neutral and charged pions are antiperiodic and the isospin symmetry is preserved. This technique comes with the cost of significantly increasing the computational expense of the calculation and requiring new, custom gauge configurations with G-parity BCs to be generated.

Due to the significantly higher cost, our most recent calculation [1] was performed with a single, rather coarse lattice spacing ($a^{-1} = 1.38$ GeV). However, we performed over 700 measurements with physical pion masses and a large volume of $(4.6\text{ fm})^3$ to control finite volume effects, and utilized three different two-pion operators to reliably extract the ground-state matrix element. We also employed the step-scaling technique to circumvent the limit on the NPR renormalization scale imposed by the coarse lattice spacing, running to a scale of $\mu = 4.006$ GeV at which the perturbative truncation systematics errors are only $O(5\%)$.

We obtained

$$\mathrm{Re}A_0 = 2.99(0.32)(0.59) \times 10^{-7}\ \text{GeV} \tag{11}$$

$$\mathrm{Im}A_0 = -6.98(0.62)(1.44) \times 10^{-11}\ \text{GeV} \tag{12}$$

where the errors are again statistical and systematic, respectively. The real part also agrees with the experimental result of $\mathrm{Re}A_0 = 3.3201(18) \times 10^{-7}$ GeV.

Despite the challenges we achieved a statistical precision of $O(10\%)$. The systematic error is dominated by finite lattice spacing effects (12%) and perturbative truncation errors on the Wilson coefficients (12%).

Combining our lattice results for the phase shifts and the imaginary components of the amplitudes with the experimental values of the real parts, which are much more precisely known, we obtained

$$\mathrm{Re}(\epsilon'/\epsilon) = 21.7(2.6)(6.2)(5.0) \times 10^{-4}, \tag{13}$$

which agrees with the experimental number of $\mathrm{Re}(\epsilon'/\epsilon) = 16.3(2.3)\times10^{-4}$. Here the first and second errors are the statistical error and the systematic error arising from lattice sources, respectively. The contribution of A_0 to the difference appearing in the parentheses of Eq. 4 is about 4× larger than that of A_2, hence it is the systematic errors on A_0 that dominate here, specifically those on the Wilson coefficients and due to discretization effects. The third error in the above is an estimate of the effects of electromagnetism and isospin breaking on ϵ', and will be discussed further below.

While further improving the statistical error remains a goal, the primary challenges are addressing the three dominant systematic errors described above. Below we will address each in turn.

4. Systematic errors on the Wilson coefficients

Despite raising the renormalization scale μ to 4 GeV in the calculation of A_0, the systematic error on the Wilson coefficients remains large due to its reliance on perturbation theory to match between the 4- and 3-flavor theories at the scale of the charm quark mass, m_c∼1.3 GeV.

At present the perturbative calculation of the Wilson coefficients is only available at NLO [3], but progress towards an NNLO calculation is underway [7] for which the authors claim a significant reduction in the systematic uncertainties; however the lack of any publications on the topic for more than 4 years suggests progress may have stalled. As an alternative, the RBC & UKQCD collaborations are exploring a direct lattice calculation of the $4 \to 3$f matching matrix [8] utilizing 4- and 3-flavor matrix elements evaluated non-perturbatively at scales much lower than the charm mass on a fixed 3-flavor background ensemble. In order to avoid unwanted mixing with irrelevant operators introduced by the gauge-fixing employed in the RI-MOM method, which becomes increasingly important at lower energies, a position-space renormalization approach is employed. A preliminary demonstration of this approach showing good potential has been performed on a $16^3 \times 32$, $a^{-1} = 1.78$ GeV domain wall ensemble.

In the longer term we intend to perform our calculation directly in the 4-flavor regime with a dynamical charm quark, eliminating the matching as a source of error. However the requirement of fine lattice spacings to control charm discretization effects coupled with the large volume and high statistics demands of the $K \to \pi\pi$ calculation likely puts this beyond the reach of present and near-term supercomputers.

5. Electromagnetism and isospin-breaking (EM+IB) effects

We perform our lattice calculation with equal up- and down-quark masses and without including electromagnetism. The contributions of these phenomena are expected to be much larger for ϵ' than the typical percent-scale effects present in most lattice calculations because the "$\Delta I = 1/2$ rule" suppression of A_2 results in a 20× relative enhancement in their size for this quantity, and a corresponding $O(20\%)$ effect on ϵ'. The current best determination [9] uses NLO chiral perturbation theory with some of the important low-energy constants estimated using the $1/N_c$ expansion, and predicts a 23% correction that we incorporate as a separate systematic error. In the future, lattice calculations might be employed to remove the dependence on the unreliable $1/N_c$ expansion and reduce the systematic error on this prediction.

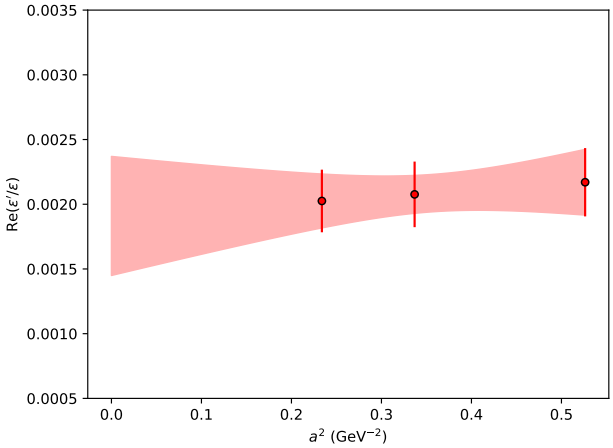

Figure 3: An illustration of the continuum extrapolation of $\mathrm{Re}(\epsilon'/\epsilon)$ using our three ensembles. The existing 32ID result is the rightmost point, and we have added representative points for the 40ID (middle) and 48ID (left) ensembles assuming comparable relative statistical errors and with a slope based on our 12% discretization error estimate.

The RBC & UKQCD collaborations are aiming to attempt a more ambitious goal of directly computing the EM+IB contributions to ϵ' via a lattice calculation. This is very challenging for a number of fundamental, theoretical reasons: The long-range nature of QED interactions must be reconciled with the finite-volume nature of lattice calculations and the locality assumptions of the Lellouch-Lüscher formalism; the mixing of two-pion states in the decay product prevents the use of isospin-definite states and requires a more complex treatment; and soft-photon emission in the decay product introduces additional multi-particle finite-volume states into an already complex problem. A promising start has been made in solving these issues [10], whereby the Coulomb gauge is employed to separate the QED contributions into those of a static Coulomb potential and of transverse photons. The dominant Coulomb potential contribution is treated with a spatial truncation method that eliminates the power-law finite-volume terms, leaving only exponentially small corrections. The truncation removes only long distance effects which can be computed analytically and corrected for. In Ref. [10] this approach was successfully demonstrated in the context of $\pi^+\pi^+$ scattering, although a complete application to $K \to \pi\pi$ will require additional work including developing an approach to computing the transverse radiation contributions, or otherwise demonstrating that they are small enough to be treated as a systematic error.

6. Discretization effects

The primary pure-lattice error is due to discretization effects on A_0, which are enhanced by our use of a coarse, $a^{-1} = 1.38$ GeV lattice. The 12% estimate for this systematic is obtained by studying the scaling behavior of the $I = 2$ operators, but the reliability of this estimate is unclear and there may be a considerable "error-on-the-error". It is therefore desirable to perform additional measurements with different lattice spacings. Unfortunately, these ensembles are substantially more expensive to generate than typical domain wall configurations due to the G-parity BCs, for which the Dirac operator is intrinsically twice as expensive numerically to apply and requires an additional and also

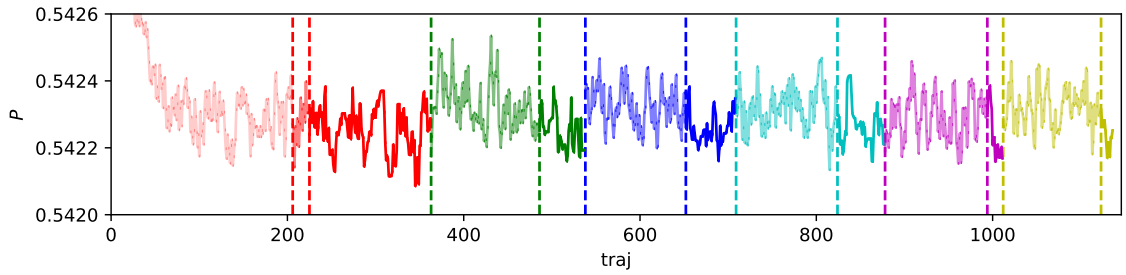

Figure 4: The plaquette history of the 40ID ensemble. 6 streams are generated in total, 5 of which are generated from the first using starting configurations after the initial thermalization period. The 6 streams are placed contiguously left-to-right and colored differently. Each stream underwent multiple phases which are demarked by regions bounded by vertical lines: a thermalization period is indicated by the lighter shaded region, and was performed without the Metropolis accept/reject enabled. This initial evolution of the first stream was performed using a lighter quark mass which was later adjusted, with this transition marked by the first red vertical line. For the other streams the thermalization phase was performed using relaxed tolerances and larger step sizes to reduce the job times by 3× and thus accelerate the decorrelation from the original stream. The last phase of each stream and indicated by the darkest color has the accept/reject enabled.

expensive square-rooting of the light-quark action (using the exact one-flavor algorithm). Similar issues apply in the context of the measurements. However, with the advent of the pre-exascale and exascale supercomputers in the U.S., tackling this issue is now computationally feasible. To this end we have invested considerable effort into porting and optimizing our configuration generation and measurement code, which use a combination of the Grid and CPS libraries, to support the NVidia, AMD and Intel GPU architectures on these machines.

Using early-access time on the NERSC Perlmutter system, we have commenced generation of two new ensembles; a $40^3 \times 64 \times 12$ with $a^{-1} = 1.723$ GeV (labeled "40ID") and a $48^3 \times 64 \times 12$ with $a^{-1} = 2.068$ GeV ("48ID"). For both ensembles we use the same Möbius domain wall fermion and Iwasaki+DSDR gauge actions as our previous ensemble. The volumes were carefully chosen to ensure that all three ensembles have the same physical volume which, coupled with G-parity BCs in 3 directions and physical pion masses, retains the physical decay matrix element as the ground-state $K \to \pi\pi$ contribution. Together these three ensembles will provide a considerable a^2 lever arm for a continuum limit, as illustrated in Fig. 3.

Thermalization and initial tuning of the 40ID ensemble was performed on a single stream, after which 5 additional streams were started, based off configurations from the first, in order to increase throughput. The plaquette history and a detailed description of the streams is given in Fig. 4. We achieve 83% Metropolis acceptance, with each trajectory requiring 5.9 hours on 32 nodes (128 NVidia A-100 GPUs) of Perlmutter with the Phase 1 (Slingshot 10) network and 4.7 hours after the upgrade to the Phase 2 (Slingshot 11) network. Some headway was also made in thermalizing the 48I ensemble but the additional cost made it challenging to achieve a good acceptance within the job constraints, and so we have chosen to focus initially on the cheaper 40ID ensemble.

7. Conclusions

We presented a summary of the RBC & UKQCD collaborations' ongoing work to improve our calculation of direct CP-violation in $K \to \pi\pi$ decays on the lattice. We have identified three primary sources of systematic error that dominate the error budget: The error arising from the truncation of the perturbative series in the calculation of the Wilson coefficients is expected to be improved by the release of NNLO perturbation theory results, and we are also pursuing a strategy of computing the $4 \to 3$ flavor matching matrix non-perturbatively, which combined with the perturbation theory can be expected to considerably reduce the uncertainty. The error resulting from not incorporating electromagnetism and isospin-breaking effects into the calculation may be addressed directly by a lattice calculation in the future, although further theoretical and computational challenges remain to be overcome. We are at present focusing on reducing or removing the discretization errors resulting from using a single, rather coarse lattice in the calculation of the $I = 0$ amplitude, and we discussed our strategy and early results for the new, finer ensembles we are generating.

In addition to the work discussed in this document, we are also in the late stages of a preliminary investigation into whether it is feasible to compute the $K \to \pi\pi$ $I = 0$ amplitude without G-parity boundary conditions. This significantly reduces the expense of the calculation and allows the reuse of existing ensembles, at the cost of requiring multi-state approaches to extract the the on-shell matrix element as an excited-state contribution.

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