Progress in the calculation of $\varepsilon'$ on the lattice

C. Kelly∗
Columbia University, 538 W 120th St., New York NY 10027
E-mail: ckelly@phys.columbia.edu

We discuss recent progress by the RBC & UKQCD collaborations in the lattice calculation of the measure of Standard Model direct CP violation, $\varepsilon'$, with physical kinematics. We present results with improved systematic errors resulting from the use of step-scaling to reduce the renormalization error, an analysis that also takes into account the one-loop-suppressed mixing with the $G_1$ two-quark operator. We also review our progress in decreasing the dominant statistical error on our result.
1. Introduction

The preponderance of matter over antimatter in the observable Universe can be explained by baryogenesis, a requirement for which is the breaking of the CP symmetry. While CP-violation (CPV) is present in the Standard Model, its magnitude appears to be too small to account for the size of the matter/antimatter asymmetry, suggesting new, Beyond the Standard Model (BSM) physics awaits discovery. Direct CPV in K-meson decays is highly suppressed in the Standard Model and therefore offers a particularly sensitive probe for BSM sources of CPV.

Direct CPV in kaon decays was discovered in the late 1990s with the following result:

\[
\text{Re}(\epsilon' / \epsilon) \approx \frac{1}{6} \left( 1 - \frac{|\eta_{00}|^2}{|\eta_{\pi\pi}|^2} \right) = 16.6(2.3) \times 10^{-4},
\]

where \( \epsilon' \) and \( \epsilon \) are the measures of direct and indirect CPV, respectively, and \( \eta_{ij} = A(K_L \rightarrow \pi_i\pi_j) / A(K_S \rightarrow \pi_i\pi_j) \). However, until recently there has not been a reliable Standard Model prediction for this quantity that can be compared to experiment because the process receives large corrections from low-energy QCD interactions that are not amenable to perturbative calculations.

The RBC & UKQCD collaborations recently published [1] the first direct calculation of \( \epsilon' \), obtained using lattice QCD via the isospin-definite amplitudes \( A_I = K \rightarrow (\pi\pi) \), where \( I \) refers to the isospin quantum number of the final \( \pi\pi \) state. These amplitudes are computed on the lattice as

\[
A_I = F \frac{G_F}{\sqrt{2}} V_{ud}^* V_{us} |z_i(\mu) + \tau y_i(\mu)| Z_j(\mu) \langle (\pi\pi)_I | Q_j(\mu) | K \rangle,
\]

where \( F \) is the Lellouch-Lüscher factor [2] that represents the finite-volume correction to the decay amplitude, \( z \) and \( y \) are c-number Wilson coefficients, \( \tau = -V_{us}^* V_{ud} V_{us}^* \), \( V_{ij} \) are CKM matrix elements, and \( Q_I \) are a set of dimension-six four-quark operators. \( Z_j \) is the renormalization matrix relating the bare lattice operators to MS operators normalized at the scale \( \mu \), thereby matching the scheme used in the calculation of the Wilson coefficients. These are computed without resorting to the use of perturbative QCD at the hadronic scale by using an intermediate ‘regularization-invariant momentum scheme’ with symmetric kinematics (RI-SMOM) [3, 4] with which we can non-perturbatively run to a high energy scale where we can legitimately match to MS using continuum perturbation theory.

The result is as follows:

\[
\text{Re} \left( \frac{\epsilon'}{\epsilon} \right) = \text{Re} \left\{ \frac{i \omega e^{i(\delta_2 - \delta_0)}}{\sqrt{2} \epsilon} \left[ A_2 \sqrt{\frac{\text{Im} A_0}{\text{Re} A_2}} \right] \right\} = 1.38(5.15)(4.59) \times 10^{-4},
\]

where the errors are statistical and systematic, respectively. Here \( \delta \) are the s-wave \( \pi\pi \)-scattering phase shifts and \( \omega = \text{Re} A_2 / \text{Re} A_0 \). Our result has roughly 3\( \times \) the experimental error and agrees with experiment to 2.1\( \sigma \). However there is a hint of a tension that has provoked much interest both within and outside the lattice community, providing strong motivation for continued study.

These proceedings summarize the collaboration’s effort to reduce the both the statistical and systematic errors on our result, with the goal of a 2\( \times \) reduction in the total error.

2. Statistical error reduction

The 30% statistical error relative to the experimental result is dominated by that on \( \text{Im}(A_0) \), despite measuring upon 216 independent configurations. (We use the experimental values for \( \text{Re}(A_0) \) and \( \text{Re}(A_2) \) as these are dominated by current-current operators that are not expected to receive large BSM contributions.) The reason for this is two-fold: first, the \( I = 0 \) two-pion state has vacuum quantum numbers and therefore receives substantial contributions from gauge field noise; and
second, the dominant contributions, those of the QCD penguin operators $Q_4$ and $Q_6$, cancel at the 50% level, enhancing the relative error on their sum.

The statistical error can be reduced by the target factor of two simply by increasing the number of measurements by a factor of four. This also grants the opportunity to correct an error [5] in the random number generator seeding used in the generation of the ensemble used in the earlier calculation. While the effects of this error numerically appear to be negligible they do damage our ability to claim an \textit{ab initio} calculation.

Unfortunately the use of G-parity spatial boundary conditions to obtain an energy conserving decay necessitates the generation of additional gauge configurations. In order to circumvent the serial nature of ensemble generation we have started a number of independent streams. In Table 1 we list the resources currently employed and the number of independent configurations we aim to obtain. To date we have generated over 250 new, independent configurations and are therefore making steady progress towards our target.

We hope to perform the majority of our measurements using early access time on the NERSC Cori II (Intel Knight’s Landing) machine. Preparation for this and the ensemble generation on the Blue Waters (Cray XE6) machine has involved substantial work porting our high-performance Blue Gene/Q (BG/Q) code based on the BFM library [6] to the more general Grid [7] framework. This work has been accompanied by significant optimization of our measurement code.

In addition to the above, we are performing an investigation into the use of the ‘exact one-flavor algorithm’ [8] (EOFA), a gauge-field evolution technique that allows the calculation of the fermion determinant for a single quark flavor. The standard approach is to take the square-root of the determinant of two quark flavors, which can be computed much more easily due to the hermiticity and positive definiteness of the two-flavor operator. G-parity boundary conditions require this root to be computed for the light quark determinant, resulting in a significant increase in computational expense over conventional simulations. Preliminary results [9] suggest that EOFA will give rise to a considerable increase in the rate of generating gauge configurations.

### 3. Systematic error reduction

The systematic error is dominated by perturbative truncation errors in the Wilson coefficients and in the matching factors that connect our RI-SMOM scheme non-perturbative renormalization (NPR) factors to $\overline{\text{MS}}$. The reason is that the matching scale at which we apply perturbation theory is limited by the lattice cutoff, and in our calculation the coarse lattice spacing forces us to choose a low matching scale of 1.53 GeV. This limit can be circumvented using the ‘step-scaling’ technique whereby the NPR factors are run between successively finer lattices up to an arbitrarily large energy scale at which perturbation theory can be applied reliably.

In these proceedings we present a preliminary analysis in which step scaling is applied between our original $32^3 \times 64$ Möbius domain wall fermion ensemble with the Iwasaki+DSDR gauge action at $\beta = 1.75 \ (a^{-1} = 1.378(7) \text{ GeV})$ and a $24^3 \times 64$ Shamir domain wall fermion ensemble with the Iwasaki gauge action at $\beta = 2.13 \ (a^{-1} = 1.785(5) \text{ GeV})$. We refer to these as the 32ID and 24I

<table>
<thead>
<tr>
<th>Resource</th>
<th>Million BG/Q equiv core-hours</th>
<th>Independent cfgs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>USQCD (BNL 512 BG/Q nodes)</td>
<td>50</td>
<td>220</td>
</tr>
<tr>
<td>RBRC/BNL (BNL 512 BG/Q nodes)</td>
<td>17</td>
<td>50</td>
</tr>
<tr>
<td>UKQCD (DiRAC 512 BG/Q nodes)</td>
<td>17</td>
<td>50</td>
</tr>
<tr>
<td>NCSA (Blue Waters)</td>
<td>108</td>
<td>380</td>
</tr>
<tr>
<td>KEK (KEKSC 512 BG/Q nodes)</td>
<td>74</td>
<td>296</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>266</strong></td>
<td><strong>996</strong></td>
</tr>
</tbody>
</table>

Table 1: A breakdown of the various resources we intend to utilize. Note that we require 4 molecular dynamics time units per independent configuration.
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Figure 1: Four-quark operator momentum configuration for the RI-SMOM operators.

ensembles, respectively. On the 24I ensemble we use a renormalization scale of $\mu = 2.29$ GeV, and on the 32ID we lower the renormalization scale from the former 1.53 GeV to 1.33 GeV in order to reduce our susceptibility to discretization errors. The step-scaled renormalization matrix is computed as follows:

$$Z(2.29 \text{ GeV}, \text{step-scaled}) = \frac{Z(2.29 \text{ GeV}, 24\text{I})}{Z(1.33 \text{ GeV}, 24\text{I})} Z(1.33 \text{ GeV}, 32\text{ID}).$$

(3.1)

Note that we do not take the continuum limit of the $Z$-factors on either lattice as the resulting error is expected to be small in comparison to our other errors.

The perturbative matching formulae between the RI-SMOM and $\overline{\text{MS}}$ schemes are thus far only available to one-loop, hence we might expect the errors to scale naively with $\alpha_s^2$: Between the low and high scales above $\alpha_s^2 = 0.1546 \rightarrow 0.0774$, suggesting a possible factor of 2 improvement in the truncation systematic using this procedure.

3.1 Summary of RI-SMOM procedure

Seven independent four-quark operators $Q'_i$, where $i \in 1, 2, 3, 5, 6, 7, 8$ (the indices indicate their relation to the conventional 10-operator basis), enter the calculation of the low-energy $K \rightarrow \pi \pi$ amplitudes at leading order in the weak effective theory, which mix at next-to-leading order in QCD. We must therefore compute the $7 \times 7$ NPR matrix relating the bare lattice operators to the chosen RI scheme, defined via

$$Q'_i^{\text{RI}}(\mu) = Z_{ij}^{\text{lat} \rightarrow \text{RI}} Q'_j^{\text{lat}}(\mu).$$

(3.2)

This matrix is computed by imposing the following set of renormalization conditions:

$$Z_q^{-2} \mathcal{P}_j \langle E_{ab} Q'_i^{\text{RI}}(2q) \rangle_{\text{amp}} = (\text{tree level value})_{ji}$$

(3.3)

where $Z_q$ is the field strength renormalization, $\langle \cdot \rangle_{\text{amp}}$ denotes the expectation value of the amputated operator and $E_{ab}$ is an operator creating four quarks with momenta as shown in Figure 1. These momenta obey the symmetric momentum condition, $q^2 = p_1^2 = p_2^2 = (p_1 - p_2)^2 = \mu^2$, where $p_i$ are the quark momenta indicated in the figure. $\mathcal{P}_j$ are a set of 7 projection operator acting on the external state $E$, which, alongside the renormalization condition on the field renormalization, define the scheme.

In order to estimate the perturbative truncation systematic we utilize two schemes labelled SMOM($\gamma, \gamma$) and SMOM($\gamma^\mu, \gamma^\mu$), where the first term in parentheses relates to the form of the projection operator applied to the four-quark operator, and the second term to that applied in the determination of $Z_q$ (cf. [10]).

3.1.1 Inclusion of $G_1$

While $Q'_i$ form a complete set of operators that contribute to the on-shell decay amplitude, there are three additional gauge-invariant dimension-6 operators, $G_1$, $G_2$ and $G_3$, that mix with $Q'_i$ under renormalization and that, by the equations of motion (EOM), either vanish or can be written as linear combinations of $Q'_i$ in the on-shell limit. The most important of these is $G_1$. 

3
\[ G_1 = -\frac{4}{\sqrt{\pi}} \gamma_\mu (1 - \gamma_5) (D_\nu G_{\nu\mu}) d , \] (3.4)

which mixes at 1-loop in QCD. While this mixing is expected to be small, we can eliminate a potential source of systematic error by including it in our operator basis as an eighth operator. We therefore define the renormalized operators

\[ Q^{R\text{I}}_i = Z^{\text{lat} \rightarrow R\text{I}}_i Q^{\text{lat}}_i + c_i^{\text{lat} \rightarrow R\text{I}} G^{\text{lat}}_1 , \quad \text{and} \quad G^{R\text{I}}_1 = d^{\text{lat} \rightarrow R\text{I}}_1 G^{\text{lat}}_1 + Z^{\text{lat} \rightarrow R\text{I}}_1 G^{\text{lat}}_1 . \] (3.5)

Below we summarize a procedure by which \( G_1 \) can be included in our calculation without a significant expenditure of computational resources. A more detailed discussion can be found in Ref. [11].

For an on-shell matrix element, the continuum EOM implies that for the bare operators,

\[ G_1 = Q'_2 + \frac{7}{3} Q'_3 - \frac{1}{3} Q'_5 + Q'_6 , \] (3.6)

which gives rise to the following condition on the Green’s functions of renormalized operators,

\[ \langle f | G^{R\text{I}}_1 (\mu) | i \rangle = s_i (\mu) \langle f | Q^{R\text{I}}_i (\mu) | i \rangle . \] (3.7)

Corrections to \( s_i \) arise due to the renormalization of the bare operators, but enter only at two-loops; for sufficiently large scales \( \mu \), the values of \( s_i \) can therefore be reliably obtained directly from Eq. 3.6: \( s_2 = 1, s_3 = 7/3, s_5 = -1/3 \) and \( s_6 = 1 \) with the remainder zero. We can then insert these relations into Eq. 3.5 and obtain a direct relation between the bare lattice matrix elements:

\[ \langle f | Q^{\text{lat}}_i | i \rangle = k_j (\mu, a) \langle f | Q^{\text{lat}}_j | i \rangle \quad \text{where} \quad k_j (\mu, a) = \frac{s_j Z^{\text{lat} \rightarrow R\text{I}}_j (\mu, a) - d^{\text{lat} \rightarrow R\text{I}}_j (\mu, a)}{Z^{\text{lat} \rightarrow R\text{I}}_1 (\mu, a) - s_k Z^{\text{lat} \rightarrow R\text{I}}_k (\mu, a)} . \] (3.8)

We can therefore write

\[ \langle f | Q^{R\text{I}}_i (\mu, a) | i \rangle = R^{\text{lat} \rightarrow R\text{I}}_j (\mu, a) \langle f | Q^{\text{lat}}_j | i \rangle \] (3.9)

where

\[ R^{\text{lat} \rightarrow R\text{I}}_j (\mu, a) = Z^{\text{lat} \rightarrow R\text{I}}_j (\mu, a) + c_j^{\text{lat} \rightarrow R\text{I}} (\mu, a) k_j (\mu, a) . \] (3.10)

In others words the inclusion of \( G_1 \) in our calculation requires only the evaluation of the renormalization coefficients \( c_i \) and the quantity \( k_j \) in our RI schemes without ever having to compute on-shell \( K \to \pi \pi \) amplitudes of the \( G_1 \) operator (a far more daunting task).

The evaluation of the renormalization coefficients requires a suitable definition of \( G_1 \) on the lattice. Here our use of the continuum EOM to relate \( G_1 \) to \( Q_i \) offers the advantage that we are free to choose a convenient discretization; had we used the lattice EOM we would be forced to use a specific and inconvenient form that is far more difficult to evaluate. We choose the following form,

\[ G^{\text{lat}}_1 = \frac{1}{2} s_\mu (1 - \gamma_5) \left[ U_{x, \mu} L_{\lambda, \mu} + L_{x, \bar{\mu}, \mu} U(x - \bar{\mu}, \mu) \right] \tau A d , \] (3.11)

where \( L_{x, \mu} \) is the standard, \( \mu \)-oriented staple and \( \left[ \right]_{TA} \) indicates the traceless, antihermitian form of the contents. It remains to define a suitable external state, projector and compute the tree-level value per Eq. 3.3, the details of which can be found in Ref. [11]. Specifically, we use a four-quark external state

\[ E_s = s_\alpha (p_1 d_\beta (p_2) f_\gamma (p_2) \bar{f}_\gamma (p_2)) \] (3.12)

where \( f \) is a fictitious quark with flavor different from \( u, d \) and \( s \) such that it does not contract directly with the \( G_1 \) two-quark operator and instead enters only via disconnected diagrams. We choose two forms for the projector,

\[ P_{\gamma, \mu, G_1} = \delta_{\alpha \beta} \delta_{\mu \gamma} (| \gamma \rangle \langle \gamma |) \beta_\alpha (\gamma_\mu) \delta_\gamma \quad \text{and} \quad P_{\alpha, \mu, G_1} = \delta_{\alpha \beta} \delta_{\mu \gamma} (| \gamma \rangle \langle \gamma |) \beta_\alpha (\gamma_\mu) \delta_\gamma \] (3.13)

which correspond to the the SMOM(\( \gamma, \gamma \)) and SMOM(\( \gamma^\mu, \gamma^\mu \)) schemes, respectively. These are slight modifications of those defined in Ref. [10] in that we have inserted \( \gamma^\mu \) in order to project out the parity-odd component. While both parity components will have the same renormalization
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<table>
<thead>
<tr>
<th>$1.32 \text{ GeV}$</th>
<th>$2.29 \text{ GeV}$</th>
<th>$2.93 \text{ GeV}$</th>
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<tr>
<td>$\text{24I}$</td>
<td>$\text{32ID}$</td>
<td>$\text{stepscaled, no } G_1$</td>
</tr>
<tr>
<td>$\text{stepscaled inc. } G_1$</td>
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</tr>
<tr>
<td>$(1,1)$</td>
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<td>$(2,2)$</td>
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<tr>
<td>$(3,2)$</td>
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<tr>
<td>$(4,2)$</td>
<td>$0.020(42)$</td>
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<td>$(5,2)$</td>
<td>$0.283(22)$</td>
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<td>$(6,2)$</td>
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<td>$0.036954(41)$</td>
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<td>$0.080(33)$</td>
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<td>$(3,2)$</td>
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Table 2: Preliminary values of $\Xi$ obtained using the renormalization matrices obtained at various scales on the 32ID and 24I lattices, as well as using the step-scaled matrices with and without $G_1$.

coefficients, we have observed that the parity-odd component typically has smaller statistical errors. Note that the power-divergent mixing of $G_1$ with lower-dimension operators must also be removed by defining a subtracted operator, as is discussed in Ref. [11].

In Ref. [11] results were obtained for $R_{ij}$ in the SMOM($\gamma^\mu$, $\gamma^\mu$) scheme on the 24I ensemble with $\mu = 2.29$ GeV, where it was shown that, while statistically resolvable, the effects of the $G_1$ operator indeed enter only at the percent-level at this scale.

3.2 Estimation of the renormalization systematic

We seek a scheme for estimating the size of the perturbative truncation errors on our result. One possibility is to examine the difference between the results in the $\overline{MS}$ scheme obtained via our two different intermediate schemes. Rather than involving the matrix elements themselves, which are statistically noisy and vary significantly in size, it is convenient to instead study the differences between the elements of the $7 \times 7$ lattice $\to \overline{MS}$ renormalization matrix

$$R_{ij}^{\text{lat} \to \overline{MS}}(\mu) = H_{ik}^{\text{RI} \to \overline{MS}, \text{1-loop}}(\mu) R_{kj}^{\text{lat} \to \text{RI}}(\mu),$$

where $H$ is the perturbative matching matrix. The matrix $R_{ij}^{\text{lat} \to \overline{MS}}(\mu)$ is formally independent of the intermediate RI scheme up to the perturbative truncation error. We define the matrix

$$\Xi = \begin{vmatrix} 1 & R_{i}^{\text{lat} \to \text{MS via SMOM(\phi \phi)}}^{\text{1-loop}} \\ R_{j}^{\text{lat} \to \text{MS via SMOM(\gamma^\mu, \gamma^\mu)}}^{\text{1-loop}} \end{vmatrix},$$

where $|.|$ implies the absolute value of each element is taken. Under the reasonable assumption that the missing NNLO and higher terms of the matching matrix for the two schemes are comparable in size, we might expect the elements of $\Xi$ to vary between zero and roughly twice the relative size of the missing terms. We therefore choose to assign a percentage systematic error that is one half of the largest observed element of $\Xi$ at a scale $\mu$. 
3.3 Results

In Table 2 we tabulate the non-zero elements of $\Xi$. Once again we observe that the effects of including or discounting the $G_1$ operator, while harder to statistically resolve after passing through the step-scaling procedure, are at the percent scale.

As expected there is a general trend towards smaller values as we increase the scale. However the $(3, 3)$ elements are consistently larger than the others by a considerable amount, even at high scales. This occurs because the 1-loop correction to the matching matrix in the SMOM($q, q$) scheme (Table XI of Ref. [10]) is almost twice as large as the next largest entry, and is $O(25\%)$ at $\mu = 1.53$ GeV. It is therefore natural that the NNLO and higher corrections will be correspondingly larger. As this behavior is unique to the $(3, 3)$ element, and that $Q'_3$ does not contribute significantly to our final result, we ignore this outlier and instead estimate the truncation systematic from the next-largest difference. We therefore estimate a 15% error at the 1.53 GeV scale, consistent with our previous result [1]. For the new, step-scaled renormalization factors at 2.29 GeV this drops to 8%, which is consistent with the expected $\alpha_s^2$ dependence.

4. Conclusions and outlook

In order to improve on our first complete calculation of $\varepsilon'$ in the Standard Model we are aiming to reduce the statistical and systematic errors by a factor of two or more. To this end we are utilizing significant computational resources to extend the number of measurements by the required factor of four, which we expect will be achievable within the next year.

The dominant systematic errors arise from the 1-loop truncation of the perturbative calculations used to match our non-perturbative renormalization scheme to $\overline{\text{MS}}$ and to compute the Wilson coefficients. Both can be reduced by increasing the renormalization scale using step-scaling. In this document we presented preliminary results for the step-scaled renormalization factors obtained with a high energy scale of 2.29 GeV, and we observe a factor of two reduction in our estimated error. We have also discussed the inclusion of the $G_1$ operator in this procedure and demonstrated that its effects are small as expected. A similar reduction might be expected in the truncation systematic for the Wilson coefficients, an analysis of which will be forthcoming.

References