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Update on the lattice calculation of $K \to \pi\pi$ decays with G-parity boundary conditions on a second lattice spacing

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We review the status of the RBC & UKQCD collaboration's lattice calculations of direct CP violation in $K \to \pi\pi$ decays, and discuss the implications of recent results showing that periodic boundary conditions coupled with modern multi-operator methods offer a competitive approach to the G-parity boundary conditions previous employed. We then present early, preliminary results for a second, finer-lattice-spacing calculation of the $I = 0$ $K \to \pi\pi$ decay amplitude in the 3 flavor theory with physical kinematics and G-parity boundary conditions. This new calculation will enable a continuum limit extrapolation, reducing/eliminating the significant finite-lattice spacing systematic error on our previous result.

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The violation of the CP symmetry is highly suppressed in the Standard Model, hence the comparison of theory to experimental measurements of CP violating processes offers a sensitive probe for new physics that may help shed light on the origin of the imbalance of matter and antimatter in the observable Universe. Direct CP violation in $K \to \pi\pi$ decays, parameterized by ϵ', is a tiny, part-per-million effect that was measured to a precision of 15% in a series of experiments at CERN and FermiLab in the late 1990s; however, it was only recently that reliable first principles theory calculations have been achievable, due to the presence of significant non-perturbative contributions for which lattice QCD provides the only known *ab initio* approach. Such calculations have been a long-term focus of the RBC & UKQCD collaborations.

ϵ', can be extracted from the difference in the complex phases of the decay amplitudes, A_2 and A_0, of a neutral kaon decaying into two pions in the $I = 2$ and $I = 0$ isospin channels, respectively:

$$\epsilon' = \frac{ie^{i(\delta_2-\delta_0)}}{\sqrt{2}} \frac{\mathrm{Re}A_2}{\mathrm{Re}A_0} \left(\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0} \right), \tag{1}$$

where δ_I are the $\pi\pi$ scattering phase shifts (also measured on the lattice). These amplitudes can be computed on the lattice to high precision using leading-order weak effective theory as $A_I = \langle(\pi\pi)_I|H_W|K^0\rangle$ where

$$H_W = \frac{G_F}{\sqrt{2}} V_{us}^* V_{ud} \sum_{i=1}^{10} c_i(\mu) Q_i(\mu) \tag{2}$$

is the 3-flavor weak Hamiltonian, G_F is the Fermi constant, V_{us} and V_{ud} are CKM matrix elements, Q_i are ten weak effective four-quark operators and c_i are the corresponding Wilson coefficients encapsulating the high-energy behavior. Both c_i and Q_i are renormalization scheme/scale (μ) dependent. We renormalize the operators using a non-perturbative (RI-SMOM) scheme that is run to a high energy where perturbation theory can be reliably employed to match to the $\overline{\mathrm{MS}}$ scheme in which the Wilson coefficients are conventionally derived. A Lellouch-Lüscher [1] finite-volume correction (not shown in the equation) is also necessary to extract the physical amplitude.

1. Obtaining the on-shell decay amplitude

A significant challenge for a lattice calculation using conventional, periodic spatial boundary conditions (BCs), is that the ground-state of the two-pion system, comprising two stationary pions, has an energy of ~270 MeV, much lower than that of the kaon, m_K~500 MeV. The physical, energy-conserving decay therefore appears as a subdominant, excited-state contribution, assuming the lattice volume is sufficiently well chosen. In the $I = 2$ channel we can avoid this issue by computing A_2 directly via $K^+ \to \pi^+\pi^0$, which can be related to the unphysical decay $K^+ \to \pi^+\pi^+$ containing only charged pions via a Wigner-Eckart isospin rotation. By then imposing antiperiodic BCs on the down quark in $n \geq 1$ spatial directions, these charged pion states also become antiperiodic, raising their ground-state energy from m_π to $\sqrt{m_\pi^2 + n\pi^2/L^2}$, where L is the spatial lattice size. The ground-state two-pion energy can then be adjusted to match that of the kaon by tuning n and L. While this approach explicitly breaks the isospin symmetry, the resulting mixing of the doubly-charged two-pion final state is disallowed due to charge conservation.

Unfortunately, this approach is not applicable to A_0, for which the final states perforce comprise both charged and neutral pions, and this, and the breaking of the isospin symmetry, cannot be avoided by a convenient isospin rotation. These calculations are also hampered by the vacuum quantum numbers of the two-pion state, which allow for contributions from noisy, disconnected diagrams. One is then left with the daunting task of precisely extracting a subdominant contribution to the lattice amplitude from data with large statistical errors and a rapidly dwindling signal-to-noise ratio.

G-parity BCs [2] provide an alternative method for inducing momentum on the pion ground state. G-parity is a combination of charge conjugation and a y-axis isospin rotation by π radians, under which both the charged and neutral pions are negative eigenstates. By applying the G-parity operation at the lattice spatial boundary in n directions, we once again raise the ground-state pion energy to $\sqrt{m_\pi^2 + n\pi^2/L^2}$, only for all pion species. Furthermore, as G-parity commutes with total isospin, the isospin symmetry remains unbroken. The downside of this approach arises from the fact that we cannot directly control the BCs of the pions, only their constituent quarks, and at the quark level the G-parity transformation is non-trivial:

$$\hat{G} \begin{pmatrix} u \\ d \end{pmatrix} \hat{G}^{-1} = \begin{pmatrix} -C\bar{d}^T \\ C\bar{u}^T \end{pmatrix}, \tag{3}$$

where $\hat{G}$ is the G-parity operator and C is the charge conjugation spin matrix. As the up and down quarks mix at the lattice boundary, we are forced to treat them explicitly as distinct flavor degrees of freedom in the lattice Dirac operator, thus doubling the computational cost of obtaining the quark propagator. Additional challenges arise due the fact that the unitary treatment of the quarks in the context of disconnected diagrams requires generating custom ensembles with G-parity BCs applied to the sea quarks, and, not only are these naïvely twice as expensive to generate as a regular, periodic ensemble, a further cost is incurred because the conventional pseudofermion method for estimating the fermion determinant provides $\det(\mathcal{M}^\dagger\mathcal{M})$, where $\mathcal{M}$ is the Dirac operator, and in the G-parity context this is a *four-flavor* determinant. For 2 + 1 flavor domain wall fermion simulations we have therefore historically employed the Exact One-Flavor Action [3, 4] (EOFA) to optimally compute the square-root of this determinant in the light-quark sector, and the rational hybrid Monte Carlo method (RHMC) to estimate the fourth-root for the strange quark. We estimate the overheads of employing these algorithms to amount to an additional factor of $O(2\times)$ in computational cost.

2. Overview of published G-parity calculations

Despite the computational challenges, G-parity BCs have been successfully employed by the RBC & UKQCD collaborations to compute the $I = 0$ decay amplitude. Combined with our earlier precise calculation of A_2 [5], we published in 2015 the first ever *ab initio* Standard Model calculation of ϵ' with systematically improvable errors [6]. This first calculation of A_0 was hampered by the presence of an excited two-pion state with an energy close to the ground state, which, alongside the intrinsically large statistical noise and the rapid decay in the signal-to-noise ratio, made the reliable extraction of the ground-state amplitude highly challenging. This issue was resolved in a follow-up calculation published in 2020 [7], which more than tripled the statistics and also introduced two additional two-pion operators that were combined with our original operator and treated collectively using multi-operator, multi-state simultaneous fits. These multi-operator techniques were ultimately crucial to reliably extracting the ground-state amplitude.

Both calculations of A_0 were performed on a single, $32^3 \times 64$ Möbius domain wall fermion ensemble labeled "32ID", with $L_s = 12$, $b + c = 32/12$, $b - c = 1$, and the Iwasaki+DSDR gauge action with $\beta = 1.75$, corresponding to an inverse lattice spacing of $a^{-1} = 1.378(7)$ GeV. We simulated with physical pion and kaon masses and used G-parity BCs in all three spatial directions, giving a two-pion ground-state energy that agrees with the kaon mass to 2%.

ϵ' is conventionally quoted as $\mathrm{Re}(\epsilon'/\epsilon)$, where ϵ parametrizes kaon indirect CP-violation. We obtained $\mathrm{Re}(\epsilon'/\epsilon)_{\mathrm{lat}} = 21.7(26)(80) \times 10^{-4}$, where the errors are statistical and systematic, respectively. This result agrees with the experimental value $\mathrm{Re}(\epsilon'/\epsilon)_{\mathrm{expt}} = 16.6(23) \times 10^{-4}$, albeit with a 3.6× larger error, dominated by systematic effects. The largest, $O(23\%)$ systematic error arises from neglecting the effects of isospin breaking and electromagnetism. A second $O(12\%)$ systematic error arises from using perturbation theory at the charm mass scale, $m_c \sim 1.3$ GeV, to match the 4 and 3-flavor weak effective theories when computing the Wilson coefficients. We are presently investigating strategies for non-perturbatively matching these theories in order to reduce the latter [8]. The former is more challenging to address, requiring theoretical developments to learn how to control long-distance electromagnetic effects in the context of a calculation that intrinsically relies on the finite-volume Lüscher and Lellouch-Lüscher prescriptions. A promising strategy, described in Ref. [9] , is presently being pursued, although it will likely require several more years before a complete calculation is performed. The remaining dominant systematic error arises due to computing A_0 on only a single, rather coarse lattice spacing. We estimate these discretization effects to be $O(12\%)$ based on the known continuum scaling of the matrix elements entering A_2, although this estimate is subject to considerable uncertainty. Addressing this final error has been the recent focus of our efforts in improving the theoretical result for ϵ'. To this end we are in the process of repeating the calculation on a second, "40ID" G-parity ensemble (detailed below) with a finer, 1.72 GeV lattice spacing, which will allow for a continuum-limit extrapolation.

3. Multi-operator methods and periodic BCs

The success of the multi-operator methodology in treating the excited two-pion states has recently prompted a largely independent investigation by the RBC & UKQCD collaborations into whether these techniques can be used to reliably obtain the physical amplitude as an excited state in a conventional, periodic calculation, thus circumventing the need for G-parity BCs entirely. In Refs.[10, 11], the authors provide first results from a physical pion mass calculation performed upon a coarse $a^{-1} = 1.0$ GeV ensemble, with a number of measurements comparable to our first, 2015 G-parity calculation. The results of this pilot calculation were very promising, producing a well-resolved value for A_0 consistent with our 2020 result and with comparable estimated systematic errors (excluding finite lattice spacing effects). Preliminary results were presented at this conference [12] of a follow-up calculation which not only doubles the statistics on this coarse measurement but also introduces a second calculation on a finer, $a^{-1} = 1.4$ GeV ensemble with the same lattice parameters as our G-parity calculation. This allowed for a preliminary continuum result for ϵ' that was found to be highly consistent with the experimental value, although there remains considerable scope for higher-order lattice spacing corrections to the coarse ensemble result.

Aside from the reduced cost from using a single-flavor Dirac operator, these calculations benefited significantly from the ability to reuse existing ensembles and eigenvectors generated for other projects, and were therefore much cheaper to perform than the G-parity calculations. Given these advantages it is natural to question the value of continuing with our planned G-parity calculation programme. To address this we first note that these approaches are expected to differ significantly in finite-volume and excited-state effects. The latter is particularly important to these calculations as noted above. As the RBC & UKQCD collaborations are the only lattice group presently working on computing $K \to \pi\pi$ decay with physical kinematics, there is considerable value in pursuing multiple, largely independent results with competing approaches that have different systematic errors. Second, the relative cost of the G-parity approach may be expected to be offset by the advantage of the desired matrix element being the dominant contribution to the lattice amplitude rather than a subdominant, excited state contribution, although at present no detailed cost comparison has been performed. Finally, the computational cost landscape for G-parity calculations has changed considerably in recent years through the advent of the "X-conjugate" algorithms described in Ref. [13] and below, which exploit a subtle symmetry in the G-parity Dirac matrix that allows certain operations to be expressed in terms of a conventional, single-flavor Dirac operator with unusual boundary conditions on the quark fields that involve a complex conjugation and multiplication by a spin matrix. This relationship allows for the decomposition of the fermion determinant such that the 2+1 flavor path integral can be evaluated directly via this X-conjugate Dirac operator without needing to root the determinant, thus reducing the cost of G-parity ensemble generation to that of a conventional, periodic calculation. Furthermore, as we show below, it allows for 2× cost reductions in eigenvector generation and in generating quark propagators, thus also reducing the measurement cost to a level comparable to a periodic calculation. While this doesn't remove the advantage of the periodic approach being able to reuse existing ensembles and eigenvectors, we note that these calculations rely on having a lattice volume both sufficiently tuned that a two-pion state with an energy close to that of the kaon mass appears as a low-lying state, and sufficiently small that these states remain well separated. The trend towards large-volume ensembles to control finite-volume errors in calculations such as that of the muon anomalous magnetic moment may mean that custom ensembles will also be required for measurements using the periodic approach in the future.

4. Finer G-parity calculation status and preliminary results

The 40ID ensemble employs a $40^3 \times 64$ Möbius domain wall fermion lattice with physical quark masses, $L_s = 12$, $b + c = 2$, G-parity BCs in three directions and the Iwasaki+DSDR gauge action at $\beta = 1.848$, corresponding to $a^{-1} \approx 1.72$ GeV. As described in Ref. [13], the X-conjugate algorithms resulted in a 5.4× reduction in computational cost, allowing completion of a trajectory in just 1.61 hours on 16 nodes of the NERSC Perlmutter supercomputer. As a result, we have now generated ∼9700 trajectories, excluding thermalization.

In Ref. [13] we estimated an integrated autocorrelation time $\tau_{\rm int} \approx 15 - 20$ trajectories based on a variety of quantities including the topological charge and Wilson flow scales ω_0 and $t_0^{1/2}$, suggesting 30-40 trajectories lie between effectively uncorrelated samples. This is considerably larger than the $\tau_{\rm int} \approx 3 - 4$ of our 32ID ensemble (6-8 trajectories between independent samples) due to the finer lattice spacing. In the 2020 calculation we measured every fourth trajectory, on the order of $\tau_{\rm int}$, yet observed only relatively minor autocorrelation effects on our primary observables, easily incorporated into our error analysis. Thus, assuming we measure at every 20 trajectories on the 40ID ensemble, we have sufficient data for 485 measurements, close to the target of $O(750)$ measurements required to match the statistics of our 2020 calculation.

In this document we present first, preliminary results for $\pi\pi$ and $K \to \pi\pi$ measurements performed on the 40ID ensemble. Per our conventional strategy [7], we use three different two-pion sources and employ all-to-all propagators computed using a variant of the TrinLat approach [14], with 2000 exact eigenmodes obtained using the block Lanczos algorithm and stochastic estimation of the high-mode contribution with dilution in all indices including the G-parity "flavor" index. The eigenvector generation is accelerated by a factor of two by instead solving for the eigenmodes $v_X^{(i)}$ and eigenvalues $\lambda_X^{(i)}$ for $i \in \{1..N_{\rm ev}\}$ of the X-conjugate Dirac operator $\mathcal{M}_X$ [13], which are trivially related to those of the G-parity Dirac operator, $v_G^{(i)}$ and $\lambda_G^{(i)}$, respectively, as $\lambda_G^{(i)} = \lambda_X^{(i)}$ and

$$v_G^{(i)} = \begin{pmatrix} v_X^{(i)} \\ -X[v_X^{(i)}]^* \end{pmatrix} \tag{4}$$

where the vector is in flavor space and $X = C\gamma^5$, for which $X^2 = -1$, $X^\dagger = X^{-1} = -X$, $X^* = X$. We also employ the "split-grid" method to parallelize the 1536 Dirac matrix inversions required over single-node subdomains, reducing the burden on the network.

We achieved an additional factor of two acceleration of the inversions using the fact that the solution $\hat{\psi} = \mathcal{M}_G^{-1}\hat{\eta}$ of inverting the G-parity Dirac operator $\mathcal{M}_G$ upon an "X-conjugate" vector of the form $\hat{\eta} = \begin{pmatrix} \eta \\ -X\eta^* \end{pmatrix}$ can be computed as

$$\hat{\psi} = \begin{pmatrix} \psi \\ -X\psi^* \end{pmatrix} \quad \text{where} \quad \psi = \mathcal{M}_X^{-1}\eta, \tag{5}$$

at half the computational cost. To exploit this relation for all-to-all propagators we first require spin, color and flavor matrix-valued stochastic sources $\theta^{(i)}$ with the usual property

$$\frac{1}{N}\sum_{i=1}^{N}\theta^{(i)}(\vec{x},t)[\theta^{(i)}(\vec{y},t)]^\dagger \xrightarrow{N\to\infty} \mathbf{I}_{24\times 24}\delta_{\vec{x}\vec{y}} \tag{6}$$

but for which either the columns are also X-conjugate,

$$\theta^{(i)} = \begin{pmatrix} A^{(i)} & B^{(i)} \\ -X[A^{(i)}]^* & -X[B^{(i)}]^* \end{pmatrix} \tag{7}$$

or can be transformed into this form by right-multiplication by another, constant matrix. Here $A^{(i)}$ and $B^{(i)}$ are spin-color matrices satisfying Eq. 6 only with the 12×12 unit matrix. In an as-yet unpublished study, performed on a smaller lattice, we investigated a variety of such sources searching for those for which the statistical errors resulting from the stochastic high-mode approximation are similar or less in size than for our original approach. We identified the following "U1H" source, for which the statistical errors were found to be no more than 10% greater than the original, and up to 40% *smaller* for some observables:

$$\theta^{(i)}_{U1H} = \begin{pmatrix} \rho^{(i)} & 0 \\ 0 & [\rho^{(i)}]^* \end{pmatrix}\begin{pmatrix} P_\pm & P_\mp \\ -XP_\mp & -XP_\pm \end{pmatrix} \tag{8}$$

where $P_\pm = \frac{1}{2}(1 \pm iX)$, $P^*_\pm = P_\mp$, and $\rho^{(i)} \in U(1)$. We allow the source to fluctuate between the $+-$ and $-+$ signature for the upper row based on the spatial parity of the site, $(x + y + z) \bmod 2$, which results in the flavor structure of the noise contributions coming from $\theta_{U1H}(\vec{x},t)\theta^\dagger_{U1H}(\vec{y},t)$ for $\vec{x} \neq \vec{y}$ oscillating between off-diagonal and diagonal as $\vec{x}$ and $\vec{y}$ are varied. Although not definitively tested, we expect this to contribute some of the benefit observed for the size of the high-mode noise.

With the above optimizations we achieved per-measurement times of 6.2 hours on 80 nodes of the ALCF Polaris supercomputer. To-date we have measured on 111 configurations separated by 50 (ensemble generation stream 1) or 40 trajectories (streams 2-4). We also performed 21 measurements using the original stochastic source approach for an additional, successful, comparison with the U1H sources. Below we present preliminary results from 81 measurements with the U1H source. Note that we make no attempt here to estimate the systematic errors on the quoted results. Also, due to the relatively small number of measurements, we do not attempt to bin the data to account for autocorrelations; however, the large measurement separation, comparable to $2\tau_{\rm int}$, should make our statistical errors sufficiently reliable for a preliminary analysis. In all cases we perform correlated fits with the covariance matrix estimated from the data, and the errors are estimated using the jackknife method.

In Fig. 1 we plot the effective masses and single-state fit results for the (moving) ground-state pion and (stationary) kaon with the indicated fit range. The fit results converted to physical units

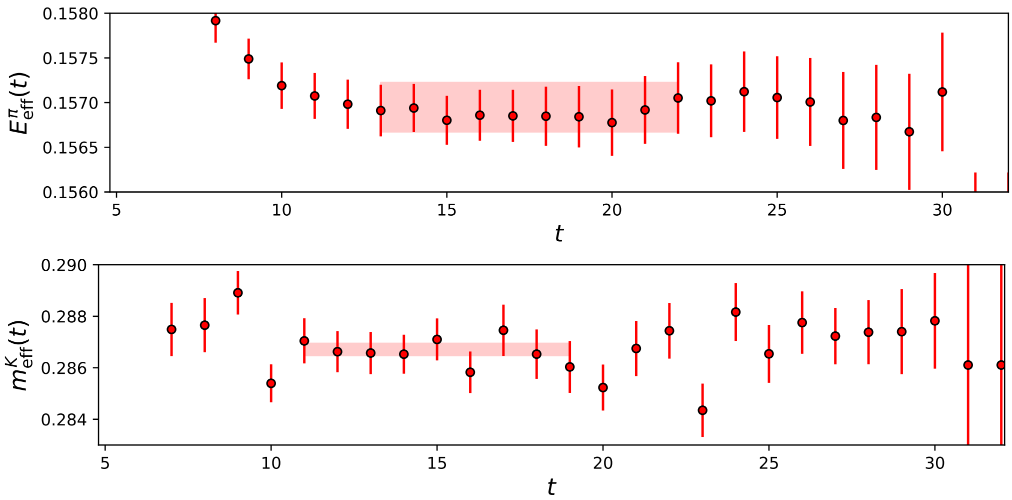

Figure 1: The pion (upper) and kaon (lower) effective energies overlaid by the single-state fit result.

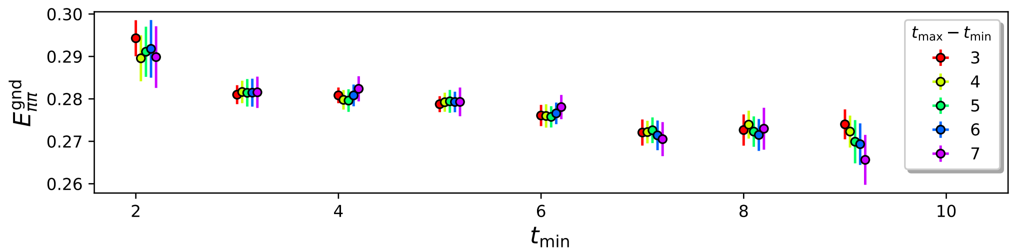

Figure 2: The fitted $\pi\pi$ ground-state energy as we vary the fit lower bound, $t_{\rm min}$, and range, $t_{\rm max} - t_{\rm min}$.

give $E_\pi = 271.6(5)$ MeV and $m_K = 496.0(4)$ MeV. Applying the (näive) dispersion relation to the pion energy gives $m_\pi \approx 135.3$ MeV. Both this and the kaon mass are very close to our target values. For the two-pion data we can vary the number of $\pi\pi$ operators and fitted intermediate states as well as the fit range. At this stage we have not exhaustively compared the different fit results for all these cases; rather we focus on the 3-operator, 2-state case found optimal for our 2020 analysis. In Fig. 2 we plot the fit result as we vary the lower and upper bounds of the fit range, showing only weak time dependence after $t_{\rm min} = 3$. Allowing for small excited-state contamination we choose a more conservative $t_{\rm min} = 7$ that agrees well with later values, giving $E_{\pi\pi} = 470(6)$ MeV, which has a small, 1.3% statistical error and a value that agrees with the kaon mass to within 5%, indicating our $K \to \pi\pi$ decay ground-state is very close to energy conserving.

For the $K \to \pi\pi$ analysis we deviate slightly from our 2020 approach by peforming a weighted average over the 6 different $K \to \pi$ separations prior to fitting, so as to reduce the size of the covariance matrix (this approach applied to our 2020 data does not significantly change the fit results). As before, we focus on the 3-operator, 2-state case and vary both the minimum separation between the kaon and four-quark operator, $t^{K\to Q}_{\rm min}$, and between the operator to the two-pion sink, $t^{Q\to\pi}_{\rm min}$. In Fig. 3 we plot these results for the Q_1 and Q_2 operators, the dominant contributions to $\mathrm{Re}(A_0)$, and for the Q_4 and Q_6 operators, the dominant contributions to $\mathrm{Im}(A_0)$. We observe only weak dependence on the fit range and well resolved values. We are unable to provide preliminary results for ϵ' and its continuum limit as we have not yet computed the RI-SMOM non-perturbative renormalization factors for this new ensemble. In principle these can be computed directly on the G-parity ensemble, but further theoretical developments are required as the concepts of flavor and

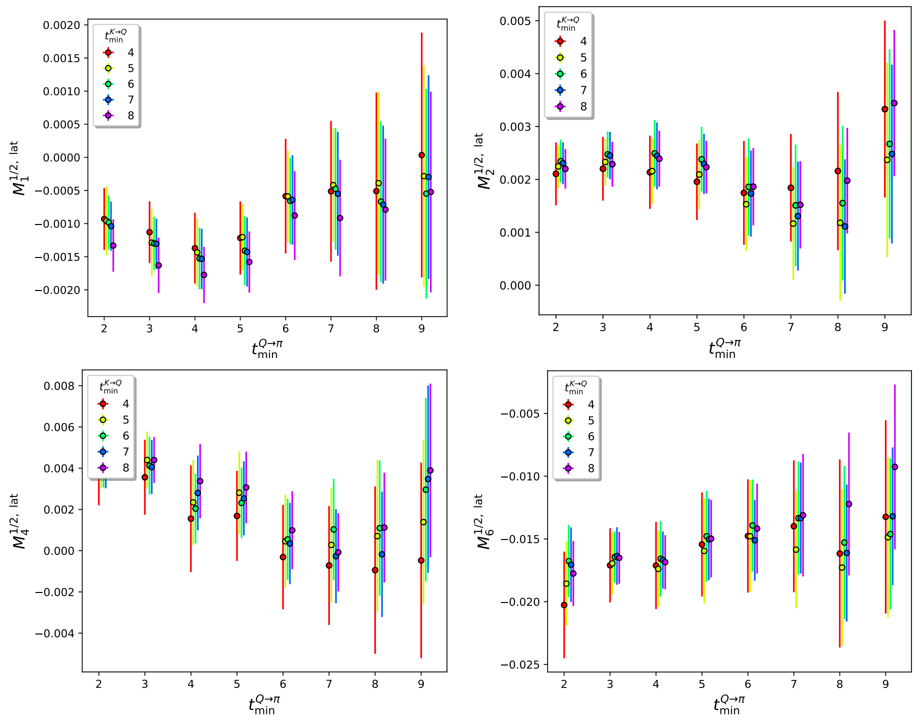

Figure 3: The fitted values of the Q_1 (upper-left), Q_2 (upper-right), Q_4 (lower-left) and Q_6 (lower-right) lattice matrix elements over variations in $t_{\min}^{K\to Q}$ and $t_{\min}^{Q\to\pi}$.

momentum are non-trivially bound in this framework. To avoid this difficulty, we are following our previous approach and generating a cheap partner ensemble with periodic BCs but otherwise equivalent ensemble parameters, and expect to have results for the renormalization factors shortly.

5. Conclusions

In this document we have reviewed the status of the RBC & UKQCD collaboration's calculations of kaon direct CP-violation. We presented arguments justifying the continued use of G-parity BCs despite the apparent success of employing multi-operator techniques on periodic BC ensembles in obtaining results of similar precision, based on differences in the key finite-volume and excited-state systematic errors and the fact that the cost of G-parity calculations has been reduced to a level comparable to periodic calculations. We then detailed the measurement strategy for our new, finer "40ID" G-parity ensemble, focusing on new developments that gave rise to the aforementioned cost reductions. Combining this second calculation with our existing result will enable a continuum extrapolation of the decay amplitude, reducing the significant discretization error. Finally we presented a preliminary analysis of 81 measurements – roughly 10% of our target statistics – finding pion and kaon masses that agree well with our expected values; two-pion energies resolved at the 1.5% scale and in good (5%) agreement with the kaon mass; and promising early results for the critical $K \to \pi\pi$ matrix elements. Complete physical results for the decay amplitude await measurements of non-perturbative renormalization factors that are presently underway. Based on current cost measurements, we anticipate achieving our target statistics for the 40ID ensemble within the 1-2 year timescale.

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