Progress Towards an *ab initio*, Standard Model Calculation of Direct CP-Violation in K-decays

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For the RBC and UKQCD collaborations

We discuss the RBC&UKQCD collaboration's progress towards a first-principles calculation of direct CP-violation in the Standard Model via $K \to \pi\pi$ decays. In particular we focus upon the calculation of the $I = 0$ channel amplitude A_0, for which obtaining physical kinematics requires more sophisticated techniques than those used for the $I = 2$-channel decay. We discuss our chosen techniques along with preliminary demonstrations of their application to simpler lattice quantities, and finally present early results for the tuning of the gauge-evolution of the large-volume, physical-pion-mass ensembles that will be used to perform the A_0 calculation.

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1. Introduction

Direct CP-violation in $K \to \pi\pi$ decays manifests as a difference in phase between the complex amplitudes, A_2 and A_0, of the decay in the $I = 2$ ($\Delta I = 3/2$) and $I = 0$ ($\Delta I = 1/2$) channels respectively (the $I = 1$ channel being forbidden by Bose symmetry):

$$\varepsilon' = \frac{i\omega e^{i(\delta_2 - \delta_0)}}{\sqrt{2}} \left(\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0} \right), \tag{1.1}$$

where $\omega = \mathrm{Re}A_2/\mathrm{Re}A_0$ and δ_i are the scattering phase shifts of the final-state pions.

Low energy strong interactions play an important role in the dynamics of these decays; for example they are largely responsible [1] for the factor of ~ 20 enhancement of the $I = 0$ decay amplitude over the $I = 2$ amplitude that is known as the "$\Delta I = 1/2$-rule". As a result we must use lattice QCD in order to study these processes. As the hadronic scale of ~ 1 GeV is much smaller than the W-boson mass, the decay can be described using the weak effective theory. The interaction takes the form of a local operator:

$$H_W^{\mathrm{eff}} = \frac{G_F}{\sqrt{2}} V_{us}^* V_{ud} \sum_{i=1}^{10} [z_i(\mu) + \tau y_i(\mu)] Q_i(\mu), \tag{1.2}$$

where z_i and y_i are Wilson coefficients determined in the perturbative regime, Q_i are the effective four-quark operators, and $\tau = -V_{ts}^* V_{td}/V_{ud} V_{us}^*$ is responsible for the direct CP-violation in the decay. On the lattice we measure Euclidean Green's functions, $\langle \pi\pi | Q_i | K \rangle$, and non-perturbatively renormalize at the scale μ. The finite-volume amplitudes are then corrected to the infinite volume by applying the Lellouch-Luscher factor [2].

The first-principles calculation of ε' has long been a goal of the lattice community, but it is only recently that the techniques and raw computing power have become available to perform a realistic calculation. The difficulties are two-fold: firstly, performing the calculation requires both large physical volumes and light quark masses, which in turn require the use of advanced algorithms and powerful computers; and secondly it requires the development of strategies for calculating diagrams with vacuum intermediate states (in the $I = 0$ channel), and for obtaining physical kinematics in the decay.

Using large-volume but relatively coarse ensembles of domain wall fermions with the Iwasaki+DSDR gauge action and near-physical pion masses, the RBC and UKQCD collaboration have performed the first realistic *ab initio* calculation of the decay amplitude in the $I = 2$ channel [3, 4], and a calculation with finer lattices and a full continuum extrapolation is underway that will substantially reduce the discretization systematic, which was the largest contribution to the error on the earlier calculation. Unfortunately the techniques used to obtain physical kinematics in this channel (discussed further below) are not applicable to the $I = 0$ case, and an alternative strategy must be found. For this we have chosen G-parity boundary conditions, the discussion of which will be the focus of these proceedings.

2. Obtaining physical kinematics

We are interested in measuring the on-shell, physical decay. The kaon mass is 500 MeV and the pion mass is 135 MeV, hence the final state pions are required to each have non-zero momentum. As this is an excited state of the $\pi\pi$ system (the ground state being that in which both pions are stationary) its contribution is sub-dominant and some consideration is required as to how best to extract it. In principle it is possible to directly measure the excited state contribution on the lattice providing one has sufficient statistical precision to resolve it over the dominant ground-state contribution. However for this calculation it is unlikely that a precise-enough measurement could be performed within a reasonable time, particularly in the $I = 0$ case where the presence of vacuum diagrams is expected to lead to considerably noisier measurements.

Another possibility is to use a moving kaon in the initial state with a two-pion final state comprising one moving pion and one stationary. The ground state of the $\pi\pi$ system with these kinematics has non-zero total momentum, which can be tuned to match the kaon energy. However, in order to satisfy $\sqrt{p_K^2 + m_K^2} = \sqrt{p_\pi^2 + m_\pi^2} + m_\pi$ (here we ignore the interaction between the pions) we would require $p_\pi = p_K \approx 780$ MeV. As the signal-to-noise ratio for the kaon state is related to the difference between the kaon energy and the pion mass of 135 MeV, such a calculation is expected to be too noisy.

For the $\Delta I = 3/2$ measurement it is possible to modify the valence quark boundary conditions in order to induce momentum on the final state pions: With antiperiodic valence boundary conditions (BC), the finite-volume discretization of the lattice momentum changes from integer multiples of $2\pi/L$ with periodic BC to odd-integer multiples of π/L, where L is the lattice spatial side length. Imposing these conditions on the down-quark propagator while retaining periodic BC for the up quark results in a charged pion state that is antiperiodic: $\pi^+(x+L) = \bar{d}(x+L)u(x+L) = -\bar{d}(x)u(x)$. However, the neutral pion, which is needed for the physical decay $K^+ \to \pi^+\pi^0$, remains periodic as $\bar{d}(x+L)d(x+L) = \bar{d}(x)d(x)$. This can be avoided using the Wigner-Eckart theorem to relate the physical decay to an unphysical one containing only charged pions:

$$\langle (\pi^+\pi^0)_{I=2}|Q^{\Delta I_z=1/2}|K^+\rangle = \frac{\sqrt{3}}{2}\langle (\pi^+\pi^+)_{I=2}|Q^{\Delta I_z=3/2}|K^+\rangle. \tag{2.1}$$

This trick circumvents another issue; that imposing different boundary conditions on the up and down quarks manifestly breaks the isospin symmetry, allowing mixing between states of different isospin. This is prevented here by charge conservation, as the final state is the only charge-2 state that can be formed with the remaining quantum numbers. Using this technique, the RBC and UKQCD collaboration were able to obtain A_2 [3, 4].

Unfortunately the strategy described above cannot be employed for the calculation of A_0: This calculation requires the measurement of $K^0 \to \pi^+\pi^-$ and also $K^0 \to \pi^0\pi^0$, where for $I = 0$ there is no Wigner-Eckart relation to remove the neutral pions from the latter. There is also no means of avoiding the isospin-breaking induced by imposing different BC on the down and up quarks. G-parity boundary conditions (GPBC) [5, 6, 7] offer a means to avoid these issues.

3. G-parity Boundary Conditions

G-parity is a combination of charge conjugation and an isospin rotation by π radians about the y-axis: $\hat{G} = \hat{C}e^{i\pi\hat{I}_y}$, where the hat-symbol is used to denote operators. The charged *and* neutral pions are all eigenstates of this operation with eigenvalue -1, hence applying the operation at a spatial boundary causes the pion states to become antiperiodic in that direction, removing the zero-momentum ground state.

At the quark level,

$$\hat{G}\begin{pmatrix} u \\ d \end{pmatrix} = \begin{pmatrix} -C\bar{d}^T \\ C\bar{u}^T \end{pmatrix}, \tag{3.1}$$

where $C = \gamma^2\gamma^4$ in our conventions. In order to efficiently handle the mixing between the quark flavours at the lattice boundary, we were required to perform extensive modifications to the Columbia Physics System (CPS) and BFM/Bagel libraries (which contains assembly-optimized code that takes full advantage of the power of the IBM BlueGene/Q machines). Further discussion of the implementation strategy can be found in ref. [8].

Additional complications arise from the fact that the Dirac operator for the fields across the boundary involves complex conjugated gauge links which necessitates the generation of new ensembles obeying complex conjugate BC. (Note that using antiperiodic BCs rather than G-parity BCs in this calculation would also require new ensembles to be generated due to the presence of vacuum diagrams.)
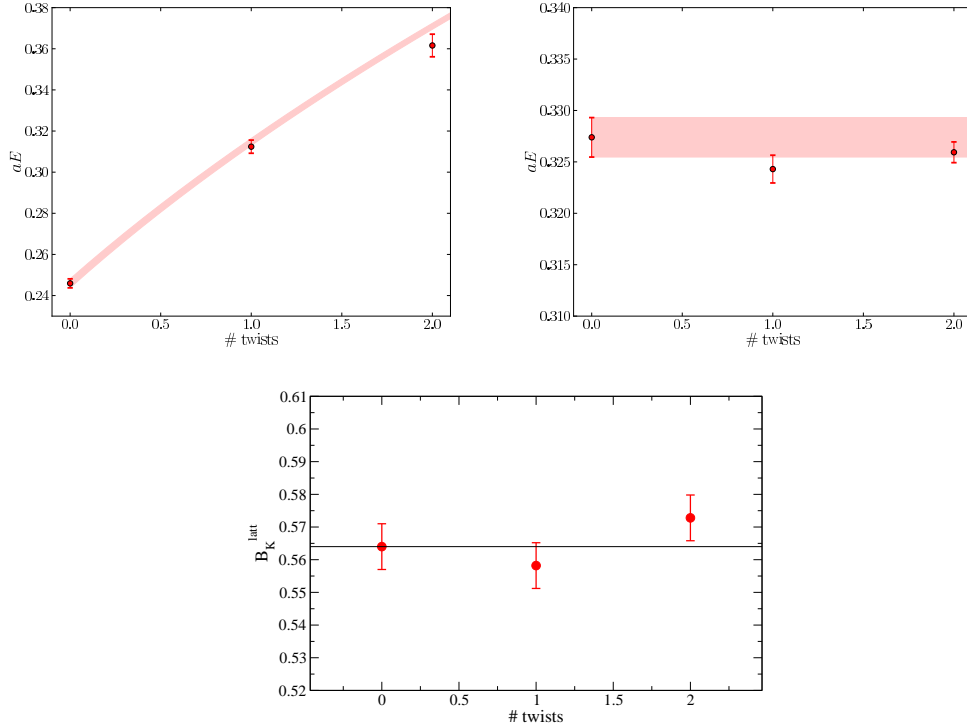
Figure 1: Top: the measured pion and kaon energies respectively as a function of the number of G-parity directions (twists), overlaid by the expected continuum dispersion relations. Bottom: B_K as a function of the number of G-parity directions.

In order to describe states involving strange quarks, in particular the stationary neutral kaons required for the A_0 calculation, with the quarks interacting with gauge fields that obey complex-conjugate BC, we place the strange quark in an isospin doublet with a fictional degenerate partner, referred to as s', and impose GPBC on this pair. We can then form a state comprising the usual kaon and a fictional meson containing the partner quarks: $\tilde{K} = \frac{1}{\sqrt{2}}(\bar{s}d + \bar{u}s')$. This is an eigenstate of G-parity with eigenvalue $+1$, and thus obeys periodic BC and has a stationary ground state. If we restrict ourselves to operators involving only the physical strange quark, then the fictional partner to the kaon can only contribute by propagating through the boundary, an effect which is suppressed exponentially in the lattice size and the kaon mass, and is expected to be on the sub-percent level. Of course this theory now has one too many quark flavours, hence we must take the square-root of the s/s' fermion determinant. Unfortunately this results in a non-local determinant, although the non-locality is confined to the boundaries and should be benign at sufficiently large volumes. Further investigation is required into this source of systematic error, perhaps using some variant of staggered chiral perturbation theory, but to-date we have not observed any evidence of its impact.

The use of GPBC impacts the forms of the diagrams involved in a given calculation: The mixing of quark flavours allows for the Wick contraction of up and down quark field operators resulting in non-zero values for the Green's functions:

$$\mathscr{G}_{y,x}^{(2,1)} = \langle C\bar{u}_y^T \bar{d}_x \rangle, \qquad \mathscr{G}_{y,x}^{(1,2)} = \langle -d_y u_x^T C^T \rangle. \tag{3.2}$$

As a result we must evaluate additional diagrams involving propagators that cross the boundary. In the first of the above contractions, quark flavour flows towards the boundary on both sides. Likewise, quark flavour flows away from the boundary in the second contraction. We may interpret this as the boundary destroying/creating flavour, violating baryon number conservation. In practise
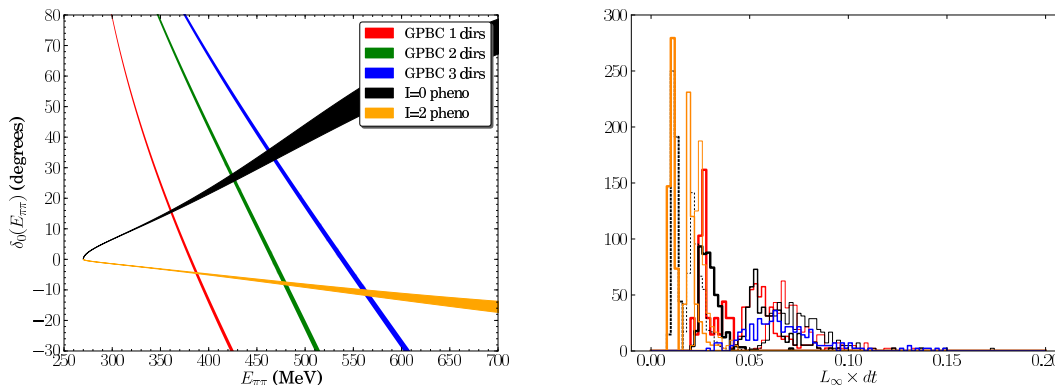
Figure 2: (Left) The s-wave $\pi\pi$ scattering phase shift δ_0 as a function of the energy of the $\pi\pi$ state obtained using Lüscher's quantization condition for G-parity boundary conditions in 1,2 and 3 directions on our 32^3 spatial box. The error band is obtained by varying the inverse lattice spacing by its combined systematic and statistical error. These are overlaid by the phenomenological curves from ref. [13]. The points at which these curves meet are the allowed finite-volume two-pion energies. Note that both of these curves assume a physical pion mass. (Right) The histogram of the molecular dynamics 'impulse' $L_\infty \times dt$ for each component of the integrator, broken down according to the timestep. The blue distribution is for the first Hasenbusch step, the red for the second Hasenbusch step (this term is nested below the first and hence has components with different time-steps), orange for the heavy quark and black for the DSDR (twisted mass) term.

this means that baryon-number eigenstates are not eigenstates of the system; for example the proton (uud) mixes with the anti-neutron ($\bar{d}\bar{d}\bar{u}$). However this is not important for calculations involving only mesonic states.

In order to demonstrate that the GPBC have the desired effect, we generated fully dynamical ensembles of domain wall fermions with the Iwasaki gauge action at $\beta = 2.13$, ($a^{-1} = 1.73(3)$ GeV) using a lattice volume of $16^3 \times 32 \times 16$ and a pion mass of ~ 420 MeV, and G-parity boundary conditions in one and two directions (with periodic BCs in the remaining directions). We compared several quantities measured on these to those calculated on our existing ensembles [9] with the same lattice parameters. In figure 1 we plot the measured pion and kaon energies as a function of the number of directions with GPBC. We see clearly the increase in pion energy associated with the increasing number of G-parity boundaries, and that it agrees well with the continuum dispersion relation. We also see that stationary kaon states can be produced in this framework. In addition, we consider the quantity B_K, which represents the amplitude of mixing between neutral kaon states via the weak interaction. As it involves only kaons, we expect this quantity to be invariant under changing the number of G-parity boundaries; from the figure we see that this is indeed the case.

4. Generation of Physical Ensembles

With the modifications to our codebase now complete, we have commenced the generation of the ensemble for our A_0 calculation using 512 nodes of the USQCD BlueGene/Q machine at Brookhaven National Laboratory. In order to avoid tuning the lattice parameters in the more complicated G-parity environment, we have retained the parameters used for our first calculation of A_2: a lattice volume of $32^3 \times 64$ with the Iwasaki+DSDR gauge action at $\beta = 1.75$ ($a^{-1} = 1.37(1)$ [10]) and input dimensionless quark masses of $m_l = 0.001$ and $m_h = 0.045$, which results in a lightest unitary pion of 171(1) MeV. We deviate slightly from the previous runs in using Möbius domain wall fermions with $L_s = 16$ for the evolution, with the Möbius parameters b and c set to 1.5 and 0.5 respectively. The Möbius action with these parameters is equivalent [11] to the Shamir domain wall fermion action with $L_s = 32$ that we used for the previous calculation, hence we achieve a factor of two reduction in L_s for the same physics. We are currently investigating the feasibility of

reducing the input quark mass to $m_l = 0.0001$ in order to bring down the pion mass to 143(1) MeV, and possibly tuning the Möbius parameters further to reduce the computational cost.

For the calculation of A_2 it was necessary to impose APBC in two directions in order to match the kaon and two-pion energies. In the $I = 2$ state the pion interaction is repulsive whereas it is attractive for $I = 0$, hence the energy of the latter state for a given choice of boundary conditions will be smaller than the former. We can estimate the energy by combining Lüscher's quantization condition [12], which relates the allowed lattice $\pi\pi$ energies to the s-wave scattering length, and a phenomenological curve [13] of the dependence of the scattering length on the energy. The points at which these two curves intersect for a given lattice spacing and box size correspond to the allowed finite-volume $\pi\pi$ energies. As the Lüscher formula depends on the boundary conditions due to the sum over allowed momenta in the zeta function, different curves are obtained as we vary the number of directions with GPBC. In figure 2 we plot the two sets of curves for both $I = 0$ and $I = 2$ $\pi\pi$ states. We see that we can achieve $E_{\pi\pi} \sim 470$ MeV using GPBC in three directions, which is close to the kaon mass of 500 MeV. Of course this estimate assumes physical quark masses, whereas in practise the lightest unitary pion will be somewhat heavier. Any remaining difference between the $\pi\pi$ energy and the kaon mass introduces a systematic error that must be included in the final error budget.

The layout of the molecular dynamics integrators used for Monte Carlo evolution of this ensemble is somewhat unusual. In a typical $2 + 1$ flavour calculation the contributions of the two flavours of degenerate light quarks are determined using the pseudofermion method with kernel $(M^\dagger M)^{-1}$, where M is the Dirac matrix. Using the square of the matrix is necessary to ensure that the matrix is positive-definite and as such can be represented as a Gaussian integral over the pseudofermion fields. For domain wall fermions we must also evaluate the determinant of Pauli-Villars fields that are used to cancel the bulk infinities in the $L_s \to \infty$ limit arising from unphysical heavy modes; as these are bosonic fields, the calculation of their determinant is combined with that of the pseudofermion determinant, such that we evaluate ratios $M(1)^\dagger M(1)/M(m_f)^\dagger M(m_f)$, where m_f is the fermion mass and the Pauli-Villars mass is unity. Reductions in the molecular dynamics fermion force can be achieved using the Hasenbusch technique [14] of splitting this ratio into a number of intermediate steps with masses in the numerator and denominator that are closer in value and with independent pseudofermion fields. By re-using the solutions of previous Hasenbusch steps as inputs to the next inversion, the use of many Hasenbusch steps typically has little overhead. For the single flavour of heavy quark, the Rational Hybrid Monte Carlo algorithm (RHMC) is typically used to evaluate the psuedofermion integral with kernel $(M^\dagger M)^{-1/2}$. This requires the evaluation of $(M^\dagger M + s)^{-1}$, for a number of shifts s. In order to do this efficiently, multi-shift Krylov solvers are typically used. These have the limitation that the input "guess" to the solver must be zero (this can avoided [15] at the expense of introducing possible instabilities into the solver), which prevents us from re-using the results of the previous Hasenbusch steps to speed up the evolution. As a result we cannot use multiple Hasenbusch steps for the evaluation of the heavy quark determinant without incurring significant overheads. Usually this is not important as the total force is dominated by the light quarks.

In the G-parity case the Dirac matrix is intrinsically two-flavour, hence we must use RHMC for both the light and strange quark determinants to take the square-root and fourth-root of det $M^\dagger M$ respectively. In addition, the cost of inverting the two-flavour Dirac matrix is roughly a factor of two larger than usual. These additional overheads force us to use fewer Hasenbusch steps for the light quark determinant, making the tuning more difficult. We have been able to achieve a good balance of forces using two Hasenbusch steps with masses $(m_f, m_{PV}) = (0.001, 0.007)$ and $(0.007, 1)$ with the second step nested beneath the first (i.e. with a smaller time-step). The cheaper heavy quark and twisted mass (DSDR) terms were further nested. We use Omelyan integrators for each term in the nested hierarchy. In figure 2 we show a histogram of the quantity $L_\infty \times dt$ for each

term, where dt is the time-step and L_∞ is the global maximum of the matrix-norm of the molecular dynamics force: $L_\infty = \max(||F||)$ and where F is the force (a matrix in the $su(3)$ Lie algebra). We have found that the distribution of this quantity gives a good indication as to whether a particular term or set of terms are dominating the integration error. We see that the impulses are well balanced such that no single term dominates in the acceptance. At the time of writing we have achieved a theoretical acceptance of around 60% and a generation time of 10.5 hours per-configuration on 512 nodes of BlueGene/Q, although further tuning is still taking place.

5. Conclusions and Outlook

After performing the calculation of the $\Delta I = 1/2 \; K \to \pi\pi$ amplitude we will have all of the pieces required for a complete *ab initio* determination of the measure of direct CP-violation in the Standard Model. This calculation requires significant computational and theoretical advances to be made, particularly in the strategy used to obtain physical kinematics in the decay. Much of this work has now been completed, and the RBC and UKQCD collaboration have begun generating the large-volume, near-physical pion mass ensembles for the calculation.

Our work now is focused upon formulating and testing the measurement strategy, including the technique we will use to evaluate the vacuum diagrams. Further testing of the systematic errors associated with the G-parity technique is also required, although thus far we have observed no evidence of any sicknesses. Further afield we might also consider the uses of G-parity boundary conditions in other frontier calculations performed by the collaboration, particularly those with significant noise contributions from intermediate pion states such as the calculation of the $K_L - K_S$ mass difference [16].

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