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Lattice Measurement of the $\Delta I = 1/2$ Contribution to Standard Model Direct CP-Violation in $K \to \pi\pi$ Decays at Physical Kinematics: Part I

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For the RBC and UKQCD collaborations

The RBC and UKQCD collaborations have recently published lattice results for the $K \to \pi\pi$ decay amplitude in the $I = 2$ channel, A_2, and improved results were presented at this conference. Here we discuss the determination of the $I = 0$ channel amplitude, A_0, which, when combined with A_2, allows for the determination of ε', the measure of direct CP-violation in the Standard Model. In this part I we provide an overview of the project and detail our use of G-parity boundary conditions to achieve physical kinematics in the decay, as well as discussing the ongoing generation of the specialized lattices required; part II [1] focuses on the measurement itself.

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1. Introduction

Direct CP-violation is the decay of a CP-odd state to a CP-even state (or *vice versa*), and was first observed in the decays of neutral kaons into two pions (CP-even). Due to indirect CP-violation, the physical eigenstates K_L and K_S are admixtures of the CP-eigenstates, hence the isolation of direct CP-violation in experimental measurements requires the observation of K_L and K_S decays in two channels. Traditionally the isospin zero and two $\pi\pi$ final states are used to define a measure of direct CP-violation as follows:

$$\varepsilon' = \frac{\omega}{\sqrt{2}}\left(\eta_2 - \eta_0\right), \text{ where } \eta_I = \frac{\langle(\pi\pi)_I|\mathscr{T}|K_L\rangle}{\langle(\pi\pi)_I|\mathscr{T}|K_S\rangle}, \ \omega = \frac{\langle(\pi\pi)_2|\mathscr{T}|K_S\rangle}{\langle(\pi\pi)_0|\mathscr{T}|K_S\rangle}, \tag{1.1}$$

and $\mathscr{T}$ is the interaction matrix. The quantity ω is small: $|\omega| \sim 1/22.5$, mainly due to low-energy strong interaction effects [2, 3, 4] (the so-called "$\Delta I = 1/2$ rule").

The first principles Standard Model determination of ε' is very important as this quantity is highly sensitive to Beyond the Standard Model sources of CP-violation, which are required in order to describe the observed matter-antimatter asymmetry in the Universe. However, because non-perturbative strong interactions play such an important role, reliable theoretical determinations of ε' can only currently be performed using lattice methods.

The lattice measurements proceed as follows. Rewriting ε' in terms of the strong interaction eigenstates, we obtain

$$\varepsilon' = \frac{i\omega e^{i(\delta_2-\delta_0)}}{\sqrt{2}}\left(\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}\right), \tag{1.2}$$

where the amplitudes A_I are defined via $\langle(\pi\pi)_I|\mathscr{T}|K_0\rangle = A_I e^{i\delta_I}$, and δ_I are the $\pi\pi$-scattering phase shifts. In terms of A_I, $\omega = \mathrm{Re}A_2/\mathrm{Re}A_0$. As these processes occur at a much lower energy scale than the underlying weak interactions, we describe the interaction using the weak effective theory:

$$H_W^{\text{eff}} = \frac{G_F}{\sqrt{2}} V_{us}^* V_{ud} \sum_{i=1}^{10} \left[z_i(\mu) + \tau y_i(\mu)\right] Q_i(\mu), \tag{1.3}$$

where z_i and y_i are perturbative Wilson coefficients, Q_i are the effective four-quark operators, and $\tau = -V_{ts}^* V_{td}/V_{ud}V_{us}^*$. On the lattice one measures the matrix elements, $\langle\pi\pi|Q_i|K\rangle$, with energy-conserving kinematics $E_{\pi\pi} = m_K$. The operators are non-perturbatively renormalized at a high energy-scale, typically 3 GeV, and perturbatively matched to the renormalization scheme of the Wilson coefficients. The finite-volume amplitudes are then corrected to the infinite volume by applying the Lellouch-Luscher factor [5].

The RBC and UKQCD collaborations have now successfully performed a physical calculation of A_2 [4]; the determination of the remaining amplitude, A_0, is therefore of high priority. In practise this measurement is significantly more difficult than that of A_2 for two reasons, the first being that the $I = 0$ $\pi\pi$ state mixes with the vacuum, giving rise to disconnected diagrams which introduce significant statistical noise that must be overcome using advanced techniques; the solution of this is discussed in part II [1] of these proceedings.

The second difficulty arises from the necessity of using physical kinematics: the Euclidean time dependence of a general Green's function has the form $C(t) = \sum_i a_i e^{-E_i t}$, with increasing energies E_i, and lattice quantities are typically extracted using single-exponential fits to the large-time behavior, where the ground-state dominates. For a standard lattice calculation with periodic spatial boundary conditions, the lightest states of the $I = 0$ $\pi\pi$ system are first the vacuum and then two pions at rest, for which the energy is $2 \times 135\,\text{MeV} \ll m_K = 496\,\text{MeV}$. In order to match the kaon and $\pi\pi$ energies we must therefore use the second excited state, which comprises two pions moving back-to-back with momentum $p = 2\pi/L$, which can be tuned by varying the lattice size L. While

the vacuum component can be explicitly subtracted, the stationary pion state cannot, hence such a calculation requires multi-exponential fits to the time-dependence; these are typically very noisy, especially when applied to measurements with disconnected diagrams. This can be circumvented by changing one or more of the spatial boundary conditions from periodic to G-parity boundary conditions (GPBC) [6, 7, 8, 9, 10].

2. G-parity Boundary Conditions

G-parity is the combined action of charge conjugation and an 180-degree isospin rotation about the y-axis: $\hat{G} = \hat{C}e^{i\pi\hat{I}_y}$, where the hat-symbol is used to denote operators. At the quark level,

$$\hat{G}\begin{pmatrix} u \\ d \end{pmatrix}\hat{G}^{-1} = \begin{pmatrix} -C\bar{d}^T \\ C\bar{u}^T \end{pmatrix}, \tag{2.1}$$

where $C = \gamma^2\gamma^4$ in our conventions.

The charged and neutral pions are G-parity odd, thus applying the operation at a spatial boundary is equivalent to imposing antiperiodic boundary conditions on the pions: $\pi(x+L) = -\pi(x)$. Therefore, with GPBC in $n \leq 3$ directions, the lightest pion state has energy $E_\pi = \sqrt{m_\pi^2 + n(\pi/L)^2}$, allowing us to instead tune the energy of the *first* excited state above the vacuum to match the kaon energy, avoiding the necessity of multi-exponential fits.

The use of GPBC introduces a number of difficulties that have been identified and elaborated upon in our previous publications [9, 10]. Here we summarize the issues and their solutions, and we refer the reader to the aforementioned documents for more detailed discussion.

- The u and d fields couple to the regular gauge links U, whereas the $\bar{u}^T$ and $\bar{d}^T$ fields couple to the complex-conjugated links U^*. Consistency across the boundary therefore requires that the gauge field obeys complex conjugate (equivalently charge conjugation) boundary conditions. This necessitates the generation of entirely new ensembles for measurements with GPBC. In section 4 we discuss in detail the ensembles that we have generated.

- Quark propagators spanning the boundary allow for unusual Wick contractions of the form $\overbrace{\bar{u}^T d}$ and $\overbrace{d u^T}$, resulting in a number of additional diagrams that must be evaluated for a given quantity. For the determination of the $K \to \pi\pi$ diagrams we wrote a symbolic computer algebra system to automate the process, and compared to a separate by-hand determination.

- The boundary conditions explicitly break flavor (baryon number) conservation, although this is not an issue for mesonic quantities.

- The neutral (and charged) kaon states, $K_0 = d\bar{s}$ and $\bar{K}_0 = s\bar{d}$, are not eigenstates of the system as GPBC transform the down quark but not the strange. In addition, modifications to the strange quark Lagrangian are required to make it consistent with the charge-conjugation boundary conditions of the gauge fields. The solution is to place the s-quark in an isospin doublet with a fictional degenerate quark field s' and impose GPBC on that pair. We can then form an operator, $\tilde{K}_0 = \frac{1}{\sqrt{2}}(d\bar{s} + \bar{u}s')$, which is G-parity even and hence projects only onto states with zero momentum.

  For the $K \to \pi\pi$ interaction we use the physical four-quark operator, which acts solely on the $d\bar{s}$ component and hence only couples to the $\bar{u}s'$ through terms spanning the boundary that are exponentially suppressed in the kaon mass and lattice size.

  In order to revert to a three flavor simulation we must take the square-root of the s/s' determinant in the RHMC, which, due to the coupling between the fields at the boundary, results

in a non-local determinant that potentially introduces universality violations; however, it can be shown that such effects are exponentially suppressed in the lattice size at low energies.

In ref. [10] we performed several dynamical domain wall fermion (DWF) simulations with GPBCs in 0,1 and 2 directions. We demonstrated that the pion states obey the continuum dispersion relation, and that we could produce stationary kaon states whose masses are independent of the number of G-parity twists within statistics. In addition we demonstrated that we could compute the $K - \bar{K}$ mixing amplitude, B_K, in this framework and that this also remains independent of the number of G-parity twists; this is a valuable test because the four-quark operator involved has a similar form to that used for the $K \to \pi\pi$ calculations. More recently we have used these ensembles to compute the $\Delta I = 3/2$ $K \to \pi\pi$ amplitude, and successfully compared to results obtained with the traditional approach used in refs. [2, 3, 4].

3. Implementation

We simulate with two independent fermion fields per lattice site and explicitly impose the flavor-mixing at the lattice boundary. The implementation is written in the Columbia Physics System (CPS) with the BFM/Bagel package for optimized fermionic inversions on IBM BlueGene/Q machines. Details of the implementation can be found in refs. [9, 10].

As we simulate with two fermion flavors we would naively expect a factor of two increase in simulation cost. However, for DWF the situation is complicated by the necessity of using the square of the Dirac matrix in the Hybrid Monte Carlo (HMC) algorithm in order to obtain a positive-definite fermion matrix. For conventional 2+1f simulations with a single-flavor Dirac matrix the resulting determinant is identical to that of two fermion flavors. However the G-parity Dirac matrix mixes the flavor fields at the boundary and is therefore intrinsically two-flavor: using the square of the Dirac matrix therefore results in a four-flavor determinant which must be square-rooted using the Rational HMC (RHMC) algorithm. Similarly the four-flavor fermion matrix for the strange sector must be fourth-rooted to revert to a single flavor.

The RHMC algorithm uses a rational approximation to the root that is valid over an eigenvalue range governed by the number of rational poles. As the light-quark Dirac matrix has a very wide eigenvalue range it was necessary to use over 20 poles, a factor of two larger than a typical strange-quark RHMC. The algorithm makes use of multi-shift conjugate gradient (CG) to perform the necessary inversions, which for such a large number of poles has substantial linear algebra overheads associated with updating the search and solution vectors. On a 512-node BG/Q machine with our target local volume, the speed of the linear algebra (as well as the matrix multiplication) is limited by the memory bandwidth, and as such achieves roughly 7.2 Gflops/s performance in the multi-shift CG. We were able to partly redress this by performing the matrix multiplication in single precision, halving the bandwidth usage. The downside is that the residual vector, which is used for the stopping condition, quickly accumulates finite-precision errors such that the algorithm either terminates too early or not at all. This was rectified by a 'reliable update' step every 200 iterations where the stored residual vector is replaced with the exact (double-precision) residual. Coupled with maximal re-use of cached data to reduce the memory load in the linear algebra, we have demonstrated a 70% improvement in performance during the RHMC update, reaching 12.3 Gflops/s. The resulting solution vectors were then used as inputs to a restarted single-precision CG solve for each pole independently in order to guarantee satisfactory convergence.

In the future we intend to investigate the use of the 'exact one-flavor action' [11], for which the fermion matrix is natively positive-definite and hence removes the need for RHMC for the light quarks.

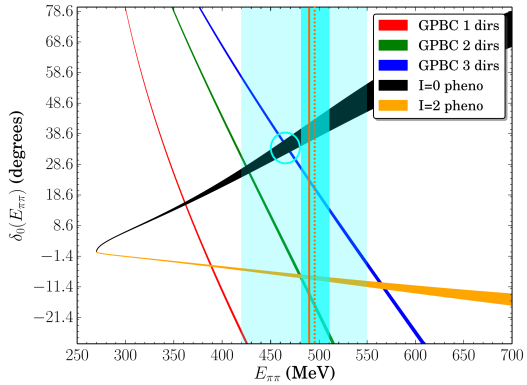

Figure 1: The s-wave $\pi\pi$ scattering phase shift δ_0 as a function of the energy of the $\pi\pi$ state obtained using Lüscher's quantization condition for G-parity boundary conditions in 1,2 and 3 directions on our 32^3 spatial box. The error band is obtained by varying the inverse lattice spacing by its combined systematic and statistical error. These are overlaid by phenomenological curves obtained from ref. [14]. The points at which these curves meet are the allowed finite-volume two-pion energies. The vertical dotted and full orange lines are the physical and measured kaon masses respectively, and the blue circle indicates the intercept at which we can predict the $(\pi\pi)_{I=0}$ energy on our physical ensemble. The wide and thin vertical blue bands are the measured values of the $(\pi\pi)_{I=2}$ energy with and without vacuum contributions respectively.

After our substantial developments in the evolution algorithms and code, we now have well-tested, efficient BG/Q code.

4. Ensemble for $K \to \pi\pi$ measurements

As initially described in ref. [10], we have generated an ensemble with a $32^3 \times 64$ lattice volume, using DWF with the Iwasaki+DSDR gauge action at $\beta = 1.75$ ($a^{-1} = 1.379(7)$ GeV [12]) and physical quark masses. Here the DSDR term in the gauge action is used to suppress the dislocations or 'tears' in the gauge field that are largely responsible for the residual chiral symmetry breaking on these coarse lattices. This ensemble is essentially the same as that used for our first measurement of A_2 [2, 3], although we have reduced the input quark mass such that the pion mass is reduced from 171(1) MeV to 141.3(2.4) MeV ($E_\pi = 273.8(1.8)$ MeV). We have also changed from Shamir to Möbius DWF, which with Möbius parameters $b-c=1$ and $b+c=32/12$ allows us to simulate with a fifth-dimensional extent of $L_s = 12$ while retaining the same physics as the original $L_s = 32$ Shamir DWF simulation, resulting in a significant reduction in computational cost.

In figure 1 we plot the curves relating the lattice $\pi\pi$ energies to the s-wave scattering length for GPBC in 1, 2 and 3 directions, obtained using Lüscher's quantization condition [13] applied to a 32^3 spatial box. We also plot phenomenological curves [14] of the dependence of the scattering length on the energy. The intercepts of these curves correspond to the allowed finite-volume $\pi\pi$ energies. Based on this figure we previously determined that GPBC in three directions provide the closest match between the kaon and $\pi\pi$ energies for the $I = 0$ case. In practise we found $E_{(\pi\pi)_{I=0}} = 485(65)$ MeV ($E_{(\pi\pi)_{I=0}} = 496(15)$ MeV without vacuum contributions), and $m_K = 489.3(2.4)$ MeV. These measurements, and those given above, were determined using 24 configurations separated by 8 MD time units. Although the $\pi\pi$ energies are currently very noisy, these preliminary results suggest that we are close to on-shell kinematics. Any remaining mismatch introduces a systematic error that must be included in the final error budget. Note that we also observe quite impressive agreement between our computed $I = 2$ $\pi\pi$ energy, $E_{(\pi\pi)_{I=2}} = 571.6(3.5)$

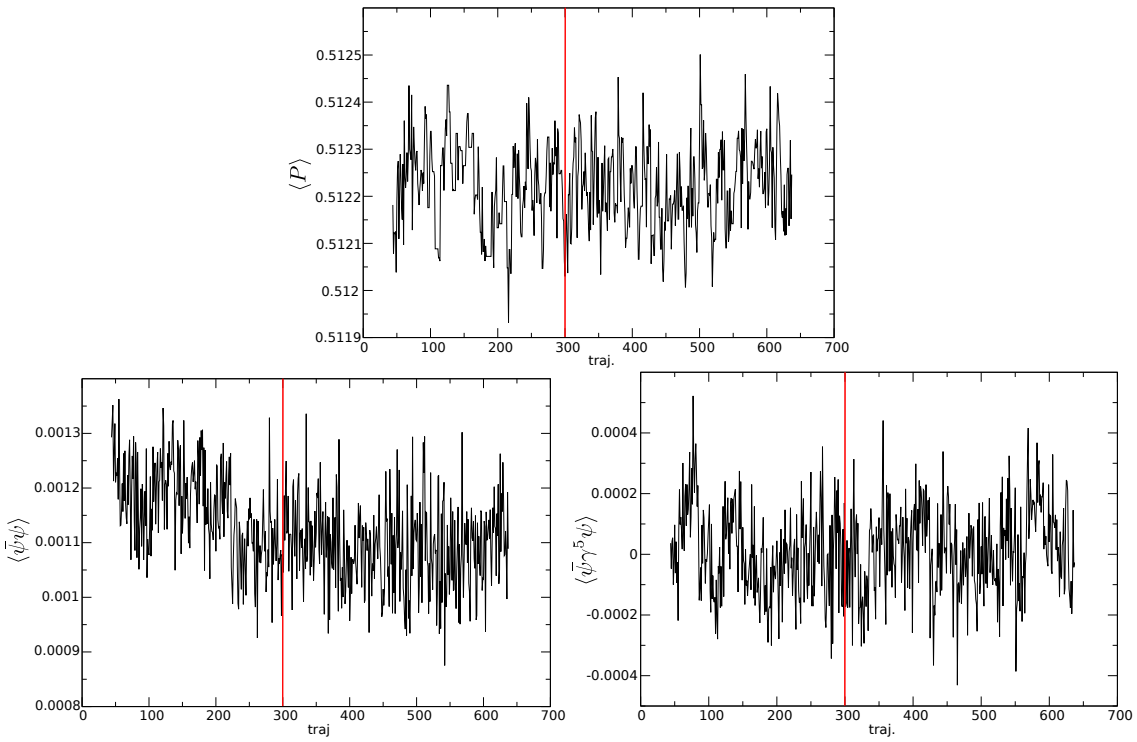

Figure 2: The evolution of the plaquette (top), chiral condensate (lower-left) and pseudoscalar condensate (lower-right) measured on the first 650 configurations of our ensemble. The red line indicates the point at which we began measurements (trajectory 300).

MeV, and the value of ~ 570 MeV that one would estimate from figure 1. A more detailed explanation of our measurement strategy and sources of systematic error is given in discussed in part II [1] of these proceedings.

The generation of the ensemble has been performed using the USQCD 512-node BlueGene/Q machine at BNL, as well as on various partitions of the 'Mira' BG/Q installation at Argonne via a USQCD allocation. In the past year we have performed a substantial amount of tuning and optimization (as discussed above), such that one configuration now requires 6.8 hours per configuration on a 512-node machine, down from 10.5 hours previously [10]. To date we have accumulated over 900 trajectories (MD time units) with an 89% Metropolis acceptance. The plaquette, chiral condensate and pseudoscalar condensate are shown in figure 2, from which we determine that the ensemble has thermalized at around trajectory number 250; we therefore currently have ~ 650 thermalized configurations. The measurements presented in these documents were performed from configuration 300.

5. Conclusions

The measurement of the $K \to \pi\pi$ amplitude in the $I = 0$ channel, A_0, is the last remaining step towards the first *ab initio* determination of the measure of direct CP-violation in the Standard Model, ε'. Comparison of this result with experiment may provide evidence of new sources of CP-violation that could help explain the observed matter-antimatter asymmetry in the Universe. Due to significant strong interaction effects, lattice methods must be used. The lattice calculation is extremely difficult due to the presence of disconnected diagrams that vastly increased the statistical noise, and also due to the requirement of an energy conserving decay process.

We have detailed a successful technique for performing a measurement with energy conserving kinematics that does not rely on multi-exponential fits to the time dependence of noisy lattice correlation functions, namely the use of G-parity spatial boundary conditions (GPBC). This approach engenders a number of technical difficulties, including the necessity of generating new ensembles, that we have summarized in this document. We have also discussed our efforts at optimizing the generation of G-parity gauge configurations. In a separate document [1] we discuss the measurement itself.

We presented details of our $32^3 \times 64 \times 12$ Möbius domain wall ensemble with parameters tuned to match an $L_s = 32$ Shamir DWF simulation with the same space-time volume. We use GPBC in three directions. The input quark masses are such that our pion and kaon masses are nearly physical: $m_\pi = 141.3(2.4)$ MeV ($E_\pi = 273.8(1.8)$ MeV) and $m_K = 489.3(2.4)$ MeV, and the $\pi\pi$ energy is $E_{\pi\pi} = 485(65)$ MeV ($E_{\pi\pi} = 496(15)$ MeV without the vacuum contributions) suggesting that our $K \to \pi\pi$ measurements are close to being on-shell. These results were obtained using 40 configurations separated by 8 MD time units. We have thus far generated over 900 trajectories, with ~ 650 thermalized, and we intend to continue configuration generation until the statistical error on our A_0 result are $\mathcal{O}(20\%)$ or less.

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