Kaon physics and CP violation calculations on QCDOC

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Abstract. The violation of charge conjugation (C) and parity (P) in kaon decays, first observed in Nobel-prize winning experiments at Brookhaven National Lab in 1964, is allowed by the Standard Model of particle physics. Predicting indirect CP violation in kaon decays requires the values for standard model parameters and the evaluation of a four-quark matrix element inside a kaon. Using lattice QCD with domain wall fermions and the current QCDOC computers, calculations are underway that will yield, among other results, the value for this matrix element, allowing more precise comparisons between theory and experiment for CP violation in kaon decays.

1. Introduction
Symmetry plays a vital role in particle physics and, over the last fifty years, violations of symmetries have played an important role in the development of the current Standard Model of particle physics. The suggestion and experimental verification of the violation of parity symmetry (P), which takes a physical process into its mirror image, in the weak interactions was the first major demonstration that long cherished symmetries could be violated in Nature. Subsequently in 1964, the combined symmetry of parity and charge conjugation (C), which takes a particle into its antiparticle, was soon shown to be violated in kaon decays. For many years, CP violation was only observed in kaon decays, a situation which has now changed with the observation of CP violation in B-quark systems. For a more extensive review, see [1].

Figure 1 outlines the observation of CP violation that occurs when a $K_L$ decays to two pions. The $K_L$ is a superposition of a $K^0$ and a $\bar{K}^0$ and the CP violation first observed in 1964, called indirect CP violation now, comes about because $K^0$ and $\bar{K}^0$ can mix with each other. In the Standard Model, $K^0 - \bar{K}^0$ mixing comes about through loop diagrams involving heavy quarks and gauge bosons. These loop diagrams can be evaluated analytically, and, for low energy processes like kaon decay, their effects are given by a four-quark operator multiplied by an effective coupling strength which is a function of the masses and couplings of the underlying electroweak theory. The resulting four-quark operator must be evaluated inside a kaon - a calculation that can only be done from first principles through lattice QCD. Figure 2 depicts this calculation and shows the resulting operator of interest, $Q^{\Delta S=2}$.

A precise value for $\langle \bar{K}^0 | Q^{\Delta S=2} | K^0 \rangle$ is needed to go from the measured indirect CP violation in kaon decays to Standard Model parameters, or from Standard Model parameters to a prediction. The importance of calculating $\langle \bar{K}^0 | Q^{\Delta S=2} | K^0 \rangle$, or the value of $B_K$, which differs only by known factors, has been stressed since the beginning of lattice QCD simulations. With the development
Figure 1. The decay $K_L \to \pi\pi$ violates CP and has a small branching ratio. It was first observed in 1964 and the isospin independent CP violating process, which does not depend on whether charged or neutral pions are in the final state, is now called indirect CP violation.

Figure 2. In the Standard Model, $K^0 \leftrightarrow \bar{K}^0$ mixing comes about through electroweak physics appearing in loop diagrams. Analytically evaluating the loop diagrams yields a four-quark operator that needs to be evaluated inside a kaon.

of the domain wall fermion formulation, the deployment of multi-Teraflops computers like QCDOC [2] and improvements in algorithms, a calculation with controlled systematic errors is now underway. We overview the improvements that we have made thus far and report the first preliminary results from these calculations here.
2. Domain Wall Fermions

The discretization of the continuum Dirac operator has presented a major theoretical challenge to particle physics since the formulation of lattice QCD. While discretizations have been available from the beginning of lattice QCD, they have all broken some of the global symmetries of the continuum Dirac operator. In the continuum, these symmetries restrict the operators that $Q^{S=S=2}$ can mix with under renormalization; breaking these symmetries at finite lattice spacing leads to mixings which are difficult to control numerically, and which make calculations of $B_K$ problematic.

Domain wall fermions introduce an extra, fifth dimension into the problem and localize the physically relevant, light quark states on opposite boundaries in this new dimension [3]. The breaking of the continuum symmetries is now controlled by the extent of the fifth dimension, making it possible to recover the desired continuum symmetries at finite lattice spacing. In practice, one has to only make the fifth dimension large enough to control the unwanted mixings. This is numerically costly, since the computer time grows linearly in the size of the fifth dimension, but is far cheaper than controlling the breaking by decreasing the lattice spacing.

An additional feature of domain wall fermions, of critical importance to the calculation of $B_K$, is the demonstrated usefulness of the non-perturbative renormalization technique to relate the value of $B_K$ calculated on the lattice to the desired continuum quantity [4, 5]. While, in principle, such renormalization factors can be calculated using analytic perturbation theory, such calculations are difficult and are the frequently the dominant source of error in the determination of $B_K$ with other lattice QCD fermion methods.

Here we have focused on the value of domain wall fermion lattice QCD in the determination of $B_K$. It is important to point out that many other QCD quantities also benefit from calculations using the gluon configurations generated with domain wall fermions, because of the preservation of the continuum global symmetries of the Dirac operator.

3. Improved Monte Carlo Algorithms

Lattice QCD simulations are done via importance sampling of the Euclidean space Feynman path integral, and the inclusion of the light quark determinants in the importance sampling is numerically costly. The Hybrid Monte Carlo (HMC) techniques in use today, which are exact algorithms for sampling phase space, use a molecular dynamics evolution to move between points in phase space, with an accept/reject step to remove errors introduced by the finite step size molecular dynamics integration. To handle the physically important case of two light quarks (the up and down quarks) and the heavier strange quark (this is called QCD with 2+1 flavors) and maintain the general structure of HMC algorithms, one needs a tractable numerical technique to handle the square root of the determinant of the Dirac operator. While polynomial approximations are in use for this purpose, the new Rational Hybrid Monte Carlo (RHMC) algorithm of Clark and Kennedy uses a rational function to approximate any desired fractional power of the determinant [6].

The RHMC provides an accurate, low cost representation of the desired fractional power, and has also been augmented by the incorporation of other techniques. To briefly describe these, we define $D(m_i) = D_{DWF}^1(M_5, m_i)D_{DWF}(M_5, m_i)$, where $D_{DWF}(M_5, m_i)$ is the domain wall fermion Dirac operator. The continuum contribution of the two light quarks, with mass $m_i$, and the strange quark, with mass $m_s$, to the path integral is $\det[D(m_i)] \det[D(m_s)]^{1/2}$. Optimizing our current production calculations has led us to implement this as

$$\det \left[ \frac{D(m_l)}{D(m_s)} \right] \det \frac{D(m_s)}{D(1.0)}^{1/2} \det \left[ \frac{D(m_s)}{D(1.0)} \right]^{1/2} \det \left[ \frac{D(m_s)}{D(1.0)} \right]^{1/2}$$

(1)

The contribution to the molecular dynamics force from each ratio above is determined with a separate stochastic estimator. The first term, involving $m_l$ and $m_s$ is handled by conventional
Figure 3. The evolution of $\langle \bar{q}q \rangle$ on a lattice with a 3 fermi volume. The calculation after the dotted line is almost 6 times faster than the calculation before the dashed line, due to algorithmic improvements.

HMC, while the remaining terms are implemented via the RHMC algorithm. The ratios are an example of Hasenbusch preconditioning [7], with the first ratio markedly reducing the force from the light quarks, which is the most expensive to calculate. This has allowed us to use different time scales for the molecular dynamics integration. Employing all of these improvements with an Omelyan integrator has made our current production calculations almost six times faster than our initial implementation.

Figure 3 shows the evolution of $\langle \bar{q}q \rangle$ for 2+1 flavors of domain wall fermions with a light quark mass of about 1/2 the strange quark mass. The space-time volume is almost 3 fermis. The first 750 time units, using the original RHMC implementation took almost 6 months on a 4,192 node QCDOC partition, while the final 1500 time units took about 2 months on the same hardware.

4. Preliminary Results
With the first available working QCDOC hardware, the RIKEN-BNL-Columbia (RBC) Collaboration and the UKQCD Collaboration began simulations with 2+1 and 3 flavor QCD to determine an optimal gauge action and lattice spacing to begin production running. The Iwasaki gauge action was chosen, since it yields an acceptably small breaking of the continuum global symmetries and an adequate motion through different topological sectors of phase space. With this choice, we have produced gauge ensembles with three values for the light quark mass, $m_l \approx 3m_s/4$, $m_s/2$ and $m_s/4$ on two volumes of approximately 2 and 3 fermis. The extent of the fifth dimension is 16 and our preliminary value for the lattice spacing is $a^{-1} = 1.62(8)$ GeV.

A wide range of quantities are being calculated on these ensembles, including $B_K$. Figure 4 shows $B_K$ plotted versus lattice spacing, with our preliminary 2+1 flavor value for a 2 fermi volume given by the black triangle. (For a recent review of kaon phenomenology from Lattice QCD, see [8].) The earlier work of the RBC [9] and CP-PACS [10] collaboration using quenched DWF has given a consistent value for $B_K$ in the continuum limit, with statistical errors of less than 5% and systematic errors, neglecting quenching errors of less than 10%.

The current ensembles, plus planned simulations at a smaller lattice spacing which will begin in the fall, will provide a value for $B_K$ in the continuum limit for 2+1 flavor QCD with statistical errors comparable to the quenched case. This will markedly improve the comparison of the theoretical and experimental results for CP violation, where a 10% quenching error is assigned to current values for $B_K$ [8].
**Figure 4.** Some results for $B_K$ from lattice QCD plotted versus lattice spacing.

**Acknowledgments**

The calculations discussed in this paper are being done by the RIKEN-BNL-Columbia Collaboration and the UKQCD Collaboration. The collaborations acknowledged the support of the RIKEN Laboratory of Japan, the US Dept. of Energy and PPARC of the UK. UKQCD participants are: C. Allton, D. Antonio, K. Bowler, P. Boyle, M. Clark, J. Flynn, A. Hart, B. Joo, A. Juettner, A. Kennedy, R. Kenway, C. Kim, C. Maynard, J. Noaki, B. Pendleton, C. Sachrajda, A. Trivini, R. Tweedie, A. Yamaguchi, J. Zanotti. RBC participants are: T. Blum, M. Cheng, N. Christ, S. Cohen, C. Dawson, T. Doi, K. Hashimoto, T. Izubuchi, C. Jung, M. Li, S. Li, H. Lin, M. Lin, R. Mawhinney, S. Ohta, S. Sasaki, E. Scholz, A. Soni, T. Yamazaki.

**References**

[1] For a review of CP violation see the Review of Particle Physics, S. Eidelman, et. al., Physics Letters B592 (2004) 1, particularly http://pdg.lbl.gov/2005/reviews/cpvio1rpp.pdf.

[2] P. A. Boyle, et. al., IBM Journal of Research and Development, Volume 49, Number 2/3 (2005) 351.

[3] D. B. Kaplan, Phys. Lett. B288 (1992) 342; Y. Shamir, Nucl. Phys. B439 (1995) 54.

[4] G. Martinelli, C. Pittori, C. T. Sachrajda, M. Testa and A. Vladikas, Nucl. Phys. B445 (1995) 81.

[5] T. Blum, et. al., Phys. Rev. D68 (2003) 114506.

[6] M. A. Clark, Ph. de Forcrand and A.D. Kennedy, PoS LAT2005 (2006) 115 and hep-lat/0510004.

[7] M. Hasenbusch, Nucl. Phys. Proc. Suppl. B129 (2004) 27.

[8] C. Dawson, PoS LAT2005 (2006) 007.

[9] Y. Aoki, et. al., (RBC) Phys. Rev. D74 (2006) 094507.

[10] A. Ali Khan, et. al., (CP-PACS) Phys. Rev. D64 (2001) 114506.