Weak interactions of kaons from lattice QCD

Norman H Christ

Physics Department, Columbia University, New York, NY 10027, USA

E-mail: nhc@phys.columbia.edu

RBC and UKQCD Collaborations

Abstract. The methods of lattice QCD and available computer resources are now sufficient that predictions for many of the Standard Model properties of kaons can be made from first principles with accurately bounded uncertainties. We discuss two relatively new areas where lattice methods are having or will soon have a large impact: calculation of the two complex amplitudes A_0 and A_2 describing the decay of the kaon into two-pions with $I = 0$ and 2 and calculation of long-distance contributions to second-order electro-weak processes including the $K_L - K_S$ mass difference ΔM_K, the CP-violating parameter ϵ_K and certain rare kaon decays.

1. Introduction

Over the past thirty years lattice QCD has evolved from providing a first non-perturbative demonstration of confinement and chiral symmetry breaking in QCD to allowing much of low energy QCD to be accurately computed from first principles with controlled uncertainties. By replacing the space-time continuum by a regular, four-dimensional, hyper-cubic lattice and using powerful Monte Carlo methods to evaluate the Euclidean Feynman path integral which defines QCD, the previously intractable complexities of low-energy, strongly-coupled QCD are reduced to the problem of obtaining very large computational resources and developing increasingly powerful and efficient numerical strategies – two areas in which advancing technology and the growing importance of computational methods throughout science work to our advantage.

In the past two years, lattice QCD calculations have crossed an important threshold and can now determine directly the physics of the up, down and strange quarks using their physical masses, or in the case of most calculations, a single, isospin-symmetric average mass of ≈ 3 MeV, (expressed in the $\overline{\text{MS}}$ renormalization scheme at 3 GeV) for the up and down quarks, giving three degenerate pions of mass 135 MeV. Earlier calculations used light quark masses as large as 30 or 40 MeV and relied on chiral perturbation theory to extrapolate to the physical value, introducing significant, uncontrolled errors.

This ability to work at a physical value for the light quark mass is especially advantageous for calculations performed with chiral fermions where the light quark mass can be the largest source of unphysical, chiral symmetry breaking. For example, the calculations of the RBC and UKQCD collaborations typically use the domain wall fermion formulation in which an extra fifth dimension, whose size varies between 12 and 32 lattice units, literally separates the right- and left-handed fermion chiralities. While the Wilson and staggered fermion formulations achieve physical chiral symmetry in the continuum limit, the breaking of chiral symmetry at short

distances complicates the definition of the $\Delta S = 1$ weak Hamiltonian where the number of operators whose mixing must be controlled is dramatically reduced by chiral symmetry.

In addition, the explicit breaking of chiral symmetry by lattice artifacts for Wilson and staggered fermions is often the largest source of finite lattice spacing errors, errors which are absent when a chiral formulation is used. This is illustrated in Figure 1 where dimensionless ratios for a number of quantities are compared between two calculations, with inverse lattice spacings of $1/a = 1.73$ GeV and 2.28 GeV. These two calculations give results which agree on the $\approx 1\%$ level for lattice spacings which are not especially small by current standards.
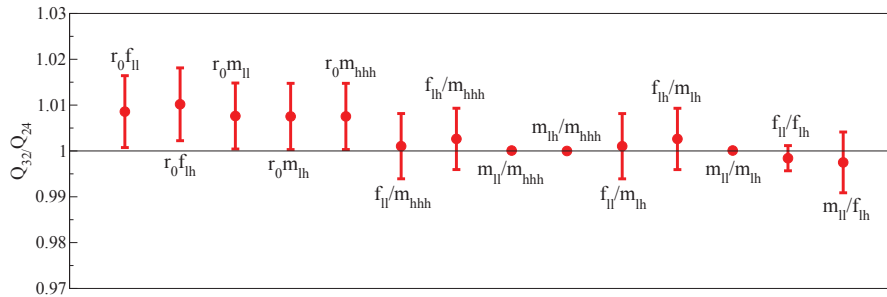
Figure 1. Comparison of a series of dimensionless ratios obtained from calculations at two inverse lattice spacings: $1/a = 1.73$ GeV and 2.28 GeV. The ratio of each ratio is plotted on the y axis. The subscripts indicate the masses of the quarks used where h indicates a near strange quark mass while l is a less massive quark. Further explanation can be found in Ref. [1].

This combined ability to work at physical quark masses and the empirically small finite lattice spacing errors found with chiral fermions implies that results accurate on the percent level can be obtained from a single lattice QCD calculation without chiral or even continuum extrapolations. For example, in a recent calculation on a $48^3 \times 96$ lattice with $1/a = 1.73$ GeV and light and strange quark masses chosen close to their physical values, we have obtained the result $f_\pi = 130.7(2)$ MeV directly from the computer with no extrapolations or corrections beyond the normalization factor for the axial current. The 0.2% error is statistical and a satisfactory agreement with the experimental value of $f_\pi = 130.4$ MeV is seen even for this simple, direct result. While added calculations with a smaller lattice spacing and heavier quark masses allow sub-percent corrections to be made that adjust for the small mismatch of the input and physical quark masses and $O(a^2)$ discretization errors [2], a result for f_π with percent accuracy can be obtained from a direct calculation of this quantity on a single lattice QCD ensemble.

Since the methods and available resources for lattice QCD are now sufficient to allow a basic quantity such as f_π to be so easily computed, it is natural to turn to more complex quantities which are more difficult to compute using lattice methods but also less well known and possibly of greater fundamental interest. In this paper we describe progress in two such directions: the calculation of the complex $\Delta I = 3/2$ and $1/2$, $K \to \pi\pi$ decay amplitudes A_2 and A_0 and the calculation of the long-distance contributions to $K^0 - \overline{K}^0$ mixing and rare kaon decays.

2. Computing A_0 and A_2 using lattice QCD

Three ingredients are needed for a first-principles lattice QCD calculation of amplitudes contributing to $K \to \pi\pi$ decay: the properly normalized, four-quark, $\Delta S = 1$ weak Hamiltonian $H_W^{\Delta S=1}$; the ability to exploit the energy quantization of two-pion, finite-volume states to create a final $\pi - \pi$ state with energy equal to M_K and an understanding of the finite volume effects which must be removed to obtain a physical, infinite-volume decay amplitude. Fortunately, reliable techniques are now available to address each of these issues.

The effective $\Delta S = 1$ weak Hamiltonian which should describe $K \to \pi\pi$ in the Standard Model is known from pioneering work in the 1970's and has been described in a comprehensive way [3] that can be accurately adapted to support lattice QCD calculations. The Rome-Southampton non-perturbative renormalization scheme [4] can be used to express the lattice-regularized versions of the seven independent four-quark operators which enter $H_W^{\Delta S=1}$ in terms of operators that have a well-defined continuum limit and can be related using continuum, QCD perturbation theory to the $\overline{\text{MS}}$ renormalization scheme used to determine the Wilson coefficients which appear in continuum expressions for $H_W^{\Delta S=1}$. These methods have been used successfully in recent lattice calculations [5] and are expected to be accurate at the 10-20% level.

This uncertainty is caused by the use of QCD perturbation theory at the scale of ≈ 2 GeV and the use of perturbation theory to remove the charm quark to obtain operators appropriate for a three-flavor theory. While this level of accuracy may be appropriate for present calculations, it can be improved to whatever extent is required by simply increasing the energy scale at which the lattice and continuum calculations are compared. A first step is to include the charm quark in the lattice calculation. By using a four-flavor theory we will avoid the problem of using perturbation theory at the charm quark scale and the uncertain validity of assuming that the charm quark mass is much larger than the energy scale relevant for K meson decay. Of course, if the charm quark is to be included in a lattice calculation, a lattice spacing must be used that is sufficiently small that $O\big((m_c a)^2\big)$ errors can be controlled. The second step in eliminating potential errors caused by the use of perturbation theory is to exploit "step-scaling" [6] and carry out the Rome-Southampton operator renormalization at a series of smaller lattice spacings and corresponding smaller lattice volumes until the scale of momentum employed is sufficiently large to guarantee sufficiently small perturbative errors. Note, this is much less demanding than performing the entire $K \to \pi\pi$ calculation at such small lattice spacings.

The next ingredient in this calculation is the creation of a physical two-pion final state. This can be done in a lattice calculation by following Lellouch and Lüscher [7], exploiting the finite-volume quantization of the two-pion energy and adjusting the volume so that the energy of a finite-volume, excited two-pion state matches M_K. In a Euclidean-space Green's function calculation the contribution of an excited two-pion state falls exponentially with increasing time relative to states with lower energy. This difficulty can be partially overcome if we introduce boundary conditions chosen to select the pion momentum that is present in the two-pion state of interest [8, 9]. For example, Figure 2 suggests the effects on the pion wave function of boundary conditions which are anti-periodic in one of the three spatial directions.

Of course, in a lattice calculation we can only impose boundary conditions on the underlying quarks and not directly on the pions. For the case of the $I = 2$, two-pion final state this is not difficult since we can use isospin symmetry to relate the amplitude of interest to the unique state in which both pions have charge $+1$ and then impose anti-boundary conditions on the down anti-quark, leaving the up quark to obey periodic boundary conditions. While this condition breaks isospin symmetry it cannot alter the $I = 2$ character of the finite-volume state in question because that state is uniquely determined by its charge.

The problem of imposing boundary conditions which will insure that the lowest energy, $I = 0$, $\pi - \pi$ state will have an energy equal to that of the K meson is much more challenging. Since the $I = 0$ state has the same electric charge as that with $I = 2$ we must impose boundary conditions which are consistent with isospin symmetry to avoid mixing these two states. This can be done by imposing G-parity boundary conditions [8, 10] which have the unusual feature of mixing particle and anti-particle. This is illustrated in Figure 3.

In a calculation in which the effects of finite volume are being critically used to create a final two-pion state with the proper energy, we should be concerned that other finite-volume effects may introduce significant systematic errors. Fortunately in the paper [7] pointing out the utility of exploiting finite volume to create a physical two-pion state, Lellouch and Lüscher also provide

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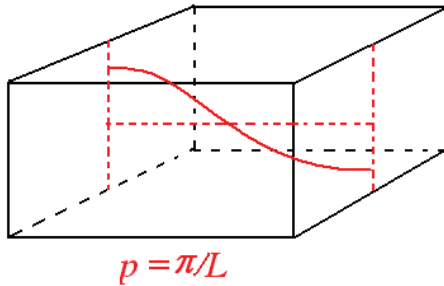
Figure 2. Diagram suggesting behavior of the pion wave function that will result if anti-periodic boundary conditions in one direction are obeyed by the pion.
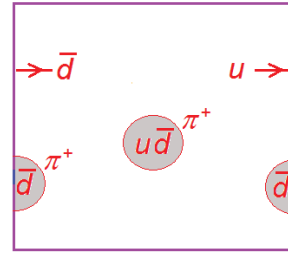
Figure 3. Diagram illustrating the unusual features of G-parity boundary conditions: a u quark passes through the boundary on the right and emerges on the left as a $\overline{d}$ while the $u - \overline{d}$, π^+ state in the center of the box is represented by a $\overline{d}\,\overline{d}$ pair when that pion state straddles the boundary.

a concrete formula for removing the leading finite-volume effects so that for volumes of linear extent L with $m_\pi L \geq 4$ one expects sub-percent residual finite-volume corrections.

While the easier calculation of the $\Delta I = 3/2$ amplitude was a pioneering effort in 2012 [11] it is now a well developed and routine part of the computational package run by the RBC and UKQCD Collaborations at increasingly small lattice spacing [12]. Our present preliminary result for A_2 at physical quark mass in the continuum limit is

$$\mathrm{Re}(A_2) = 1.606(61)_{\mathrm{stat}}(145)_{\mathrm{sys}} \times 10^{-8}\mathrm{GeV}, \quad \mathrm{Im}(A_2) = 7.35(24)_{\mathrm{stat}}(88)_{\mathrm{sys}} \times 10^{-13}\mathrm{GeV}. \quad (1)$$

The real part of A_2 agrees reasonably well with the experimental value of $1.436(4) \times 10^{-8}$ GeV while $\mathrm{Im}(A_2)$ cannot be directly measured in experiment and has not been previously computed.

Calculation of the $\Delta I = 1/2$ amplitude is much more difficult because the quantum numbers of the $I = 0$, $\pi - \pi$ final state are the same as those of the vacuum and the G-parity boundary conditions still allow the vacuum as a final state. Although this state can be subtracted, the noise left behind grows exponentially as $e^{M_K t}$ relative to the $\pi - \pi$ signal, when the final state propagates for the time t.

However, after much preparation we have begun a realistic calculation of A_0 using G-parity boundary conditions in all three spatial directions on a $32^3 \times 64$ lattice with $1/a = 1.37$ GeV and physical values for the light and strange quark masses. All seven operators entering $H_W^{\Delta S=1}$ are being evaluated. The two pions are absorbed on time slices separated by four time units and hydrogen atom wave functions with a radius of two lattice units are used for each of the pion states, an arrangement which is realized by using all-to-all propagators. These two features of the calculation have been shown in earlier studies [13, 14] to give improvements which reduce the noise coming from the vacuum subtraction by more than a factor of four. This calculation is now underway and we expect to have results with 20-30% errors within the coming year. If successful, this will give the first Standard Model prediction of the direct CP-violating parameter ϵ'. For the real parts of A_0 and A_2 we can already compare unphysical results for $\mathrm{Re}(A_0)$ with the physical calculation of $\mathrm{Re}(A_2)$ and recognize an emerging explanation for $\Delta I = 1/2$ rule [15]: the two amplitudes which add to give $\mathrm{Re}(A_0)$ cancel when combined to form $\mathrm{Re}(A_2)$.

3. Long distance contributions to second-order weak processes
Given the ability to work with physical quark masses and to control all systematic errors it is natural to ask if there are additional areas in kaon physics where lattice QCD might advance our understanding of Standard Model processes. One such new and promising direction is the

use of lattice QCD to calculate what are often referred to as long distance, second-order weak phenomena. Such phenomena include the $K_L - K_S$ mass difference ΔM_K, the contribution of the up and charm quark loops to the indirect CP-violation parameter ϵ_K and certain rare kaon decays where the change of quantum numbers requires that the decay occur at second order in the weak interactions. Such second-order weak processes are of great interest because their small size implies increased sensitivity to other, non-Standard-Model phenomena.

Such second order weak phenomena usually involve internal loops containing W bosons and receive contributions from both short distances on the order of the inverse W or top quark mass and long distances on the order of the inverse charm quark mass $1/m_c$ or the QCD scale $1/\Lambda_{\mathrm{QCD}}$. Here the notions of short and long distances are best defined as the scales at which QCD perturbation theory is or is not applicable. While in the past, the charm quark scale has been included in the short-distance category, recent perturbative studies of ΔM_K [16] which is dominated by distances of order $1/m_c$ suggest that non-perturbative methods are required even at this scale to obtain reliable results.

The largest contribution to ϵ_K comes from a top-quark loop which implies that at long distances, this second-order weak process can be expressed as a local $\Delta S = 2$ operator multiplied by a Wilson coefficient which can be accurately computed in perturbation theory. However, up and charm quarks contribute at the few-percent level and such amplitudes involve two local W exchanges (each accurately represented by a $H_W^{\Delta S=1}$ or $H_W^{\Delta C=1}$ vertex), which may be separated by distances of the order of $1/\Lambda_{\mathrm{QCD}}$. For ΔM_K the top quark is suppressed by the relatively small size of the real parts of its CKM matrix element and the dominant contribution comes from the long-distance contributions of up and charm quarks.

While non-trivial, the computation of such long-distance mixing effects is possible using lattice QCD [17]. The challenge of such calculations arises both from the complexities of the second-order amplitudes involved and the fact that the calculation is performed in Euclidean space. The quantum mechanical strategy underlying the calculation is straight-forward. We compute the matrix element between K^0 and $\overline{K}^0$ as the product of two, four-quark, weak operators integrated over a volume of time extent T as is illustrated in Figure 4. In such a Euclidean time calculation there will be a number of physical process that contribute. The process of interest is simple propagation of a K-meson state with the exponential time dependence $e^{-(M_K + \Delta M_K)T}$ which when evaluated at second order in ΔH_W will give the term $\Delta M_K T$, linear in T, from which ΔM_K can be easily extracted.

Unfortunately this term of interest must be distinguished from exponentially larger terms in which the factors of H_W allow the energy-non-conserving decay of the kaon state to an intermediate vacuum, single pion state or $\pi - \pi$ state with energy below M_K. For example, the contribution of an intermediate, single-pion state will fall much less rapidly with increasing T as $e^{-M_\pi T}$. However, these larger terms can be computed independently and subtracted in a correlated fashion, yielding a linear term which can be accurately identified as shown in Figure 5. The data presented in this figure comes from a complete calculation [18], including all graphs, which obtains ΔM_K with a $\approx 15\%$ statistical error but which must be repeated at smaller lattice spacing if the $O\big((m_c a)^2\big)$ discretization errors associated with the charm quark mass are to be controlled. A similar calculation of the long-distance contributions to ϵ_K has now been started. This calculation is more difficult because there is reduced GIM suppression and a non-perturbative subtraction combined with a perturbative correction is needed to properly join the non-perturbative long-distance with the perturbative short-distance results.

For rare kaon decays such as $K_L \to \pi^0 \ell^+ \ell^-$ or $K^+ \to \pi^+ \nu \overline{\nu}$ such non-perturbative, long-distance contributions are important at the few percent level and their calculation using lattice methods promises to extend the physics reach of experiments studying these decays. Calculation of such decays using lattice QCD [19] is now practical and exploratory calculations are now being carried out by RBC and UKQCD. These decays are more accessible to lattice QCD than the
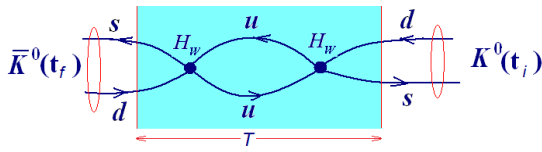
Figure 4. Diagram showing schematically a calculation of the long-distance parts of ΔM_K or ϵ_K using lattice QCD. The two first-order weak opeartors H_W are integrated over a region of time extent T lying between the operators which create the initial K^0 and destroy the final $\overline{K}^0$.
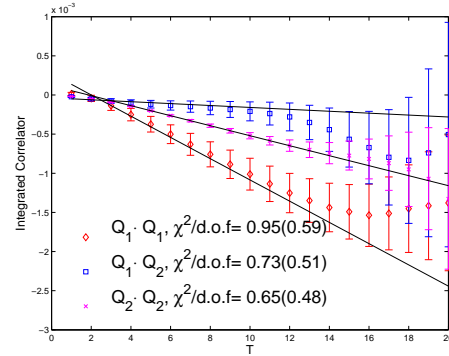
Figure 5. Plots of the linear T behavior in the calculation of ΔM_K for products of the operators O_1 and O_2 appearing in $H_W^{N_f=4}$.

$K \to \pi\pi$ calculations described in the previous section because of the absence of final state interactions, allowing the final state particles to be directly assigned the momenta carried by the physical decay products. However, the diagrams that must be evaluated are more complex and the presence of additional, Euclidean-time processes which are exponentially larger than the transition of interest (described above for the calculation of ΔM_K) must be overcome.

4. Conclusions

The ability to work directly with physical quark masses and to employ a fermion formulation which respects chiral symmetry makes possible the calculation of a variety of important quantities in kaon physics such as the complex, two-pion decay amplitudes A_0 and A_2, the $K_L - K_S$ mass difference and the long distance contributions to ϵ_K and rare kaon decays. Current calculations and future calculations at sufficiently small lattice spacing to allow accurate treatment of the charm quark, open the possibility to discover new phenomena beyond those predicted by the Standard Model at increasingly high energy and with increasing precision.

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