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LATTICE QCD AND FLAVOR PHYSICS

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ABSTRACT

Now that lattice QCD simulations are able to include effects of light sea quarks, the prospects are good for constraining quark flavor phenomenology. This review talk for particle physics experimentalists begins with an introduction intended to describe broadly the steps of lattice Monte Carlo simulations. The remainder of the talk is a brief survey of recent and ongoing calculations relevant for quark flavor physics.

1 Introduction

In principle lattice QCD is an *ab initio* method for numerically computing the QCD spectrum and many hadronic matrix elements. In practice there are several difficulties which must be overcome. Getting to the point where all uncertainties in the calculations can be reduced systematically has taken (at least) 2 decades. Are we there yet? Possibly. Recently it has been shown that the inclusion of light sea quark effects, via an improved staggered fermion action, removes the uncontrollable errors of the quenched approximation. This allows for more accurate investigation of quark mass extrapolations as well as finite volume and discretization effects.

Given that the dominant uncertainty for most of the constraints on the CKM parameters ρ and η comes from hadronic transitions [1, 2], little more needs to be said to motivate lattice QCD calculations. Several speakers at this conference have already remarked on the importance of lattice results for flavor physics phenomenology, and Lubicz talked at length about the impact that lattice QCD results have in fits to the CKM parameters at the Lattice Field Theory Symposium this year[3]. Furthermore, the CLEO-c experiment will make measurements which will allow for greater tests of lattice phenomenology [4, 5].

Since this is a conference mainly for experimentalists, I will give an introduction to lattice QCD calculations which touches upon important ingredients but skips many details not related to the rest of the talk. The quenched approximation and the use of improved staggered quarks to unquench are of particular relevance. The second half of the talk presents a selection of results, some preliminary, which are important for high energy phenomenology. Due to time and space constraints, this presentation is focused by the lens of my interests. A more thorough review of recent results is in preparation [6].

2 Lattice Monte Carlo Calculations

The goal of this section is to give the nonexpert a broad outline of lattice QCD simulations and to highlight where recent progress has made a substantial improvement. The interested reader may find more details in reviews such as Ref. [7] (and the many references therein).

QCD is a strongly coupled theory at energy scales below approximately 1 GeV: processes with 23 gluon exchanges are just as important as a single gluon exchange. Matrix elements involving low energy hadrons cannot be calculated directly using a perturbative expansion about small coupling. Instead a nonperturba-

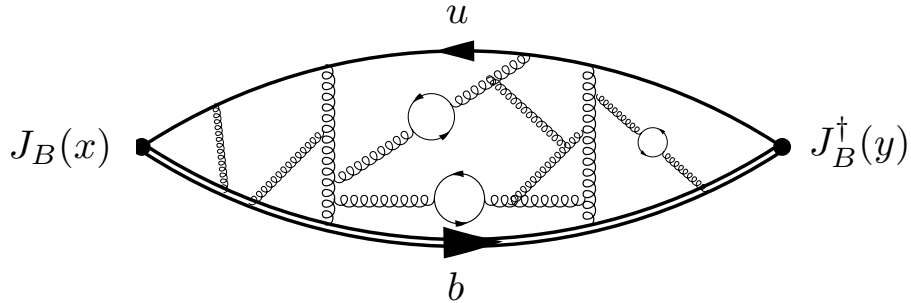


Figure 1: *Cartoon of a B^- meson propagator. The b and \bar{u} quarks propagate through nonperturbative glue.*

tive way of evaluating path integrals is needed. Lattice field theory provides this, and moreover it is the only known way to regulate a quantum field theory nonperturbatively. By rotating the time coordinate 90° in the complex plane (“going to Euclidean spacetime”) and working with a discrete and finite spacetime, the path integral representations of hadronic matrix elements can be computed numerically by Monte Carlo simulation.

2.1 Generating Important Samples of Glue

Monte Carlo simulations of lattice QCD rely on the same principles used for simulations of classical statistical mechanical models, *e.g.* the Ising model. Recall that any quantum observable, like the propagator of some hadron from x to y (*e.g.* Fig. 1), can be computed from the path integral,

$$\langle J^\dagger(y)J(x) \rangle = \frac{1}{\mathcal{Z}} \int [d\psi][d\bar{\psi}][dU] J^\dagger(y)J(x) e^{i\mathcal{S}_M} \quad (1)$$

where ψ represents the quark field and U the glue field, and $\mathcal{Z} \equiv \langle 1 \rangle$. J creates (J^\dagger annihilates) the hadron, and all possible paths are included with a phase determined by the action $\mathcal{S}_M = \int d^3x' dt' \mathcal{L}_M$, where \mathcal{L}_M is the QCD Lagrangian in Minkowski spacetime. If we change from physical Minkowski spacetime to Euclidean spacetime by introducing an imaginary time coordinate $\tau \equiv it$, then

$$\langle J^\dagger(y)J(x) \rangle = \frac{1}{\mathcal{Z}} \int [d\psi][d\bar{\psi}][dU] J^\dagger(y)J(x) e^{-\int d^3x d\tau \mathcal{L}_E}. \quad (2)$$

Let us compare (2) to the expectation value for the magnetization in the Ising model

$$\langle s_i \rangle = \frac{1}{Z'} \sum_{s_i=\pm 1} s_i e^{-H/T}. \quad (3)$$

Z' is the corresponding partition function. One can identify the Ising spins with the fermion and gluon degrees of freedom, and the statistical mechanical Hamiltonian with the integral of the QCD Lagrangian (*viz* the action). The role of temperature in the Ising model is played by the couplings in the QCD Lagrangian, the gauge coupling and the quark masses. (Recall we are discussing zero temperature QCD simulations. Finite temperature QCD simulations will not be discussed here.)

The Euclidean path integral still has one peculiarity not present in the classical statistical system: the fermion fields are anticommuting variables. Formally integrating out the fermions, we obtain

$$\begin{aligned} \langle J^\dagger(y)J(x) \rangle &= \frac{1}{Z} \int [d\psi][d\bar{\psi}][dU] J^\dagger(y)J(x) \exp\left(-\bar{\psi}(\gamma^\mu D_\mu + m)\psi - \mathcal{S}_g\right) \quad (4) \\ &= \frac{1}{Z} \int [dU] J^\dagger(y)J(x) \det Q[U] e^{-\mathcal{S}_g[U]} \quad (5) \end{aligned}$$

where $Q = \gamma^\mu D_\mu + m$ is a matrix with spacetime, color, and spin indices, and it depends on the glue field through the gauge-covariant derivative D . Finally, assuming we have been lucky or clever enough to ensure that $\det Q > 0$, we can consider quantum observables like (5) to be equivalent to statistical mechanical expectation values like (3): the sum over all possible field values, or configurations, weighted by a positive ‘‘Boltzmann’’ factor.

Now we are ready to use Monte Carlo methods to evaluate path integrals. Since the Boltzmann weights are exponentials, most configurations give an exponentially small contribution to the integral. Thus, the QCD path integral can be evaluated by generating an ensemble of ‘‘important’’ glue field configurations, ones which maximize the Boltzmann weight. One starts with some initial configuration and uses an algorithm to create successive configurations with a probability

$$\mathcal{P}[U] = \det Q[U] e^{-\mathcal{S}_g[U]}. \quad (6)$$

Using a finite number of configurations, N , gives rise to statistical uncertainty which decreases like \sqrt{N} .

The main obstacle lattice QCD calculations face is the difficulty in computing $\det Q[U]$ for realistic quark masses. The fastest algorithms include the determinant by introducing wrong-statistics fermions ϕ , such that

$$\mathcal{P}[U] = \exp\left(-\mathcal{S}_g[U] - \phi^* Q^{-1}[U] \phi\right). \quad (7)$$

The cost of numerically inverting Q increases (nominally) like the ratio of the largest eigenvalue to the smallest, and the smallest eigenvalue vanishes as the quark mass is taken to 0. This, and other complications, make simulations with realistically light quarks prohibitively expensive.

The valence, or quenched, approximation saves computer time by mutilating the theory: the determinant is simply neglected in (5) and (6), and configurations are generated with a weight determined solely from the gluon action. Consequently, effects of virtual quark loops like those shown in Fig. 1 are omitted. As a phenomenological model, quenched lattice QCD is not a bad one up to the 10–20% level (look ahead at Fig. 3). However, disagreement between calculation and experiment at this level leads to ambiguities which cannot be removed within the quenched approximation. In order to obtain the accuracy necessary to be relevant for flavor physics, lattice simulations have to include sea quark effects.

2.2 Improved Staggered Quarks

The improved staggered fermion discretization is most expedient method to include light sea quark effects in present lattice QCD simulations. Below a short description of the main ideas behind staggering and improvement is given, followed by an important caveat and my opinion of its relevance for phenomenology.

If we discretize the fermion Lagrangian by simply replacing the derivative operator by a finite difference operator, we find that the free massless fermion propagator,

$$G(p) = \frac{1}{ia \sum_{\mu} \gamma^{\mu} \sin(p_{\mu}a)}, \quad (8)$$

has poles not only at $p = 0$, but also when any component $p_{\mu} = \pi/a$. (a denotes the lattice spacing.) The simplest solution, due to Wilson, is to add a term which gives the extra 15 states, the “doubblers,” a mass. This term, however, necessarily breaks chiral symmetry causing problems such as additive mass renormalizations which make numerical simulation at small masses intractable.

Instead of solving the doubling problem, the staggered formulation embraces the extra fermions. By using a lattice symmetry the 16 species are reduced to 4 which are interpreted as artificial flavors, called tastes. Quarks of different tastes can interact by exchanging a gluon which has at least one momentum component close to π/a (see left diagram of Fig. 2). The effect of this is that a low energy, light meson propagator contains important contributions not just from valence quarks with small momentum, but also from valence quarks with large momentum components in opposite directions. This mixing breaks the taste symmetry of the free

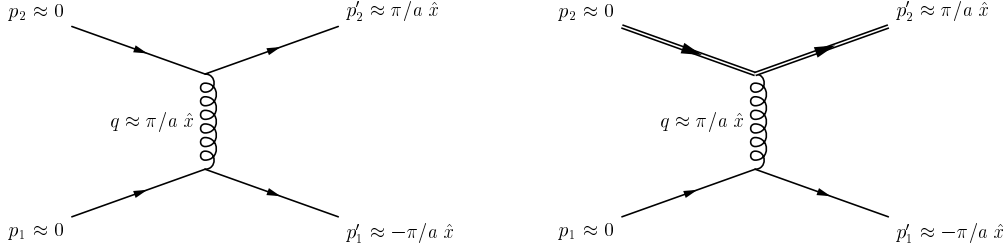


Figure 2: *Quark-quark scattering by a gluon with a large momentum component.*

fermion action and, left untreated, leads to large discretization errors. Based on quenched studies it appears that without improvement, one would have to simulate on lattices with spacings less than 0.06 fm to have control over discretization errors [8]; if one also requires the lattice volume to be bigger than $(2 \text{ fm})^3$, simulations with light staggered sea quarks would not be feasible today. Happily the leading taste-changing interactions can be suppressed by modifying the lattice action [9, 10]. This improvement allows one to obtain accurate results with attainable lattice spacings and sizes, *e.g.* the coarse set of MILC collaboration lattices which have $a = 0.13 \text{ fm}$ and $V = (2.5 \text{ fm})^3$.

The news is even better for studies of heavy-light mesons. In these simulations, one uses a non-staggered discretization for the b or c quark: either a nonrelativistic action or a Wilson-like discretization. Since the heavy quark formulation *does* get rid of the doublers, the heavy quark in Fig. 2 (right) becomes very energetic when it absorbs or emits a hard gluon ($p_\mu \approx \pi/a$). Such high energy effects give negligible contributions to heavy-light meson propagators [11].

Results using the improved staggered action for light sea quarks look very promising [12]. Figure 3 shows a series of lattice calculations divided by the corresponding observed physical values. The quantities in the plot are some of the simplest ones to compute cleanly and correctly in lattice QCD.¹ The contrast between quenched results (left) and unquenched results (right) is striking.

Alas, there is a fly in the ointment. Even while we can tame the taste-changing interactions, we cannot reduce the number of tastes below 4. Using a weight given by

$$\det Q_{\text{stag}} e^{-S_g} \tag{9}$$

¹“Correctness” here means that we have a valid expectation for the simulation to agree with experiment. The ρ mass is a counterexample: it can be computed very cleanly in lattice simulations; however, we should have no expectation of obtaining $m_\rho = 770 \text{ MeV}$ until the simulated ρ is above the simulated $\pi\pi$ threshold.

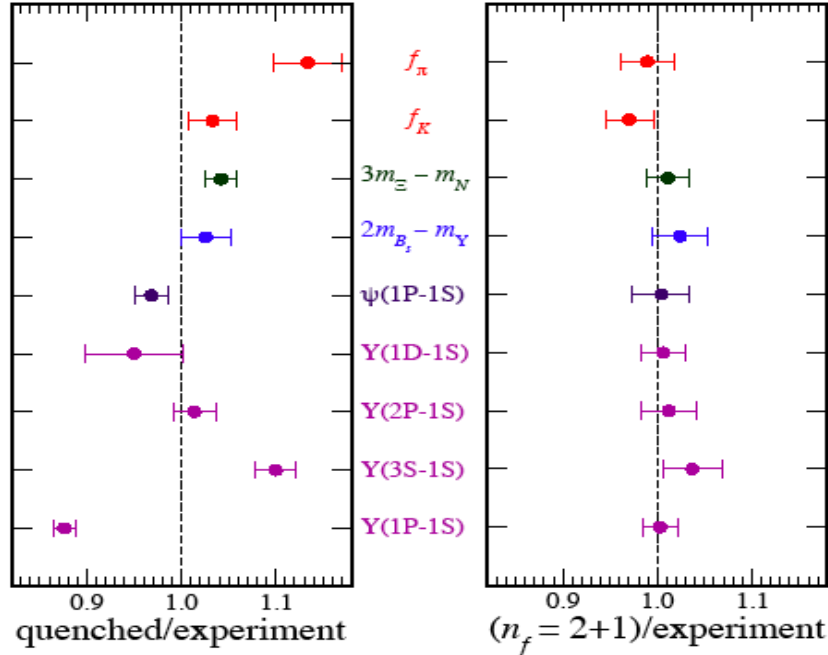


Figure 3: Comparison of quenched and unquenched results to experiment [12].

produces an ensemble of configurations which include the effects of 4 degenerate tastes of sea quarks. In order to simulate a theory with 2 light and 1 strange flavor of sea quark using staggered fermions (improved or not), one takes a square root and a fourth root of the determinant

$$\left(\det Q_{\text{stag}}^{m=m_{ud}}\right)^{1/2} \left(\det Q_{\text{stag}}^{m=m_s}\right)^{1/4} e^{-S_g}. \quad (10)$$

The problem is that the roots of the determinants cannot be exponentiated to give a local fermion action. The open question remains, does there exist a matrix Q_{local} which is QCD in the continuum limit (*i.e.* $\lim_{a \rightarrow 0} \bar{\psi} Q_{\text{local}} \psi = \bar{\psi} (\not{D} + m) \psi$) such that

$$(\det Q_{\text{stag}})^{1/4} = \det Q_{\text{local}}? \quad (11)$$

If so, then 2+1 flavor staggered fermion simulations are *ab initio* QCD calculations; if not, then the simulations merely model QCD.

In my opinion, this open question is an important one to study, but it should not temper one's excitement over the success of Fig. 3. We can leave behind the quenched approximation, a theory which we know is not QCD and disagrees with experiment, in exchange for light quark simulations which agree with experiment but may or may not be formally QCD in the continuum limit. Enthusiasm for this approach is shared by those outside the field (see e.g. [13]).

Eventually nonstaggered lattice actions will replace staggered ones. The beauty of lattice QCD is that, in the continuum limit, it is formally QCD. Presently the fourth-root trick spoils this beauty. On the other hand, phenomenology dictates that results be obtained with physical values for the quark masses, so extrapolations are necessary. Chiral perturbation theory tells us how to extrapolate, but its domain of convergence is limited to small quark masses. With current and near-future resources, nonstaggered simulations barely overlap with the chiral regime. Consequently, the empirical extrapolations that are performed using data at and beyond the border of the chiral regime are under no better theoretic control than staggered simulations which use the fourth-root trick.

2.3 Miscellany

Several important parts of lattice calculations for flavor physics could not be addressed here. Nevertheless the interested reader should be aware of work in these directions and may wish to consult the following review articles. (1) Heavy quarks on the lattice cannot be treated the same as light quarks when $m_Q a \geq 1$. There are several approaches for treating heavy quarks on the lattice, and Kronfeld discussed these last year [14]. (2) Much effort recently has been invested in fermion discretizations which preserve the full flavor symmetries of the continuum, namely *overlap* and *domain wall* fermions. These methods require significantly more computer resources, so they presently cannot explore as deeply into the chiral regime as staggered fermions. Nevertheless, the full flavor symmetry simplifies many analyses and no fourth-root trick is required to simulate with 3 light flavors (*e.g.* see Ref. [15] and therein). (3) People are exploring *twisted mass* fermions, which combine good features of both Wilson and staggered quarks and require no fourth-root trick. Frezzotti gave a review this year [16].

3 Some Recent Results

Many of the preliminary results reported below were presented at *Lattice 2004*. Since several months pass between the conference and submission of proceedings, it is not uncommon in our field to update results in the interim. For “official” Summer 2004 numbers, readers should consult the authors’ write-ups as they appear or Ref. [6].

3.1 Heavy-light Decay Constants and $B^0 - \overline{B}^0$ Mixing

The B_s and D_s decay constants are relatively straightforward to compute in lattice QCD since the strange quark mass can be tuned to its physical value. Figure 4

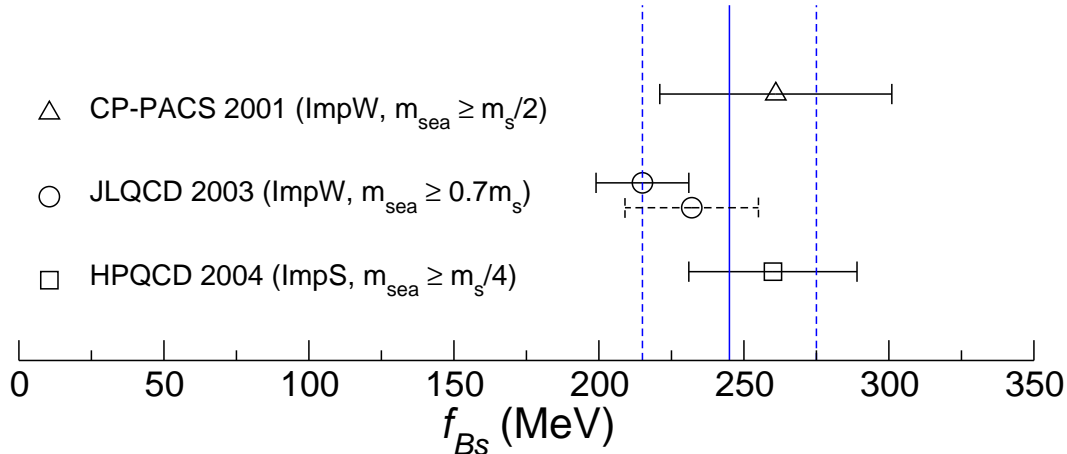


Figure 4: Summary of unquenched f_{B_s} calculations [17, 18, 19]. I have symmetrized the CP-PACS central value and averaged to obtain the solid vertical line, 245 MeV. The dashed vertical lines denote 30 MeV systematic uncertainties. The dashed point includes my estimate for the JLQCD result taking into account the lattice spacing ambiguity observed by CP-PACS (see text).

shows 3 results which compute f_{B_s} on unquenched lattices [17, 18, 19]; the first 2 use improved Wilson fermions as light as $m_s/2$, and the last uses improved staggered fermions as light as $m_s/4$. Ref. [17] observed a 10-20% lattice scale ambiguity, which they include in their error estimate. Ref. [18] did not compute the Υ splittings, but given the similarity in the sea quark mass range simulated, I suspect that they will see a similar effect; I indicate my prejudice with the dashed point in Fig. 4. See Ref. [6] for a more detailed argument. A straight average of the 3 published results (shifting the CP-PACS central value so that the error bars are symmetric) gives $f_{B_s} = 245$ MeV. Since all 3 calculations have similar dominant systematic errors (due to truncating perturbative expansions) averaging does not reduce this uncertainty: 30 MeV is the typical estimate of these truncations.

Refs. [17, 18] give unquenched results for f_B (and the ratio f_{B_s}/f_B which gives a more restrictive constraint on $|V_{td}|$). However, in my biased opinion, unquenched simulations with light quark masses below $m_s/2$ are necessary to have a trustworthy overlap with chiral perturbation theory. Work using improved staggered fermions is underway, and progress is reported in Ref. [20].

Figure 5 shows preliminary results for the D_s and D decay constants computed using Fermilab heavy quarks and improved staggered light quarks on the MILC configurations [21]. Since they have a large set of “partially quenched” data (where the valence quark mass is allowed to be different than the sea quark mass),

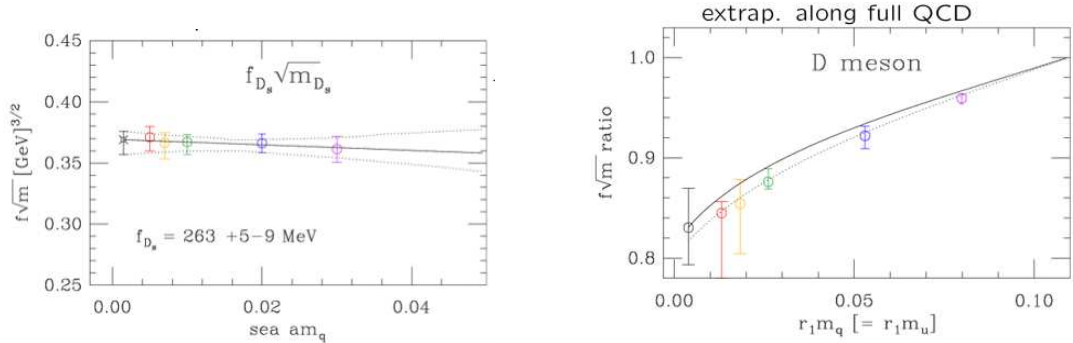


Figure 5: Preliminary Fermilab/MILC calculation of f_{D_s} (left) and f_D/f_{D_s} (right) [21]. The physical strange quark mass corresponds to $am_s = 0.04$ and $r_1 m_s = 0.11$. On the right, the solid line is a fit to chiral perturbation theory which includes finite lattice spacing effects.

they can do sophisticated global fits to partially quenched chiral perturbation theory, even including leading taste-breaking effects [22]. I will delay quoting results until Ref. [21] appears, but the dominant uncertainty in f_{D_s} and f_D has been estimated to be 10% from the heavy quark matching to QCD. This uncertainty largely cancels in the ratio, so they anticipate the dominant uncertainty for f_{D_s}/f_D to be 5% coming from statistics and the chiral fits.

The $\Delta B = 2$ hadronic matrix elements relevant for the $B^0 - \overline{B}^0$ mass and lifetime differences can be directly calculated, although the numerics are more difficult than for the decay constant. JLQCD has calculated these with 2 flavors of dynamical improved Wilson fermions in [18, 23]. Calculations using improved staggered fermions are underway [20].

3.2 Semileptonic B , D , and K Decays

Calculations of the semileptonic form factors parameterizing B and D semileptonic decays have recently been carried out on the unquenched MILC configurations [24, 25]. The form factors f_+ and f_0 are shown as functions of q^2 , the momentum carried away by the lepton pair, in Fig. 6. The dominant uncertainties in these calculations come from the truncation of the heavy quark effective action.

The data are fit well by the Bećirević-Kaidalov ansatz [26], which is used to extrapolate (for B) or interpolate (for D) to $q^2 = 0$. Furthermore one can integrate f_+ over $0 \leq q^2 \leq q_{\text{max}}^2$ and combine the result with experimental branching ratio and lifetime to determine the corresponding CKM matrix element. In the case of $B \rightarrow \pi \ell \nu$, one cannot presently simulate at small q^2 without inducing large

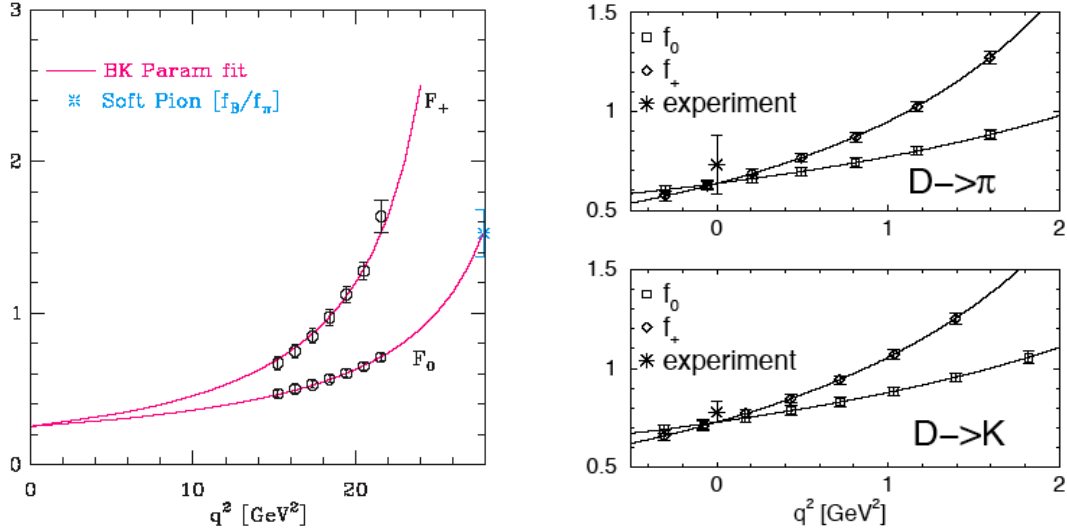


Figure 6: $B \rightarrow \pi \ell \nu$ form factors (left) [24], and $D \rightarrow \pi \ell \nu$ and $D \rightarrow K \ell \nu$ form factors (right) [25].

discretization effects. Restricting both the form factor integration and the branching fractions to decays with $q^2 \geq 16$ GeV 2 [27] reduces the theoretical error in $|V_{ub}|$ but increases the experimental error [24].

Unprecedented precision is being obtained in lattice calculations of K decays. Figure 7 shows the $K \rightarrow \pi \ell \nu$ form factor $f_+(q^2)$ in the quenched approximation (left) [28] and the unquenched K (top right) and π (bottom right) decay constants [29]. The calculation of f_+ is notable for several technical innovations which allow a signal to be extracted. The calculation of f_K/f_π is now precise enough lead to a value for $|V_{us}|$ competitive with the semileptonic determination [30, 29].

3.3 Quarkonia and B_c Masses

We have already seen in Fig. 3 the improvement in the bottomonium spectrum when light sea quark effects are included [12]. Preliminary charmonium results were presented last year [31]. Work is underway to finalize these results.

The B_c meson mass has been computed using the unquenched MILC configurations [32]. Fig. 8 (left) shows the result as the rightmost point and comes from computing $m_{B_c} - (m_{J/\psi} + m_\Upsilon)/2$ on the lattice and using the experimental quarkonium masses. Fig. 8 (right, upper points) shows this mass difference vs. sea quark mass as well as a check using the difference $m_{B_c} - (m_D + m_B)$ (lower points); only statistical errors are plotted. The systematic uncertainties are also larger using the

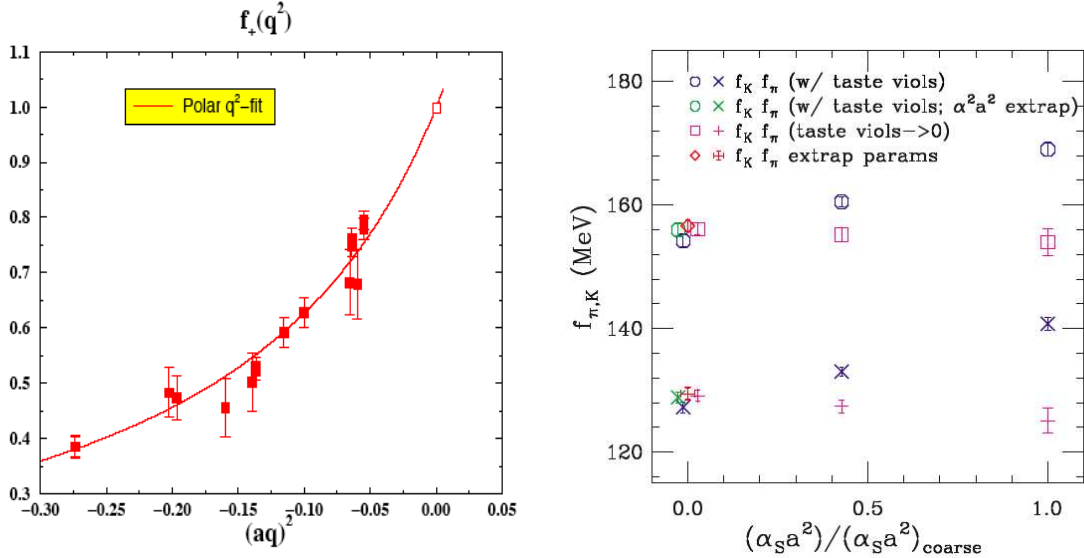


Figure 7: K semi-leptonic form factor f_+ vs. momentum transfer [28] and K decay constant (upper points) vs. lattice spacing [29].

B and D – about 50 MeV compared to 10 MeV for the mass difference from J/ψ and Υ – so while the 2 results agree, the more precise one is taken for the preliminary result. Given the precision of the lattice result compared to experiment, this will be an interesting prediction to compare to Tevatron Run II data.

4 Conclusions

In my opinion the next few years will be exciting ones for lattice QCD. Having shed the quenched approximation, lattice calculations can reach enough precision and accuracy to help constrain the CKM matrix elements. In order to do so, hard work is still required to reduce uncertainties from extrapolations in quark mass, finite spacing and size effects, and operator matchings. In the absence of a theoretical proof, the open question behind the staggered fourth-root trick will hang over our heads. Even so, the accumulation of empirical agreement between staggered simulations, experiment, and eventually non-staggered simulations, is enough to have give important contributions to phenomenology. Finally, there are still classes of problems which are difficult to address with current techniques – decays with multiple final-state hadrons, in particular – which will receive much more attention if the simpler problems can ever be said to be done.

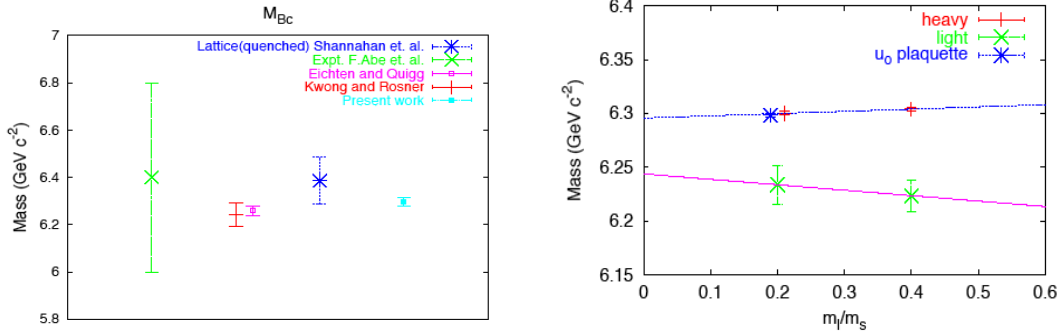


Figure 8: *Left: B_c mass from experiment (far left point), models (2nd and 3rd points), and lattice (4th point quenched, 5th point unquenched) (see [32] and Refs. within). Right: Comparison of m_{B_c} computed using two mass differences (see [32] and the text); results agree within errors.*

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