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Predictions with lattice QCD

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Abstract. In recent years, we used lattice QCD to calculate some quantities that were unknown or poorly known. They are the q^2 dependence of the form factor in semileptonic $D \to Kl\nu$ decay, the leptonic decay constants of the D^+ and D_s mesons, and the mass of the B_c meson. In this paper, we summarize these calculations, with emphasis on their (subsequent) confirmation by measurements in e^+e^-, γp and $\bar{p}p$ collisions

1. Introduction and Background

The central theme of elementary particle physics is to find new interactions of matter, energy, space and time. When the matter in question is the quarks, one is faced with quark confinement: quarks never appear freely; they are always bound inside hadrons—baryons like the proton, or mesons like the pion or kaon. In the Standard Model of elementary particles, confinement is a phenomenon of quantum chromodynamics (QCD), the gauge theory of the strong force.

Since only hadrons can be detected, the effects of quark confinement must be calculated with QCD, before the experimental data can be interpreted in terms of quarks. In many cases, the best technique for doing the calculations is to formulate QCD on a space-time lattice. Lattice QCD and the Feynman path integral reduce the problem of to an integral whose dimension scales as N^4, where N is the (linear) lattice size. The problem cries out for supercomputing.

In recent years, lattice QCD has reached the stage where many calculations of hadron masses, mass splittings and operator matrix elements agree with experimental measurements. The key has been the inclusion of sea quarks, which are pairs of virtual quarks swirling around inside hadrons. The progress has been especially striking [1] when the sea quarks are implemented as staggered quarks, using an action designed to reduce discretization effects.

One ingredient of these calculations is controversial. Sea quarks are always computationally demanding, although staggered quarks are by far the fastest. Staggered quarks introduce some extra unwanted quarks, however. The computer algorithms [2] and subsequent analysis of the numerical data [3] remove them, but do so differently for valence and sea quarks. The difference can lead to violations of unitarity. In the cases discussed here, it is plausible that such effects are small, but a proof is not yet at hand [4].

Less controversial is the treatment of heavy quarks. In practice, the lattice spacing is not small enough to resolve the Compton wavelength of charmed and b quarks. Fortunately, chromodynamics at this length scale is simple enough to factor it out from the computer simulation, and several methods exist [5]. Nevertheless, it is good to have check.

In this paper, we discuss three topics: the normalization and q^2-dependence of the $D \to Kl\nu$ form factor; the decay constants of the D^+ and D_s mesons; and the mass of the B_c meson. Each of these lattice-QCD calculations was subsequently confirmed by experimental measurements, satisfying a long-standing demand of experimental physicists [6]. The quantities discussed here were ideal candidates: they are straightforward to compute; they test the controversial aspects in complementary ways; and the first "good" experimental measurements were expected on the same time scale. The success of the predictions is extremely encouraging. In particular, the calculations for D mesons are, in lattice QCD, similar to those for B mesons, whose b quarks are considered likely to exhibit new, non-Standard interactions.

2. Semileptonic D Decays

Semileptonic decays such as $D \to Kl\nu$ proceed as follows. A quark (in this case, a charmed quark) emits a virtual W boson, thereby turning into a quark of a different flavor (in this case, a strange quark). The W immediately disintegrates into a lepton-neutrino ($l\nu$) pair. The rate depends on q^2, which is the invariant-mass-squared of $l\nu$. Some of the q^2 dependence stems from QCD through a function called a form factor (in this case, denoted $f_+(q^2)$). The momentum transfer q^2 falls in the range $0 \leq q^2 \leq q^2_{\rm max} = (m_D - m_K)^2$. In lattice QCD, discretization effects are smallest when the spatial momentum $\boldsymbol{p}$ of the kaon is small, which puts q^2 close to $q^2_{\rm max}$.

Experiments usually measure the branching fraction and quote the normalization $f_+(0)$, after making assumptions about the q^2 dependence. While our results were still preliminary [7], experimental results came out for the normalization of $D \to Kl\nu$ [8] and $D \to \pi l\nu$ [9]. The agreement with our final results [10] is excellent. For example, we find $f_+^{D\to K}(0) = 0.73(3)(7)$ [10] while the BES Collaboration measures $f_+^{D\to K}(0) = 0.78(5)$ [8].

In principle, the shape of the form factors can be computed directly in lattice QCD. In practice, we calculated at a few values of $\boldsymbol{p}$ and used a fit to the Ansatz of Bećirević-Kaidalov (BK) [11] to fix the q^2 dependence. It was important, therefore, to measure the q^2 dependence experimentally. In photoproduction of charm off fixed nuclear targets, the FOCUS Collaboration was able to collect high enough statistics to trace out the q^2 distribution of the decay [12]. This setup does not yield an absolutely normalized branching ratio, so one is left to compare $f_+(q^2)/f_+(0)$.

In Fig. 1(a) we plot our result for $f_+(q^2)/f_+(0)$ vs. $q^2/m^2_{D^*_s}$. The errors from $f_+(0)$ must be propagated to non-zero q^2, so for $f_+(q^2)/f_+(0)$ the errors grow with q^2. Figure 1 shows 1-σ

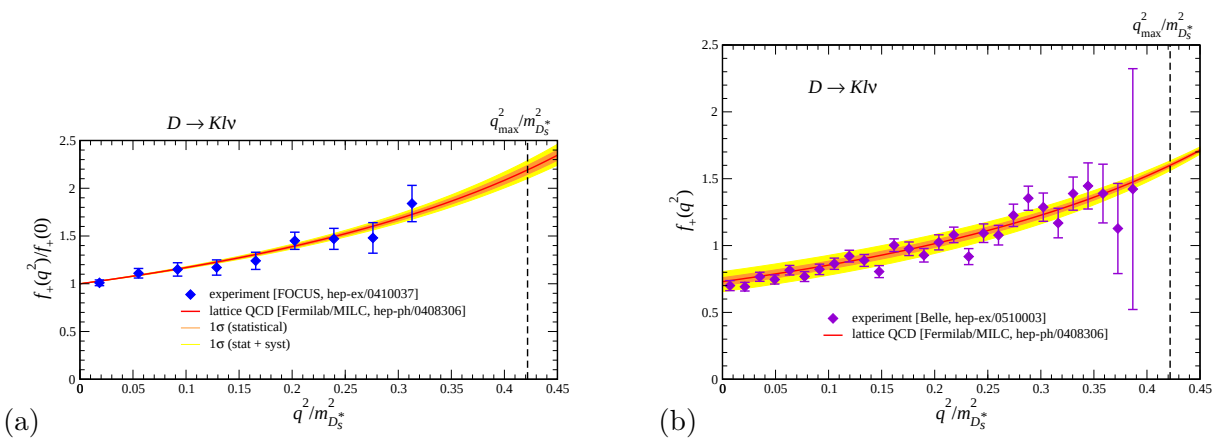

Figure 1. Form factor for $D \to Kl\nu$ vs. $q^2/m^2_{D^*_s}$: (a) shape $f_+(q^2)/f_+(0)$ compared with FOCUS [12]; (b) shape and normalization $f_+(q^2)$ compared with Belle [14].

bands of statistical (orange) and all uncertainties (yellow) added in quadrature [13]. As one can see, the q^2 dependence of lattice QCD (curve and error band) and data from the FOCUS experiment (points) agree excellently, although the uncertainties are still several per cent. The FOCUS results appeared two months after the lattice calculation. More recently, the Belle Collaboration at the e^+e^- collider KEK-B measured the shape *and* normalization of the form factor in a single experiment [14]. In Fig. 1(b) we compare our result for $f_+(q^2)$ with Belle. The color code for the lattice QCD error bands is as before, and now depict q^2 dependence of the lattice-QCD errors in a realistic way.

3. Leptonic D Decays

We also considered the leptonic decay of charmed mesons, $D^+ \to l\nu$ and $D_s \to l\nu$. Here the quark and antiquark in the meson merge into a virtual W, which disintegrates into $l\nu$. The QCD influence is a single number (for each meson), called decay constants and denoted f_{D^+} or f_{D_s}. At Lattice 2004 [15], we presented preliminary results for f_{D^+} and f_{D_s}, based on one lattice spacing, $a \approx 0.125$ fm. Our extended the running to two other lattice spacings. Details are given in the ensuing publication [16]. We find

$$f_{D^+} = 201 \pm 3 \pm 17 \text{ MeV}, \quad (1)$$

$$f_{D_s} = 249 \pm 3 \pm 16 \text{ MeV}, \quad (2)$$

where the first error is from finite Monte Carlo statistics, the second is a sum in quadrature of several systematics. A conservative (but not naïve) estimate of heavy-quark discretizations effects is the second largest (largest) systematic on f_{D^+} (f_{D_s}).

Figure 2 shows the n_f dependence of the decay constants. Quenched ($n_f = 0$) results vary widely, but we show one [17] carried out with similar choices for other aspects of the calculations. One sees a trend of f_{D_s} to increase with n_f. A similar comparison of f_{D^+}, in Fig. 2(b), is less instructive, but shown for completeness.

The CLEO-c Collaboration [19] and the BaBar Collaboration [20] have measured

$$f_{D^+} = 223 \pm 17 \pm 3 \text{ MeV} \quad \text{CLEO-}c \text{ [19]}, \quad (3)$$

$$f_{D_s} = 279 \pm 17 \pm 20 \text{ MeV} \quad \text{BaBar [20]}, \quad (4)$$

respectivelty at the CESR and PEP-II e^+e^- colliders. At the 1-σ level, the agreement with lattice QCD is fine. Even more compelling is the ratio $R_{d/s} = m_{D^+}^{1/2} f_{D^+} / m_{D_s}^{1/2} f_{D_s}$:

$$R_{d/s} = 0.786 \pm 0.042 \quad \text{lattice QCD}, \quad (5)$$

$$= 0.779 \pm 0.093 \quad \text{CLEO/BaBar}, \quad (6)$$

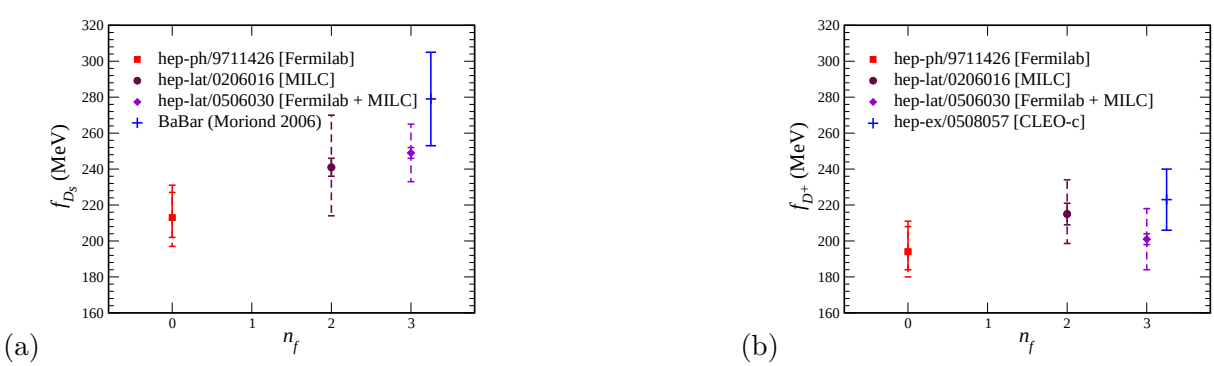

Figure 2. Dependence of (a) f_{D_s} and (b) f_{D^+} on the number n_f of sea flavors. Quenched ($n_f = 0$) [17]; $n_f = 2$ [18]; $n_f = 3$ [16]. Solid (dashed) error bars are statistical (statistical+systematic).

in which several uncertainties from lattice QCD cancel. Experimental and lattice-QCD uncertainties are reducible, so the test will sharpen over the coming few years.

4. Mass of the B_c Meson

The pseudoscalar B_c^+ meson is the lowest-lying bound state of a charmed quark and a b quark. The CDF Collaboration [21] first observed it during Run I of the Tevatron $\bar{p}p$ collider in the semileptonic decay $B_c^+ \to J/\psi l^+ \nu$. But it was clear that Tevatron Run II detectors would be able to reconstruct hadronic modes, such as $B_c^+ \to J/\psi \pi^+$, which give much much better precision on m_{B_c} [22]. At Lattice 2004 we presented results in nearly final form [23], and posted the final results on the arXiv in mid-November [24]:

$$m_{B_c} = 6304 \pm 12^{+18}_{-0} \text{ MeV}, \tag{7}$$

where the last error is a rough estimate of residual heavy-quark discretization effects. Soon afterwards, CDF announced their precise mass measurement [25]:

$$m_{B_c} = 6287 \pm 5 \text{ MeV}, \tag{8}$$

which agrees with Eq. (7) at slightly more than 1-σ.

Two comments are in order. First, the agreement at the gross level of the calculation with experiment shows that discretization effects are well under control with the heavy-quark methods of choice. These are lattice NRQCD [27] and the Fermilab method [28], which are based on effective field theories for heavy quarks [29, 30]. Indeed, as seen in Fig. 3(a), almost no lattice spacing dependence is seen in the splitting $\Delta_{\psi\Upsilon} = m_{B_c} - (\bar{m}_\psi + m_\Upsilon)/2$ that is at the crux of the calculation [26]. Moreover, it is striking how little the splitting $\Delta_{\psi\Upsilon}$ changes when sea quarks are included. Figure 3(b) compares Eq. (7) with an old quenched calculation [26] (and the measurement [25]). The solid error bar shows the non-quenching errors, and the dashed includes the estimate of the quenching error. The inclusion of sea quarks has reduced the splitting by a factor of three or four, bringing an essentially discrepant result into agreement.

5. Conclusions

In the past year, several lattice-QCD calculations have been confirmed by experiment. FOCUS [12] and Belle [14] confirmed the q^2-dependence of the $D \to Kl\nu$ form factor [10]; CLEO-c [19] and BaBar [20] respectively confirmed the D^+ and D_s decay constants [16]; and CDF [25] confirmed the mass of the B_c meson [24]. To obtain these results it is essential to have heavy-quark discretization effects under control, as one expects from theoretical foundations [27, 28, 29, 30]. Furthermore, the comparison of quenched QCD, QCD with 2+1 staggered flavors, and experiment shows that sea quarks are needed to obtain agreement, and

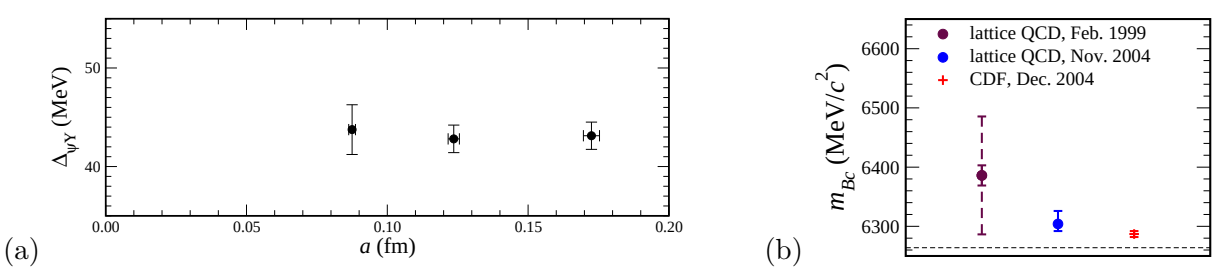

Figure 3. (a) Dependence of the splitting $\Delta_{\psi\Upsilon}$ on the lattice spacing a. (b) Comparison of the quenched [26], $n_f = 2+1$ [24] and experimental [25] values of m_{B_c}; the dashed line denotes the baseline $(\bar{m}_\psi + m_\Upsilon)/2$.

that staggered quarks (in these cases) capture the needed effect. The results are promising for the search for new b quark interactions, because a straighforward change to the D form factors and decay constants yield the corresponding results for B mesons. These are a key element to enable the experimental search for new phenomena in quark-flavor physics [6].

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