Lattice QCD and Heavy Quark Physics

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Lattice QCD results relevant to heavy quark physics are reviewed. In particular new results will be shown that, for the first time, include dynamical quarks in the QCD vacuum which are close enough to being realistic to allow accurate extrapolation to the physical point. Agreement with experiment is found for a wide range of spectral quantities and the implications of this for hadronic matrix elements needed for the extraction of CKM elements from B factory experiments is discussed.

1 Introduction

Despite being thirty years old, lattice QCD is only just coming of age as a method for calculating hadronic masses and matrix elements from first principles. Such calculations are sorely needed, particularly by the B factory programme attempting to determine the elements of the CKM matrix which couples quark flavours via the weak interaction and allows for CP violation in the Standard Model.

In this review I will describe how and where calculations in lattice QCD are needed by experiment, avoiding technical details. I will then discuss the current status of the field including new results in which the systematic errors of lattice QCD are reduced below the few percent level for the first time. The prospects for the future in the light of thesei results are very encouraging.

2 Lattice QCD Calculations

Lattice QCD calculations proceed by the discretisation of a 4-d box of space-time into a lattice. The QCD Lagrangian is then discretised onto that lattice. The spacing between the points of the lattice, a, is ≈ 0.1fm in current calculations and the length of a side of the box is $L \approx 3.0$fm. Thus our simulations can cover energy scales from ≈ 2 GeV down to ≈ 100 MeV.

The Feyman Path Integral is evaluated numerically in a two-stage process. In the first stage sets of gluon fields ('configurations') are created which are representative 'vacuum snapshots'. In the second stage, quarks are allowed to propagate on these background gluon field and hadron correlators are calculated. The dependence of the correlators on lattice time is exponential. From the exponent the masses of hadrons of a particular J^{PC} can be extracted, and from the amplitude, simple matrix elements [1].

QCD as a theory has a number of unknown parameters, which presumably make sense in some deeper theory. These parameters are the overall dimensionful scale of QCD and the bare quark masses. To make predictions, these parameters must be fixed from experiment. In lattice QCD we do this by using one hadron mass for each parameter. The quantity which is equivalent to the overall scale of QCD on the lattice is the lattice spacing. It is clearly important to use well-defined hadron masses in fixing the parameters i.e. the hadrons used should be stable ones (in QCD), well below decay thresholds. The obvious one to use to fix the u and d quark masses (taken to be equal in lattice calculations to date) is m_π and for the s quark mass, m_K. Other choices are sometimes made, however. In addition it is a good idea to set the scale using a quantity which is well-known experimentally but which is not sensitive to the quark masses, to save an iterative fixing procedure. Radial or orbital splittings in charmonium or bottomonium are optimal for this.

Lattice calculations are hard and very time-consuming. Progress has occurred in the last thirty years through gains in computer power but also, often more importantly, through gains in calculational efficiency and physical understanding. One particular area which revolutionised the field from the mid-1980s was the understanding of the origin of discretisation errors and their removal by improving the lattice QCD Lagrangian. Discretisation errors appear whenever equations are discretised and solved numerically. They manifest themselves as a dependence of the physical result on the unphysical lattice spacing. In lattice QCD, as elsewhere, they are corrected by the adoption of a higher order discretisation scheme. The complication in a quantum field theory like QCD is the presence of radiative corrections to the coefficients in the higher order scheme which must be determined.

Physical understanding of heavy quark physics on the lattice has also made a huge difference to the feasibility of calculating matrix elements relevant to the B factory programme on the lattice. The use of non-relativistic effective theories requires the lattice to handle only scales appropriate to the physics of the non-relativistic bound states and not the (large) scale associated with the b quark mass. A very fine lattice would be needed to cover an energy scale of 5 GeV and this is currently impossibly as would also be very wasteful. With the use of non-relativistic effective theories, heavy quark physics is one of the areas where lattice QCD can now make most impact.

One area which has remained problematic, but which this year's results have addressed successfully, is the handling of light quarks on the lattice. In particular the problem is that of how to include the dynamical (sea) $u/d/s$ quark pairs that appear as a result of energy fluctuations in the vacuum. We can safely ignore $b/c/t$ quarks in the vacuum because they are so heavy, but we know that light quark pairs have significant effects, for example in screening the running of the coupling constant and in generating Zweig-allowed decay modes for unstable mesons.

The inclusion of dynamical quarks is numerically very expensive, particularly as the quark mass is reduced towards the small values which we know the u and d quarks have. There are several technical issues associated with discretising the quark action on the lattice and this has led to a number of different formalisms for handling quarks. The different formalisms have different levels of discretisation errors which can be improved as above, but also handle the chiral symmetry of QCD in different ways. Some formalisms are much faster to simulate with than others, but all require supercomputers to include dynamical quarks.

Many calculations even today use the 'quenched approximation' in which the light quark pairs are ignored. Results then suffer from a systematic error of $\mathcal{O}(20\%)$. A serious problem with the quenched approximation is the lack of internal consistency which means that the results depend on the hadrons that were used to fix the parameters of QCD. Thus it is not even possible to define a result as *the* result in quenched QCD, but only the result given a particular method of fixing the parameters. This ambiguity plagues the lattice literature.

Other calculations have included 2 flavours of degenerate dynamical quarks, i.e. u and d, but with masses much larger than the physical ones. This has led to some improvements over the results in the quenched approximation but these improvements have often been hard to quantify because of remaining large systematic errors. Results must be extrapolated to the physical u/d quark mass and chiral perturbation theory is a good tool for this. However, chiral perturbation theory only works well if the u/d quark mass is light enough and, for errors at the few percent level, this means less than $m_s/2$. This has been impossible to achieve in most calculations.
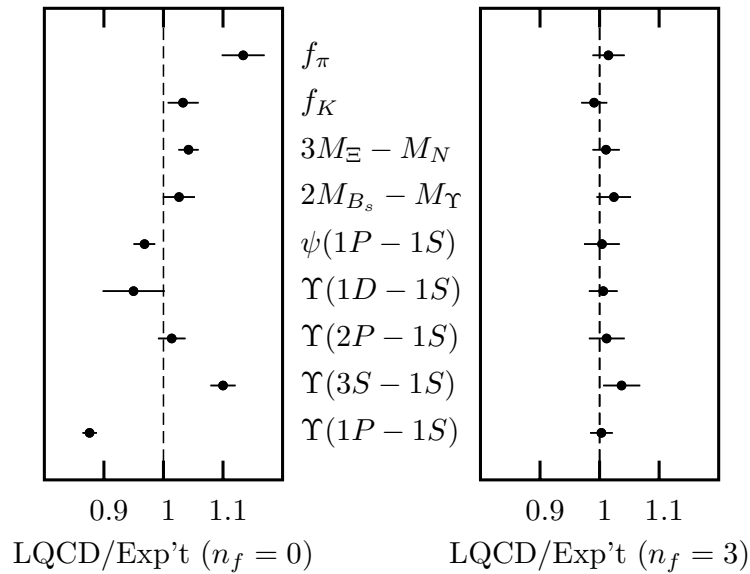
2.1   Unquenching Lattice QCD

Figure 1: A comparison of quenched (left) and unquenched (right) lattice QCD results [2]. The unquenched results use 2+1 flavours of dynamical improved staggered quarks.

Real QCD has only one set of parameters, so results should be unambiguous and independent of which (sensible) hadron masses were used to fix the parameters. Once the parameters have been fixed using a particular set of hadron masses, then other quantities calculated as predictions of QCD should agree with experiment.

This happy state of affairs has now been reached with new calculations from the MILC/ HPQCD/FNAL/UKQCD collaborations that include $2(u/d) + 1(s)$ dynamical quarks in the

vacuum and with the u/d quark mass taking a range of values from $m_s/2$ down to $m_s/8$. These are much lighter u/d masses than before and this explains the qualitative change in the outcome of the calculation. Chiral extrapolations down to the physical u/d quark mass can now be done without large uncertainties in the extrapolated results [2].

The major development has been the use of the improved staggered formalism for quarks in lattice QCD. This formalism allows for much faster numerical simulations so that light u/d masses can be reached and s quarks can also be included. A theoretical caveat is that a single staggered quark field generates 4 species, or 'tastes', of quark. When the dynamical quarks are included in the QCD action through the quark determinant, the fourth root of the determinant must then be taken. Although this is straightforward numerically, it leaves some theoretical uneasiness and so careful testing is necessary. The results above certainly confirm that no problems show up across a wide range of simple quantities.

Figure 1 shows the results for lattice QCD divided by experiment for a range of quantities from light mesons and baryons to heavy-light and heavyonium systems. The scale of QCD (lattice spacing) was fixed using the radial excitation energy in the Υ system ($M(\Upsilon') - M(\Upsilon)$) and the quark masses were fixed using m_π, m_K, m_{D_s}, m_ψ and m_Υ. The two plots contrast the situation in the quenched approximation (n_f flavours of dynamical quarks $= 0$) with the new unquenched results ($n_f = 3$) for 9 other well-defined quantities. The new unquenched results show agreement with experiment for *all* the quantities. This also demonstrates, as described above, that fixing the scale and quark masses is unambiguous since using any of the 9 quantities shown here instead of the ones used (and not plotted) would have reproduced the same results. This is clearly an enormous improvement over the situation in the quenched approximation, and shows that accurate results from lattice QCD should now be possible.

2.2   Lattice input to the Unitarity Triangle

One of the key places where lattice QCD input is needed is in (over-)constraining the unitarity triangle derived from the CKM matrix. Figure 2 shows the current status with error bars [3]. The sides of the triangle constrained to the dark and medium/light circles are given by B semi-leptonic decay and mixing rates respectively. These rates are given by a weak interaction part which contains the CKM element and the matrix element between B mesons or between the B meson and the vacuum of a weak current. This latter part must be calculated in lattice QCD. The attempt to pin down the vertex of the unitarity triangle will be limited by theoretical errors on the matrix elements unless lattice QCD calculations with few % errors can be achieved. The lattice errors will only be reliable if they are checked against other quantities well-known experimentally, for example in Υ physics. Hence the importance of covering all sectors of the theory, as in Fig. 1 above.

3   Lattice Results for B_B and f_B

Useful recent reviews of lattice QCD with an emphasis on heavy quark physics are given in [4]. I will concentrate here on the lattice calculation of the matrix element for the mixing of neutral B mesons since that has most recent progress. B mixing proceeds through the 'box' diagram

Figure 2: Recent status of constraints on the unitarity triangle, from CKMfitter [3].

of Fig. 3. On the lattice we do not simulate W bosons or t quarks so these are integrated out to give the matrix element of a 4-quark operator of the effective weak Hamiltonian. This is parameterised in terms of a 'bag parameter', B_B, according to:

$$\langle \overline{B}_q | (\overline{b}q)_{V-A}(\overline{b}q)_{V-A} | B_q \rangle = \frac{8}{3} M_{B_q}^2 f_{B_q}^2 B_{B_q}. \tag{1}$$

f_{B_q} is the decay constant, which is related to the decay rate for the (charged) B meson to decay, via a W, entirely to leptons. The motivation for separating out this matrix element is clear from Fig. 3. If we cut the right-hand diagram in half, each piece is equivalent to the leptonic decay of a B (ignoring the distinction between charged and neutral Bs).

Figure 3: B box diagram which mixes neutral B mesons.

f_B and B_B are normally calculated separately on the lattice. Both are required for the mixing matrix element to be combined with experimental results on neutral B oscillations. Once mixing of B_s mesons has been observed, useful quantities will be the ratios of f_B and B_B for B_s divided by the corresponding quantity for B_d. The required renormalisation of lattice matrix elements to match a continuum renormalisation scheme cancels in this ratio so that it should be more accurately calculated on the lattice than either number individually.

B_B has been calculated so far in the quenched approximation and with 2 flavours of dynamical quarks with masses above $m_s/2$ by the JLQCD collaboration [5]. It is a dimensionless quantity so not directly sensitive to the ambiguities of fixing the scale in the quenched approximation. It also seems to be very insensitive to the mass of the light quark in the B meson, supported by chiral perturbation theory which has a very small coefficient for the dependence of B_{B_d} on the logarithm of the d quark mass. JLQCD quote 1.02(2)(+6-2) for the ratio B_{B_s}/B_{B_d}. It seems likely then that results for B_B will not change markedly on including a more realistic dynamical quark content although this calculation has yet to be done, and could surprise us.

The calculation of f_B is a different picture and recently has become rather controversial. It had generally been assumed, without very good justification, that the ratio of f_{B_s}/f_{B_d} would also not change significantly between quenched and unquenched results. The sensitivity to ambiguities in the lattice spacing determination in the quenched approximation do cancel out. However, the ratio is still sensitive to the difference between the s quark and the d quark in the different B mesons. Chiral perturbation theory also expects f_{B_d} to exhibit a significant logarithmic dependence on m_d. The coefficient of the 'chiral logarithm' contains $(1 + 3g^2)$ where g is the $BB^*\pi$ coupling, thought to take a value $g^2 \approx 0.35$. All of these features mean that it is important to calculate this ratio using a realistic QCD vacuum and using a light u/d quark mass for which chiral extrapolations can be done reliably.

JLQCD results [5] on the same configurations as above yield a ratio of 1.13(3)(+13-2). This is obtained from a linear extrapolation from $m_{u/d} > m_s/2$ down to the physical point. The large positive error bar allows for the possibilities of chiral logarithms, but no curvature is seen in the calculated results at the large light quark masses used.

Results on configurations with 2+1 flavours of dynamical improved staggered quarks are shown in Fig. 4 [6]. The u/d quark masses extend down to well below $m_s/2$. Although the statistical errors at the lightest $m_{u/d}$ mass are still large, and fits to the full chiral perturbation theory formula including chiral logarithms have yet to be done, the results indicate a ratio significantly larger than 1.13. Once the physical ratio has been determined precisely it will be important input to CKM fits. A larger value will increase the average radius of the medium shaded circle in Fig. 2; a more precise value will reduce the width of the medium shaded band.

4   Conclusions

The impact of lattice QCD calculations has been hindered by the difficulty of including a realistic QCD vacuum. This has led to an unacceptable level of systematic error for the results needed by experimentalists, such as participating at B factories. New results this year look set to herald a brighter future in which few percent errors are at last obtainable from lattice QCD and we will be able to provide key input to the determination of the CKM matrix.
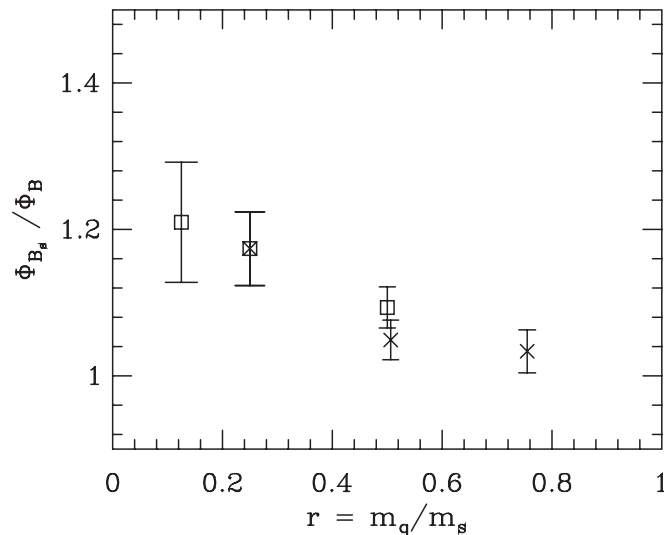
Figure 4: Results for the ratio of Φ_{B_s}/Φ_{B_d} where $\Phi = f\sqrt{M}$ and M is the meson mass. Results are plotted against valence quark masses $m_{u/d}/m_s$ for QCD with 2+1 flavours of dynamical improved staggered quarks with various dynamical u/d quark masses [6].

Acknowledgments

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