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# SHEP 96-13 LATTICE SIMULATIONS AND EFFECTIVE THEORIES

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I present a brief introduction to the lattice formulation of quantum field theory, and discuss the use of lattice simulations for studies in particle physics phenomenology. The computation of  $f_B$ , the decay constant of the *B*-meson, is used as a case study. I also explain the appearance and cancellation of "renormalons" in the evaluation of power corrections (higher-twist corrections) in hard scattering and decay processes.

#### Introduction

The lattice formulation of quantum field theories, together with large scale numerical simulations, is becoming a very powerful non-perturbative tool in many areas of particle physics, and in the evaluation of long-distance stronginteraction effects in physical processes, in particular. In these lectures I will present a brief introduction to lattice computations in QCD (lecture 1) and will then discuss, as a case study, the applications to the evaluation of the decay constant of the *B*-meson, and other physical quantities, in the Heavy Quark Effective Theory (HQET). Finally in the third lecture I will review the question of "renormalons", which arises when one evaluates power corrections (i.e. higher-twist corrections) to hard scattering and decay processes.

The principal objective of these lectures is to explain the theoretical framework needed for lattice simulations in particle physics, and to give some idea of what is possible now and what the outstanding problems are. In the first two lectures I will illustrate the discussion with numerical results obtained by the UKQCD collaboration, of which I am a member. It is not my intention, nor would it be appropriate at this school, to present a critical review of the many interesting results which have appeared in the last few years from many different groups. The proceedings of the annual symposia on Lattice Field Theory contain detailed reviews and status reports on all aspects of the subject, and provide very helpful starting points for literature searches. A selection of review talks, which are suitable as further reading to the material of these lectures, can be found in refs.<sup>1-5</sup>.

# 1 Lecture 1 – Lattice Computations of Masses and Matrix Elements

In this first lecture I will briefly review the ingredients used in evaluating hadronic masses and matrix elements in QCD. Simulations using the Heavy Quark Effective Theory will be described in the remaining two lectures.

The quantity which is evaluated directly in lattice computations is the vacuum expectation value of a multi-local operator  $O(x_1, x_2, \dots, x_n)$ , composed of quark and gluon fields:

$$\langle 0|O(x_1, x_2, \cdots, x_n)|0\rangle = \frac{1}{Z} \int [dA_\mu] [d\psi] [d\overline{\psi}] e^{iS} O(x_1, x_2, \cdots, x_n) , \qquad (1)$$

where Z is the partition function

$$Z = \int [dA_{\mu}] [d\psi] [d\overline{\psi}] e^{iS}$$
<sup>(2)</sup>

and S is the QCD action. In these introductory paragraphs all the formulae are written in Minkowski space, although, of course, the lattice simulations use a Euclidean formulation of QCD. For the computations described in these lectures, n will be either equal to 2 or 3, and we now describe the significance of the two- and three-point correlation functions respectively.

### **Two-Point Correlation Functions:** Consider the bilocal operator *O*:

$$O(x_1, x_2) = J(x_1) J^{\dagger}(x_2) , \qquad (3)$$

where J and  $J^{\dagger}$  are interpolating operators which can destroy or create the hadron H, whose mass will be denoted by  $m_H$ . Moreover, we will assume that H is the lightest hadron which can be created by  $J^{\dagger}$ . We now define the two-point correlation function:

$$C_2(t) = \int d^3x \, e^{i\vec{p}\cdot\vec{x}} \langle 0 \, | \, J(\vec{x},t) \, J^{\dagger}(\vec{0},0) \, | \, 0 \rangle \,\,, \tag{4}$$

where we take t > 0. Inserting a complete set of states,  $\{n\}$ , between the two operators we obtain

$$C_2(t) = \sum_{n} \int d^3x \, e^{i\vec{p}\cdot\vec{x}} \langle 0 \, | \, J(\vec{x},t) \, | \, n \rangle \langle \, n | J^{\dagger}(\vec{0},0) \, | \, 0 \rangle \tag{5}$$

$$= \frac{1}{2E} |\langle 0 | J(\vec{0}, 0) | H(p) \rangle|^2 e^{-iEt} + \cdots , \qquad (6)$$

where the ellipses represent contributions from states which are heavier than H, and we have used translational invariance to displace the argument of J from  $(\vec{x}, t)$  to the origin. The four-momentum p has components  $(\vec{p}, E)$ , where  $E^2 = \vec{p}^2 + m_H^2$ . In Euclidean space the exponential factor in eq.(6) is  $e^{-Et}$ , and the contributions of the heavier states have similar exponential factors. Thus for sufficiently large times t, the contribution from the heavier states is suppressed, and the ground state is isolated. By fitting the time behaviour of the computed correlation function, one obtains E, and hence the mass of the hadron H, and also the matrix element  $|\langle 0 | J(\vec{0}, 0) | H(p) \rangle|$ . For example if H is the pion, and J the axial current, then from this matrix element we can obtain the value of the pion's decay constant:

$$|\langle 0 | A_{\mu}(0) | \pi(p) \rangle| = f_{\pi} p_{\mu} .$$
<sup>(7)</sup>

**Three-Point Correlation Functions:** It will also be useful for us to consider three-point correlation functions:

$$C_3(t_x, t_y) = \int d^3x \, d^3y \, e^{i\vec{p}\cdot\vec{x}} e^{i\vec{q}\cdot\vec{y}} \langle 0 \, | \, J_2(\vec{x}, t_x) \, O(\vec{y}, t_y) \, J_1^{\dagger}(\vec{0}, 0) \, | \, 0 \rangle \,, \qquad (8)$$

where,  $J_1$  and  $J_2$  are the interpolating operators for hadrons  $H_1$  and  $H_2$  respectively, O is a local operator, and we have assumed that  $t_x > t_y > 0$ . Inserting complete sets of states between the operators in eq.(8) we obtain

$$C_{3}(t_{x},t_{y}) = \frac{e^{-iE_{1}t_{y}}}{2E_{1}} \frac{e^{-iE_{2}(t_{x}-t_{y})}}{2E_{2}} \langle 0 | J_{2}(\vec{0},0) | H_{2}(\vec{p},E_{2}) \rangle \times \langle H_{2}(\vec{p},E_{2}) | O(\vec{0},0) | H_{1}(\vec{p}+\vec{q},E_{1}) \rangle \langle H_{1}(\vec{p}+\vec{q},E_{1}) | J_{1}^{\dagger}(\vec{0},0) | 0 \rangle + \cdots$$
(9)

where  $E_1 = \sqrt{m_1^2 + (\vec{p} + \vec{q})^2}$ ,  $E_2 = \sqrt{m_2^2 + \vec{p}^2}$  and the ellipses represent the contributions from heavier states. In Euclidean space the exponential factors become  $\exp(-E_1 t_y)$  and  $\exp(-E_2(t_x - t_y))$ , so that for large time separations,  $t_y$  and  $t_x - t_y$ , the contributions from the lightest states dominate. All the elements on the right-hand side of eq.(9) can be determined from two-point correlation functions, with the exception of the matrix element  $\langle H_2|O|H_1 \rangle$ . Thus by computing two- and three-point correlation functions the matrix element  $\langle H_2|O|H_1 \rangle$  can be determined.

The computation of three-point correlation functions is useful in studying weak decays of hadrons (e.g. if  $H_1$  is a *D*-meson,  $H_2$  a *K* meson and *O* the vector current  $\overline{c}\gamma^{\mu}s$ , then from this correlation function we obtain the form factors relevant for semileptonic  $D \to K$  decays) and in determining properties of hadronic structure (e.g. if  $H_1$  and  $H_2$  both represent the proton and *O* is the electromagnetic current, then from  $C_3$  we obtain the electromagnetic formfactors of the proton).

The computation of correlation functions will be outlined in subsec. 1.2, but I start with a brief description of the formulation of QCD on a discrete space-time lattice.

## 1.1 Elements of Lattice QCD

In order to perform lattice computations it is necessary to formulate QCD in discrete space-time and in Euclidean space<sup>*a*</sup>. The quark fields  $\psi(x)$  are field variables defined on the sites,  $\{x\}$ , of the lattice. The gluon fields are conveniently introduced in terms of "link" variables  $U_{\mu}(x)$ , defined on the link between the point x and  $x + a\hat{\mu}$ , where  $\hat{\mu}$  is the unit lattice vector in the  $\mu$ direction. The gluon field  $A_{\mu}$ , is then given by

$$U_{\mu}(x) = e^{iag_0 A_{\mu}(x+a\,\hat{\mu}/2)} , \qquad (10)$$

where a is the lattice spacing and  $g_0(a)$  is the bare coupling constant defined with the lattice action being used. Under a local gauge transformation g(x), the fields transform as:

$$\psi(x) \to g(x)\psi(x)$$
 and  $U_{\mu}(x) \to g(x)U_{\mu}(x)g^{\dagger}(x+a\hat{\mu})$ . (11)

 $U^{\dagger}_{\mu}(x-a\hat{\mu})$  can be thought of as the link variable from x to  $x-a\hat{\mu}$ . From eq.(11) it can be seen that any closed loop of link variables will be gauge invariant, and this is exploited in constructing the action and the operators which represent observables. For example, the Wilson action for the gauge fields is defined in terms of the "plaquette" variable, which is the product of link variables around an elementary square of the lattice:

$$\mathcal{P}_{\mu,\nu}(x) \equiv \text{Tr} \left[ U_{\mu}(x) U_{\nu}(x+a\hat{\mu}) U_{\mu}^{\dagger}(x+a\hat{\nu}) U_{\nu}^{\dagger}(x) \right] \,. \tag{12}$$

The Wilson action is defined by

$$S_{\text{gluon}} \equiv \beta \sum_{x,\mu,\nu} \left[ 1 - \frac{1}{3} \operatorname{Re} \mathcal{P}_{\mu,\nu}(x) \right] , \qquad (13)$$

where  $\beta = 6/g_0^2$ . Expanding the right hand side of eq.(13) in powers of the lattice spacing, one can verify that, as required, it gives  $\int d^4x \frac{1}{4}F_{\mu\nu}^2$ , up to "irrelevant" terms of  $O(a^2)$ .

 $<sup>^{</sup>a}$ For excellent pedagological introductions to the lattice formulation of QCD see refs.<sup>6,7</sup>.

When trying to discretise the fermion action, one encounters the famous problem of "Fermion Doubling". For example consider the free quark propagator, corresponding to the Dirac action  $\overline{\psi}(\partial + m)\psi$ . Defing the derivative of a function as the difference of its values at neighbouring sites, one obtains the following lattice propagator in momentum space

$$S(q)_{\text{free}} = m + \frac{i}{a} \sum_{\mu} \gamma_{\mu} \sin(aq_{\mu}) . \qquad (14)$$

Consider now q satisfying the continuum mass-shell condition  $q^2 + m^2 = 0$ . The free-propagator then has a pole at this choice of q as expected (modified by terms which vanish as  $a \to 0$ ). Now there are also poles at the values of momenta with any component  $q_{\mu}$  replaced by  $\pi/a - q_{\mu}$ , leading to sixteen states instead of one. Such doubling of the fermion degrees of freedom is a general feature of lattice theories<sup>8</sup>. Wilson's solution to this problem was to add an "irrelevant" operator to the action, in such a way that the unphysical doublers have infinite masses as  $a \to 0$ . For the free theory the Wilson term takes the form:

$$-\frac{ra}{2}\overline{\psi}\partial^{2}\psi = -ra^{4}\sum_{x}\left\{\frac{1}{2a}\sum_{\mu}[\overline{\psi}(x)\psi(x+a\hat{\mu}) + \overline{\psi}(x)\psi(x-a\hat{\mu}) - 2\overline{\psi}(x)\psi(x)]\right\},$$
(15)

where r is an arbitrary parameter. Physical quantities must, of course, be independent of r. With the Wilson term, the free propagator becomes

$$S(q)_{\rm free} = m + \frac{i}{a} \sum_{\mu} \gamma_{\mu} \sin(aq_{\mu}) + \frac{r}{a} \sum_{\mu} (1 - \cos(aq_{\mu})) .$$
 (16)

from which the shift of the mass of the doublers can be deduced. The Wilson term breaks chiral symmetry, even for m = 0, but the symmetry is restored at a special value of the bare mass<sup>9</sup> (see below). Including now interactions between quarks and gluons, the Wilson action becomes:

$$S_W = S_{\text{gluon}} + a^4 \sum_x \left\{ -\frac{\kappa}{a} \sum_\mu \left[ \overline{\psi}(x)(r - \gamma_\mu) U_\mu(x) \psi(x + a\hat{\mu}) + \overline{\psi}(x + a\hat{\mu})(r + \gamma_\mu) U_\mu^{\dagger}(x) \psi(x) \right] + \overline{\psi}(x) \psi(x) \right\}, \qquad (17)$$

where the parameter  $\kappa = 1/(2m + 8r)$  contains the dependence on the mass of the quark. The fields have been rescaled by a factor of  $2\kappa$ , and of course, a new term must be included for every quark flavour (each with a different  $\kappa$  parameter).

I end this subsection with some brief comments:

- i) The only parameters of the theory are those of QCD itself, i.e. the coupling constant, and the quark masses (parametrised in terms of  $\kappa$ ).
- ii) As mentioned above, physicial quantities must be independent of r, and we set r = 1 in most of the following discussion.
- iii) There is a value of  $\kappa (= \kappa_c)$  for which chiral symmetry is restored,  $(\kappa_c = 1/8 + O(\alpha_s))^9$ .
- iv) Expanding the right hand side of eq.(17) in powers of the lattice spacing we find

$$S_W = S_{QCD}^{\text{cont}} + O(a) , \qquad (18)$$

where the superscript "cont" implies that this is the continuum QCD action. Thus, for a finite lattice spacing a, we expect there to be "discretisation" errors of O(a) (i.e. of O(pa), O(ma) or of  $O(\Lambda_{\rm QCD}a)$ , where p is the momentum of one of the hadrons). Much work is currently being done in trying to reduce these lattice artefacts, by using "improved" lattice actions and operators <sup>10</sup>.

## 1.2 Evaluation of Correlation Functions

In this subsection I will briefly describe the steps used in the evaluation of correlation functions, without explaining the algorithms which are used in the computations.

**Pure Gauge Theories:** In the pure gauge theory, and in Euclidean space the functional integral in eq.(1) becomes:

$$\langle 0|O(x_1, x_2, \cdots, x_n)|0\rangle = \frac{1}{Z} \int [dU] e^{-S(U)} O(x_1, x_2, \cdots, x_n) ,$$
 (19)

where Z is given by

$$Z = \int [dU]e^{-S(U)} \tag{20}$$

and S is the gluon action (13). Examples of interesting studies in pure gauge theories include the evaluation of the spectrum of glueball states and the determination of the potential between a static quark and an anti-quark (for a recent review, and references to the original literature, see ref. <sup>11</sup>).

On a finite lattice with V points, the right hand side of eq.(19) is a welldefined multi-dimensional integral (specifically, for an SU(n) gauge theory it is a  $4V(n^2 - 1)$  dimensional integral). Monte Carlo algorithms are an efficient way to evaluate these multi-dimensional integrals. With these algorithms gluon configurations are generated on all the links of the lattice, with a probability density  $1/Z \exp(-S(U))$ . Thus

$$\langle O \rangle = \frac{1}{N_c} \sum_{c=1}^{N_c} O(U_c) \tag{21}$$

where  $O(U_c)$  is the value of O for the field configuration  $\{U_c\}$ , and the sum is over  $N_c$  statistically independent gluon configurations. In general we do not very know much about the statistical distribution of the results, but expect that the uncertainty will typically decrease like  $1/\sqrt{N_c}$ . The "statistical" error for a quantity in a given computation is estimated from the variation of the result as gluon configurations are subtracted and added.

**Lattice QCD** We now write the Wilson action (17) in the following shorthand notation:

$$S_W = \bar{\psi} \,\Delta(U)\psi + S_{\text{gluon}} \tag{22}$$

wher  $S_{\text{gluon}}$  is the gluon action and  $\Delta$  is a matrix in position, spin and colour spaces. The functional integral over the quark fields is straightforward to evaluate formally:

$$\int [d\psi] [d\bar{\psi}] e^{S_W} = \det[\Delta(U)] e^{-S_{\text{gluon}}}$$
(23)

$$\int [d\psi] [d\bar{\psi}] \psi_i \bar{\psi}_j e^{S_W} = \Delta_{ij}^{-1}(U) \det[\Delta(U)] e^{-S_{\text{gluon}}}$$
(24)

etc. The labels *i* and *j* represent the lattice coordinates, as well as spin and colour indices.  $\Delta^{-1}(U)$  is the quark propagator in the background field  $\{U\}$ . Thus for the integration over the gluon fields, the action should now be modified to  $S_{\text{gluon}} - \ln \det[\Delta(U)]$ . The second term, which represents the effects of closed quark loops, is non-local, and its inclusion in the Monte-Carlo algorithms is very expensive in terms of computing resources. It is the focus for much of the development work in improved algorithms for lattice simulations. At present, most large scale numerical simulations are performed in the "quenched approximation", in which the determinant is not included, i.e. the effects of closed quark loops are neglected. Even where they are explicitly included, it is generally the case that the sea quarks are heavy (with masses about those

of the strange quark), so that it is likely that the effects of light quark loops are significantly underestimated in these studies.

We do not really know how large the errors introduced by the quenched approximation are, and expect that these will depend on the physical quantities being computed, as well as on the quantities being used to fix the lattice spacing (and quark masses). Over the last ten years and more, a wide variety of quantities have been computed in quenched simulations and compared to the experimental values. In almost all cases there is good agreement between the computed and measured values (of the order or better than 25% or so), giving us confidence in the predictions for unknown physical quantities, such as the decay constant  $f_B$  discussed in the second lecture. The errors due to quenching are likely to be larger when one compares physical quantities which depend on different scales (e.g. if one fixes the lattice spacing in some process which occurs at a scale of  $O(\Lambda_{\rm QCD})$  and uses it in the prediction for heavy quarkonia). Of course it is only when we are able to include light quark loops in a reliable way that we will be able to claim that lattice QCD is a truly quantitative non-perturbative technique.

For the rest of these lectures I will discuss results obtained with the quenched approximation.

### 1.3 The Pion Propagator

I conclude this lecture with a specific example, that of the evaluation of the pion's decay constant  $f_{\pi}$ . The evaluation of other matrix elements and hadronic masses follows similar steps. Consider now the correlation function of two axial currents:

$$C(t) \equiv \sum_{\vec{x}} \langle 0 | \bar{\psi}(0) \gamma^0 \gamma^5 \psi(0) | \bar{\psi}(x) \gamma^0 \gamma^5 \psi(x) | 0 \rangle$$
(25)

$$= -\frac{1}{Z} \int [dU] e^{-S_{\text{gluon}}} \operatorname{Tr}[S(0,x)\gamma^0 \gamma^5 S(x,0)\gamma^0 \gamma^5] , \qquad (26)$$

where  $x = (\vec{x}, t)$  and I have denoted the quark propagator (with the dependence on the background field implicit) by S(x, 0). This correlation function is represented by the diagram in fig. 1.

The symmetry property  $S(0, x) = \gamma^5 S^{\dagger}(x, 0)\gamma^5$  is particularly useful, as it implies that in order to evaluate the correlation function C(t), for each gluon configuration it is sufficient to determine the set of quark propagators from an arbitrary lattice point to the origin,  $\{S(x, 0)\}$ . This is achieved by using efficient algorithms for the inversion of sparse matrices. I now assume that these sets of propagators have been generated for many gluon configurations and that C(t) has been evaluated.



Figure 1: Diagramatic representation of the two-point correlation function of the pion, eq.(26). The lines represent quark propagators in the gluon background field.

Fig. 2 shows the pion's correlation function obtained on a  $24^3 \times 48$  lattice at  $\beta = 6.2$  (for which the inverse lattice spacing is about 2.9 GeV), using 60 gauge field configurations (and the SW fermion action, which is an "improvement" on the Wilson action as explained in section 2.4). The light quarks are a little lighter than the physical mass of strange quark. In the same figure is shown the fit to a single state. The fit allows for the contribution of the backward propagating meson (which arises because, with periodic boundary conditions, t is both greater than and smaller than 0, so that there are two contributions for any t), so that the exponential is replaced by a hyperbolic cosine (which makes a difference close to the centre of the lattice).

Following the discussion above we need to establish whether we can isolate the ground state, i.e. whether the correlation function is well represented by a single exponential over some interval at larger times. To this end it is useful to define the effective mass by

$$m_{\rm eff}(t) \equiv \ln\left[\frac{C(t)}{C(t+1)}\right] , \qquad (27)$$

so that if the correlation function is well represented by a single exponential, then  $m_{\text{eff}}$  will be almost independent of the time t. The criteria for the construction of good lattice interpolating operators, such that the overlap with the lightest state is enhanced, and a plateau in the plot of  $m_{\text{eff}}(t)$  as a function of t is reached at relatively small times, is an area under intensive investigation. In order to determine  $f_{\pi}$  however, we need to determine the matrix element of a local axial current. The effective mass plot for the  $\pi$ -mesons, now for light quark masses which are a little heavier than the strange quark, obtained by the UKQCD collaboration with local interpolating operators are presented in fig. 3.

Because of finite volume effects it is not possible to perform the computations with physical light-quark masses, rather one must extrapolate the results obtained for masses around that of the strange quark to the chiral  $(m_q = 0)$ 



Figure 2: Correlation function of the light pseudoscalar meson ("pion") with quarks which are a little lighter than the strange quark (from ref.<sup>12</sup>).

limit. This requires the knowledge of the value of the  $\kappa$ -parameter at the chiral limit ( $\kappa_c$ ). To determine  $\kappa_c$ , we use PCAC and plot  $m_{\pi}^2$  as a function of  $1/\kappa$  (and hence as a linear function of the quark mass), and determine the value of  $\kappa$  at which  $m_{\pi}^2 = 0$  (or  $m_{\pi}$  takes its physical value). In fig. 4(a) we show such a plot, again from the UKQCD collaboration's simulation at  $\beta = 6.2$ . In fact it can be shown using chiral perturbation theory that the PCAC relation stating that  $m_{\pi}^2$  is proportional to the quark mass is violated in quenched simulations <sup>13,14</sup>. However this effect only occurs at very low quark masses which is difficult to simulate without encountering finite volume effects. Recently Kim and Sinclair have demonstrated this violation of the PCAC in a numerical simulation on very large lattices <sup>15</sup>.

Having determined  $\kappa_c$  we now extrapolate the results for  $f_{\pi}$  to the chiral limit. Generally, in the absence of any theoretical guidance, one assumes a linear dependence on the mass of the light quark in this extrapolation. Now  $f_{\pi}$  is a dimensionful quantity, which we determine in lattice units, i.e. we compute  $af_{\pi}$ , where a is the lattice spacing. Thus to make a prediction for  $f_{\pi}$  we need to know the value of a. In lattice computations this is done implicitly using



Figure 3: The effective mass plot of the light pseudoscalar meson ("pion") with quarks which now are a little heavier than the strange quark (from ref. <sup>12</sup>).

dimensional transmutation. Instead of fixing a, and then using some physical quantity to determine the bare coupling constant  $g_0(a)$  (which is a genuine parameter of QCD), one fixes  $g_0(a)$  (or equivalently  $\beta$ ) and determines a. For example one may use the mass of the  $\rho$ -meson to determine a (an extrapolation to the chiral limit of the UKQCD results, at  $\beta = 6.2$ , is presented in fig. 4(b)). My summary of the values of the lattice spacings for two commonly used values of  $\beta$  (obtained by using light quark quantities to set the scale) is

$$a^{-1}(\beta = 6.0) = 2.0(2) \,\text{GeV}$$
 (28)

$$a^{-1}(\beta = 6.2) = 2.9(3) \,\text{GeV} \,.$$
 (29)

The errors are largely due to the variation in the results obtained using different physical quantities to set the scale, and hence are at least partially due to quenching. An inverse lattice spacing of 2 GeV corresponds to a spacing of 0.1 fm.

In this way one obtains the matrix element of the axial current (or similarly other matrix elements) from lattice simulations. The matrix element is of a bare operator which has been defined in QCD with a lattice regularization,



Figure 4: The values of (a) the pion mass squared, and (b) the rho mass plotted as a linear function of the quark mass(from ref. <sup>12</sup>).

and a specific lattice action. The ultraviolet properties of such an operator are of course different from those defined in the continuum. However, since it is the short-distance behaviour which is different, the relation between bare lattice operators defined with an inverse lattice spacing  $a^{-1} \gg \Lambda_{\rm QCD}$  and renormalized continuum operators defined at a scale  $\mu \gg \Lambda_{\rm QCD}$ , can be derived using perturbation theory<sup>b</sup>.

As an example of the results obtained for  $f_{\pi}$ , the UKQCD collaboration, from the simulation which was used to illustrate the calculational steps above, quote  $f_{\pi}/m_{\rho} = 0.14(1)$ , to be compared to the experimental result of 0.17.

## 2 Lecture 2 – Simulations in The Heavy Quark Effective Theory

In this lecture I will apply the formalism reviewed above to lattice simulations in the HQET, using the evaluation of the decay constant of the *B*-meson  $(f_B)$ as a case study. Matthias Neubert has, at this school, already described the formalism of the Heavy Quark Effective Theory (HQET) and explained its usefulness <sup>18</sup>. In this framework, predictions for physical quantities in heavy quark physics are presented in terms of a series in inverse powers of the mass

 $<sup>^{</sup>b}$  For some quantities this matching between the lattice and continuum operators represents the largest source of theoretical uncertainty. Non-perturbative methods to evaluate the matching factors are being developed  $^{16,17}$ .

of the heavy quark. The predictions are given in terms of matrix elements of operators containing the field of the heavy quark, and lattice simulations provide the opportunity for the evaluation of these matrix elements.

Before starting the presentation however, I would like to discuss why it useful to perform lattice computations in the HQET, rather than to evaluate quantities such as  $f_B$  directly in QCD. The reason is that the sizes of the lattices and lattice spacings which we can be used are limited by the available computing resources, and current quenched simulations are performed with inverse lattice spacings typically in the range of 2–3.5 GeV. Thus the lattice spacings are larger than the Compton wavelength of the b-quark, and we cannot meaningfully study its propagation directly in QCD. Since in lattice computations we have the luxury of varying the masses of the quarks, one approach to the study of *B*-physics on the lattice is to perform the computations with several smaller values of the heavy quark mass (typically in the range of that of the charm quark mass), and to extrapolate the results to the b-quark<sup>c</sup>. Of course such an extrapolation introduces uncertainties, and much effort is being spent on reducing the lattice artefacts (errors due to the finite size of the lattice spacing) by introducing improved actions and operators, in order to be able to perform the simulations with larger masses.

Simulations in the HQET, provide the results in the infinite mass limit, and in principle, also allow for a systematic program of evaluating corrections to this limit. The corresponding results can be used as a check of the extrapolations of the results obtained with propagating heavy quarks, as described above. Since the mass of the heavy quark does not enter directly into simulations in the HQET (having been scaled out), lattice artefacts are, a priori, expected to be as small as for quantities in light quark physics.

### 2.1 The Heavy Quark Effective Theory on the Lattice

The Lagrangian for the HQET, at zero three-velocity (i.e. in the static limit) in Euclidean space takes the form d:

$$\mathcal{L} = \bar{h} D_4 \frac{1 + \gamma^4}{2} h . \tag{30}$$

If we define the lattice covariant derivative by

$$D_4 f(\vec{x}, t) = \frac{1}{a} \left[ f(\vec{x}, t) - U_4^{\dagger}(\vec{x}, t-a) f(\vec{x}, t-a) \right] , \qquad (31)$$

 $<sup>^</sup>c{\rm In}$  the following I shall refer to such simulations as ones with "propagating" heavy quarks, in distinction to the "static" quarks of the HQET.

<sup>&</sup>lt;sup>d</sup>The construction of the HQET in Euclidean space, with  $\vec{v} \neq 0$  is subtle, requiring an interpretation of  $\delta^{(3)}(\vec{x} - \vec{v}t)$ , see refs. <sup>19,20</sup>



Figure 5: Quark flow diagram representing the decay of a *B*-meson into leptons.

then the propagator of the heavy quark h in the background field configuration  $\{U\}$  is given by

$$S_{h}^{\{U\}}(\vec{x},t;\vec{0},0) = \delta^{(3)}(\vec{x})\theta(t)U_{4}^{\dagger}(\vec{0},t-a)U_{4}^{\dagger}(\vec{0},t-2a)\cdots U_{4}^{\dagger}(\vec{0},0) , \qquad (32)$$

with  $S_h^{\{U\}}(\vec{0}, 0; \vec{0}, 0) = 1$ . Other choices of the lattice covariant derivative correspond to propagators with different boundary conditions at the origin. From eq.(32) we see that the propagator of the heavy quark is given directly in terms of the link variables, and so no inversion of a sparse matrix is necessary (as is the case for the quark propagator in QCD, see subsection 1.3 above).

# 2.2 Calculation of $f_B$ in the Static Limit

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The non-perturbative strong interaction effects in the leptonic decay amplitude of the *B*-meson are contained in a single parameter, the decay constant  $f_B$ . The process is illustrated in the diagram of fig. 5. To determine this parameter, in analogy to the computation of  $f_{\pi}$  discussed in subsection 1.3 above, we compute the correlation function:

$$C_{2}(t) = \sum_{\vec{x}} \langle 0 | \bar{h}(x) \gamma^{4} \gamma^{5} q(x) \bar{q}(0) \gamma^{4} \gamma^{5} h(0) | 0 \rangle$$
(33)

$$= -\sum_{\vec{x}} \langle \operatorname{Tr}[\gamma^4 \gamma^5 S_l(x,0) \gamma^4 \gamma^5 S_h(0,x)] \rangle$$
(34)

$$= \frac{|\langle 0|\bar{h}\gamma^4\gamma^5 q|0\rangle|^2}{2M_B} e^{-\mathcal{E}t} + \cdots$$
(35)

$$= \left(\frac{1}{Z_A^{\text{stat}}}\right)^2 \frac{f_B^2 M_B}{2} e^{-\mathcal{E}t} + \cdots , \qquad (36)$$

where  $S_l$  and  $S_h$  are the light and heavy quark propagators respectively. I now explain the features of the calculation represented by eqs.(33)–(36) in some more detail:

What is the interpretation of  $\mathcal{E}$ ?:  $\mathcal{E}$  itself is not a physical quantity, indeed it diverges linearly with the inverse lattice spacing. At the tree level, it is just the difference of the mass of the pseudoscalar meson and that of the quark. When higher order corrections are included the interpretation of  $\mathcal{E}$  becomes more subtle, and will be explained in the third lecture below. In the lattice theory, with the hard ultraviolet cut-off  $a^{-1}$ , quantum corrections generate a mass term in the effective theory, even if the bare action does not have such a term (as in eq.30)). This mass term is of  $O(\alpha_s/a)$ . For now I will just note that from the measured value of  $\mathcal{E}$ , it is possible to derive the value of any short-distance mass of the heavy quark (such as the  $\overline{\text{MS}}$  mass).

Heavy Quark Scaling Law: Since the action of the HQET is independent of the mass of the heavy quark, so is the correlation function (33). Thus, from eq.(36) we can deduce the well known scaling law that the decay constant of a heavy pseudoscalar meson decreases like the square-root of its mass. This scaling law is modified by logarithmic corrections contained in the matching factor  $Z_A^{\text{stat}}$  as explained below.

**"Smearing":** In practice it is difficult to isolate the contribution of the ground state in these calculations<sup>21,22</sup> using local interpolating operators. To enhance the relative contribution of the lightest state, various extended (or "smeared") interpolating operators are used. For example one might smear the field in the axial current by

$$h^{s}(\vec{x},t) \equiv \sum_{\vec{y}} f(\vec{x},\vec{y}) h(\vec{y},t)$$
(37)

in the Coulomb gauge say. Different choices of the smearing function f are used by the various groups carrying out such simulations. The Fermilab group in particular have been stressing the possibility of learning about the wave function of the heavy meson by studying its overlap with different extended operators<sup>23</sup>. However, it should be remembered that  $f_B$  is obtained from the matrix element of the local (i.e. not smeared) axial current. To determine this, one has to compute the correlation functions of two smeared currents (from which one obtains the matrix element of the smeared current as in eq.(35)) and of a smeared and a local current (from which one is then able to deduce the matrix element of the local current). A strong check that the ground state has been isolated is provided by verifying that the matrix element of the local current is independent of the smearing function f used in the calculation **Matching:** The quantity which one obtains directly in lattice simulations is the matrix element of the bare axial current in the HQET, defined with the lattice regularization. In order to obtain  $f_B$  one needs the matrix element of the axial current in QCD. The difference between the two is an ultraviolet effect and can be calculated in perturbation theory. Although not necessay, this calculation is usually performed in two steps

$$A_{\mu}^{\text{latt, HQET}}(a) \to A_{\mu}^{\overline{\text{MS}}, \text{ HQET}}(\mu) \to A_{\mu}^{\text{QCD}}$$
 . (38)

In the first of these steps lattice perturbation theory is used to obtain the matrix element of the axial current in the HQET defined in some continuum renormalization scheme, such as the  $\overline{\text{MS}}$  scheme, from the matrix element of the bare current in the lattice theory. In the second step the matrix element of the physical (QCD) current (and hence  $f_B$ ) is obtained from that in the effective theory.  $Z_A^{\text{stat}}$  in eq.(36) is the combined matching factor. It depends logarithmically on the lattice spacing, being proportional to  $\alpha_s(a)^{(-2/\beta_0)}$ , where  $\beta_0 = 11 - 2/3N_f$  is the coefficient of the first term in the  $\beta$ -function, and  $N_f$  is the number of light-quark flavours.

In these lectures it is not possible for me to describe the technical details of lattice perturbation theory. The lattice action for the HQET in eq.(30) and the QCD action in eq.(17), with the derivatives defined as differences, lead to Feynman rules where the momentum dependence is given in terms of trigonometric functions. For example the quark propagator for the Wilson action is given by the expression in eq.(16). This makes the analytic evaluation of Feynman diagrams in lattice perturbation theory prohibitatively difficult in general, and instead the integrals are evaluated numerically.

Lepage and Mackenzie have argued convincingly that the bare lattice coupling  $g_0^2(a)$  is a poor expansion parameter for lattice perturbation theory, i.e. that with this choice the higher order corrections have unnecessarily large coefficients<sup>24</sup>. As an example, consider the one-loop tadpole correction to the plaquette variable, illustrated in fig. 6. Numerically it turns out that such tadpole contributions, which are common to many quantities, are large. In particular they will appear each time that there is a link variable (from which the tadpole can emanate). Let

$$u_0^4 \equiv \frac{1}{3} \langle \operatorname{Tr} \mathcal{P}_{\mu,\nu} \rangle \tag{39}$$

where the plaquette  $\mathcal{P}$  has been defined in eq.(12). Thus one might expect that at least part of the large higher order corrections are given by  $u_0$  for each link variable present in the quantity being studied. If this is the case then we can replace each link variable  $U_{\mu}$  by  $U_{\mu}/u_0$ , compensating for this by different



Figure 6: Representation of a one loop tadpole diagram contributing to the plaquette variable. The diagram is generated by expanding one of the link variables to  $O(g_0^2)$ .

perturbative matching factors. For the gluon action one would rewrite  $\mathcal{P}/g_0^2 \rightarrow \mathcal{P}/(\tilde{g}^2 u_0^4)$ , with  $\tilde{g}^2 = g_0^2/u_0^4$ . It might therefore be expected that  $\tilde{g}^2$  is a better expansion parameter, and this appear to be the case (for numerical evidence of this feature, and of a general discussion of "tadpole resummation" see ref.<sup>24</sup>). It would, nevetheless, be very welcome to have a non-pertubative determination of the matching factor. For simulations with the Wilson action for the light quark,  $Z_A^{\text{eff}} \simeq 0.7$  for typical beta values used in current simulations, and for the "improved" SW-action described in subsection 2.4,  $Z_A^{\text{eff}} \simeq 0.8$ . These values are obtained from one-loop perturbation theory.

## 2.3 Results

Before presenting some results obtained from simulations in the heavy quark effective theory, let us recall precisely what it is that we are calculating. The decay constant  $(f_P)$  of a heavy pseudoscalar meson (P) satisfies the scaling law:

$$f_P = \frac{A}{\sqrt{M_P}} \left\{ \alpha_s^{-2/\beta_0}(M_P) \left( 1 + O(\alpha_s) \right) + O(\frac{1}{M_P}) \right\} , \qquad (40)$$

where  $M_P$  is the mass of the meson. The factor of  $\alpha_s(M_P)^{-2/\beta_0}$  arises from the matching of the HQET with QCD, and in our case above (for the *B*-meson) it is included in  $Z_A^{\text{stat}}$ . From lattice simulations in the HQET, we obtain A, the normalisation of the leading term. In order to compute the  $O(1/M_P)$ corrections, it is necessary to compute the matrix elements of the dimension-4 operators which arise in the expansion of the axial current in QCD in terms of operators of the HQET. It is also necessary to include the  $O(1/M_P)$  corrections to the heavy quark action (30). Such calculations are only just beginning to be performed <sup>25</sup>. I denote by  $f_B^{\text{stat}}$ , the value of  $f_B$  obtained by dropping the  $1/M_P$  corrections. The UKQCD collaboration obtain

$$f_B^{\text{stat}} = 266 + \frac{18}{20} (\text{stat}) + \frac{28}{27} (\text{syst}) \,\text{MeV} , \qquad (41)$$

where the quoted systematic error is due to the uncertainty in the value of the lattice spacing (which enters as  $a^{3/2}$  in this calculation). For a recent review of the status of computations of  $f_B^{\text{stat}}$  see ref.<sup>4</sup>. I will delay the interpretation of this result until after a discussion of the computations performed with propagating heavy quarks in subsection 2.4.

The calculation of  $f_B^{\text{stat}}$  is performed in a theory without any explicit large masses. A priori, one would therefore expect that the systematic errors should be similar to those in light quark physics. By repeating this calculation at several values of  $\beta$ , the Fermilab group have claimed that there are large lattice artefacts <sup>26</sup>. This conclusion relies heavily on the results at  $\beta = 5.7$  however, and a detailed study of the data of the APE collaboration leads to the conclusion that the results for  $f_B^{\text{stat}}$  are independent of  $\beta$  (i.e. of a) for  $\beta \geq 6.0^{27}$ .

# 2.4 Calculations of $f_B$ performed with Propagating Heavy Quarks

In this subsection I return to simulations performed in QCD. Now, as explained above, the *b*-quark is too heavy to use, so the calculations of decay constants and other physical quantities are performed with quark masses in the region of that of the charmed quark. Even so, the largest source of systematic uncertainty are discretisation errors which are of  $O(m_Q a)$  for a heavy quark with mass  $m_Q$ . For example, at  $\beta = 6.2$  the bare mass of the charm quark,  $m_{ch,0}$ , is about 0.35 in lattice units, where

$$m_{ch,0} a \equiv \frac{1}{2} \left( \frac{1}{\kappa_{ch}} - \frac{1}{\kappa_c} \right) \tag{42}$$

and  $\kappa_{ch}$  is the  $\kappa$ -parameter corresponding to a charm quark.

**"Improvement":** In order to reduce these discretisation errors much effort is being invested to develop the systematic "improvement" technique of Symanzik<sup>10</sup>. This technique involves the modification of the lattice action and operators in such a way that the discretisation errors are formally reduced. As an example consider the action<sup>28</sup>:

$$S_{QCD}^{II} = S_{\text{gluon}} + S_W^F - \Delta S^{II} \tag{43}$$

where  $S_{\rm gluon}$  and  $S_W^F$  are the Wilson gluon and quark actions as defined in subsection 1.1 and

$$\Delta S^{II} = -2\kappa a^4 \sum_{x,\mu} \frac{r}{8a} \Big\{ \bar{\psi}(x) U_{\mu}(x) U_{\mu}(x+a\hat{\mu}) \psi(x+2a\hat{\mu}) + \bar{\psi}(x+2a\hat{\mu}) U_{\mu}^{\dagger}(x+a\hat{\mu}) U_{\mu}^{\dagger}(x) \psi(x) - 2\bar{\psi}(x) \psi(x) \Big\} .$$
(44)

Now expanding  $S_{OCD}^{II}$  as a series in the lattice spacing we find:

$$S_{QCD}^{\text{cont}} = S_{QCD}^{II} + O(a^2) , \qquad (45)$$

where the superscript "cont" represents "continuum". A similar expansion for the Wilson action, eq.(18), gives discretisation errors of O(a) rather than of  $O(a^2)$ . When radiative corrections are included one finds that the discretisation errors are of  $O(\alpha_s a)^{29}$ , and so the use of the action (43) has formally reduced the lattice artefacts from O(a) to  $O(\alpha_s a)$ . One can also readily check that the problem of fermion doubling has not been reintroduced by the addition of the term  $\Delta S^{II}$ .

The action in eq.(43) contains next-to-nearest neighbour interactions, in addition to the nearest-neighbour interactions of the Wilson theory. By changing (the fermionic) variables in the functional integral, it is also possible to construct an equivalent improved theory with nearest neighbour interactions only  $^{30}$ 

$$S_{QCD}^{I} = S_{\text{gluon}} + S_{W}^{F} - \Delta S^{I} \tag{46}$$

with

$$\Delta S^{I} = \frac{ira\kappa}{2} g_0 \sum_{x,\mu\nu} \bar{\psi}(x) \sigma_{\mu\nu} F_{\mu\nu} \psi(x) . \qquad (47)$$

This lattice action, which was first proposed by Sheihkoleslami and Wohlert, is called the SW-action. In eq. (47),  $F_{\mu\nu}$  is a lattice definition of the field strength tensor. Several groups performing large scale numerical simulations are using this action, and the results from the UKQCD collaboration which I am using to illustrate this talk were obtained with this formulation of QCD. Even with this action however, in simulations containing the charm quark, one might expect 10% errors due to finite-*a* effects.

It is also possible to try to construct an action by subtracting  $\Delta S^I$  with a coefficient which is different from unity in order to reduce the lattice artefacts still further. This is sometimes done at the one-loop level <sup>31</sup> or by using mean field theory estimates <sup>32,33</sup> or non-perturbatively <sup>17</sup>. Finally let me mention the exciting program of constructing "Perfect Actions" <sup>34</sup>, in which, ideally, by using the renormalization group transformations on a fixed-point action, all the discretisation errors would be removed (although in practice one may have to settle for a substantial reduction of the artefacts, rather than for "perfection").

**Results:** My summary of the results obtained with propagating quarks is:

$$f_D = 200 \pm 30 \,\mathrm{MeV}$$
 (48)

$$f_B = 180 \pm 40 \,\mathrm{MeV} \,, \tag{49}$$

where the result for the B-meson was obtained, of course, by extrapolation to the b-quark of results obtained with lighter quarks. This extrapolation is illustrated in fig. 7, where the results from the UKQCD collaboration are presented for the scaling quantity

$$\hat{\Phi}(M_P) \equiv f_P \, M_P^{1/2} \, (\alpha_s(M_P) / \alpha_s(M_B))^{2/\beta_0} \,, \tag{50}$$

as a function of  $1/M_P$ <sup>35</sup>, where all quantities are given in lattice units<sup>*e*</sup>. Here P represents a heavy-light pseudoscalar meson. There are twelve "measured" points, corresponding to three light quark masses (represented by the open triangle (heaviest), circle and square(lightest)) and four heavy quark masses (represented, for each light quark mass, by the same open symbol). The full points represent the values obtained by extrapolation of the light-quark masses to the chiral limit, for each heavy quark mass. If there were no  $1/M_P$  and higher corrections then, for each choice of the light quark mass, the points would lie on a horizontal line. Clearly there are significant, negative,  $O(1/M_P)$ corrections. The violation of the heavy quark scaling law is of the correct sign to match up with the static result, although UKQCD find a (small) discrepancy between their result for  $f_B^{\text{stat}}$  and the value obtained by extrapolating the results computed at finite values of  $M_P$ . Given the different systematic errors in the computations with static and with propagating heavy quarks, the near consistency of the results is very pleasing. I would summarize the best estimate of  $F_B$  from lattice simulations as being 190(40) MeV.

Test of the Heavy Quark Symmetry: I would like to mention one important test of the lattice calculations with propagating heavy quarks, which is provided by the heavy quark symmetry <sup>36</sup>. In the infinite mass limit the decay constants of the pseudoscalar  $(f_P)$  and vector  $(f_V)$  mesons are related

$$\widetilde{U}(M) \equiv \frac{f_V f_P}{M} \frac{1}{1 + \frac{8}{3} \frac{\alpha_s(M)}{\pi}} \to 1$$
(51)

as  $M \to \infty$ , where  $f_V$  is defined by

$$\langle 0 | V_{\mu}(0) | V \rangle = \epsilon_{\mu} \frac{M_V^2}{f_V} .$$
(52)

In eq.(52),  $V_{\mu}$  is the vector current with the appropriate flavour quantum numbers, and  $\epsilon_{\mu}$  is the polarisation vector of the vector meson V. The perturbative

 $<sup>^</sup>e {\rm The}$  simulation was performed at  $\beta = 6.2$  for which the inverse lattice spacing is about 2.9 GeV.



Figure 7: The behaviour of the scaling quantity  $\hat{\Phi}$  with  $1/M_P$ . The solid line represents the linear fit to the chirally extrapolated points using the three heaviest meson masses, whereas the dashed curve results from a quadratic fit to all four.

matching factor in eq.(51), has been calculated to one-loop order. In fig. 5 I present the results of the ratio in eq.(51) as a function of 1/M, where for M I have taken the spin averaged meson mass  $(M = (3 M_V + M_P)/4)^{35}$ . It can be seen that the results obtained at finite values of the mass of the heavy quark differ substantially from the asymptotic value, but the extrapolation to  $M = \infty$  is in good agreement.

#### 2.5 Other Physical Quantities in B-Physics

To conclude this lecture I will briefly mention some other quantities in heavy quark physics which have been, or are being, computed in simulations in the HQET.

 $\mathbf{f}_{\mathbf{B}_s}/\mathbf{f}_{\mathbf{B}_d}$ : By studying the dependence on the results for  $f_B$  on the mass of the light quark, one obtains a good estimate of the ratio of the decay constants of the  $B_s$  and  $B_d$ -mesons. With both static and propagating heavy quarks one typically finds that  $f_{B_s}$  is about 10-20% larger than  $f_{B_d}$ . This can be



Figure 8: The quantity  $\widetilde{U}(M)$  plotted against the inverse spin-averaged mass. Linear and quadratic fits are represented by the solid and dashed curves respectively. Also shown are the statistical errors of the extrapolation to the infinite mass limit.

understood as being due to the fact that the  $B_s$  meson is more compact than  $B_d$ , with a larger wave-function at the origin.

**Heavy Baryons:** The detailed study of heavy baryons is just beginning in lattice simulations. In the HQET it is possible to evaluate mass differences, such as that between the  $\Lambda_b$  baryon and *B*-meson. The UKQCD collaboration find for this quantity <sup>37</sup>:

$$M_{\Lambda_b} - M_B = 420 \ ^{+100}_{-90} \ ^{+30}_{-30} \,\mathrm{MeV} \,, \tag{53}$$

to be compared with the experimental result of 346 MeV with an error of about 7 MeV (this is based on the new result from the CDF collaboration<sup>38</sup>). It must be remembered that the result in eq.(53) represents the value in the infinite mass limit. A comprehensive study of the spectrum of heavy baryons using propagating heavy quarks, can be found in ref.<sup>39</sup>, where the  $\Lambda_b$ -B mass splitting was found to be  $359 \pm 50 \pm 27$  MeV.

**B**<sub>B</sub>: One of the most important quantities in the phenomenology of *B*-physics is the parameter  $B_B$ , which together with  $f_B$  contains the strong interaction effects in  $B^0 - \overline{B}^0$  mixing. It is defined by

$$B_B = [\alpha_s(\mu)]^{-2/\beta_0} \frac{\langle \overline{B}^0 | O_L(\mu) | B^0 \rangle}{\frac{8}{3} f_B^2 M_B^2}$$
(54)

where  $O_L$  is the  $\Delta B = 2$  operator

$$O_L(\mu) = \bar{b}\gamma_{\mu}(1 - \gamma^5)q \,\bar{b}\gamma^{\mu}(1 - \gamma^5)q \;.$$
(55)

The first factor on the right hand side of eq.(54) is introduced to cancel the  $\mu$  (i.e. renormalization scale) dependence of the matrix element at leading logarithmic order.

In order to determine the physical amplitude for the  $\Delta B = 2$  transition, it is necessary to write the corresponding QCD operator, renormalized in some continuum scheme, in terms of the bare operators of the HQET defined using the lattice regularization. Because of the breaking of chiral symmetry in theories based on the Wilson formulation of lattice fermions, this requires the evaluation of the matrix elements of 3 other  $\Delta B = 2$  operators in addition to  $O_L$ ,

$$O_R = \left(\bar{b}\gamma_\mu (1+\gamma^5)q\right) \left(\bar{b}\gamma_\mu (1+\gamma^5)q\right)$$
(56)

$$O_N = (\bar{b}\gamma_{\mu}(1-\gamma^5)q) (\bar{b}\gamma_{\mu}(1+\gamma^5)q) + 2(\bar{b}(1-\gamma^5)q) (\bar{b}(1+\gamma^5)q) + 2(\bar{b}(1+\gamma^5)q) (\bar{b}(1-\gamma^5)q) (57)$$

$$O_S = \left(\bar{b}(1-\gamma^5)q\right) \left(\bar{b}(1-\gamma^5)q\right) , \qquad (58)$$

where the QCD operator  $O_L$  is given by

$$O_L^{QCD}(m_b) = Z_L O_L^{\text{latt}} + Z_R O_R^{\text{latt}} + Z_N O_N^{\text{latt}} + Z_S O_S^{\text{latt}} .$$
<sup>(59)</sup>

The matching coefficients  $Z_i$ ,  $\{i = L, R, N, S\}$ , have been calculated at one loop level for the Wilson and SW actions in references <sup>40</sup> and <sup>41</sup> respectively. The one-loop contribution to  $Z_L$  is large, for example at  $\beta = 6.2$  with the SW action (corresponding to the UKQCD simulation),  $Z_L \simeq 0.55$ . This underlines further the necessity for a non-perturbative determination of the matching coefficients.

The matrix elements of the lattice four-quark operators, normalised by the factor  $8/3f_B^2m_B^2$  as in eq.(54), can readily be obtained from the ratio of correlation functions:

$$R_i^{SS}(t_1, t_2) = \frac{K_i^{SS}(t_1, t_2)}{\frac{8}{3}C^{SL}(t_1)C^{SL}(t_2)}$$
(60)



Figure 9: Diagramatic representation of the ratio defined in eq.(60). The double (single) lines represent the propagators of the heavy (light) quark. The labels S and L indicate whether smeared or local operators have been inserted at the corresponding point.

where  $K_i^{SS}$ , with i = L, R, N, S, is the three point function

$$K_{i}^{SS}(t_{1}, t_{2}) \equiv \sum_{\vec{x}_{1}, \vec{x}_{2}} \langle 0 | \left\{ A^{\dagger^{S}}(\vec{x}_{1}, -t_{1}) O_{i}^{\text{latt}}(0) A^{\dagger^{S}}(\vec{x}_{2}, t_{2}) \right\} | 0 \rangle (61)$$

$$\stackrel{t_{1}, t_{2} \gg 0}{\longrightarrow} \frac{(Z^{S})^{2}}{2M_{B}} e^{-E(t_{1}+t_{2})} \langle \overline{B}^{0} | O_{i}^{\text{latt}} | B^{0} \rangle ; \qquad (62)$$

 ${\cal C}^{SL}$  is the two-point correlation function of two axial currents,

$$C^{LS}(t) = \sum_{\vec{x}} \langle 0 | A_4^L(\vec{x}, t) A_4^{\dagger^S}(\vec{0}, 0) | 0 \rangle , \qquad (63)$$

and the superscripts L and S stand for *local* and *smeared* respectively. The smeared currents are introduced to enhance the overlap with the ground state, and the local ones because it is from these that we are able to obtain the decay constant  $f_B$ . The ratio  $R_i$  is represented by the diagram in fig.9.

The UKQCD collaboration finds the following results from their simulations at  $\beta=6.2^{\,37}$  :

$$B_{B_d} = 1.02 \stackrel{+}{_{-}} \stackrel{5}{_{-}} (\text{stat}) \stackrel{+}{_{-}} \stackrel{3}{_{-}} (\text{syst})$$
(64)

$$B_{B_s} = 1.04 + \frac{4}{5}(\text{stat}) + \frac{2}{1}(\text{syst})$$
(65)

A discussion of the phenomenological consequences of these results can be found in ref.<sup>37</sup>. A preliminary result which is somewhat higher (by about 25%) than that in eqs.(64) and (65) was recently presented in ref.<sup>42</sup>.

Relatively few calculations have been performed for the B-parameter with propagating heavy quarks  $^{43,36,44}$ , the most recent of which quotes

$$\alpha_s^{(2/\beta_0)}(5\,\text{GeV}) \ B_B = 0.90(5) \text{ and } 0.84(6)$$
 (66)

obtained using the Wilson fermion action at  $\beta = 6.1$  and 6.3 respectively <sup>44</sup> f. Thus this result obtained with propagating Wilson quarks is a little larger (about 20% larger) than that obtained with static quarks in eq.(64). It is too early to be sure that this difference is a physical effect, rather than an artefact of lattice systematics. In particular it will be interesting to compare the calculations of the matching factors in the recent studies <sup>42,44</sup> when the details of these calculations are published, with those of ref.<sup>37,36</sup>. In reference<sup>36</sup> there is some evidence that the  $O(1/m_Q)$  corrections to the result obtained in the static limit may be negative, so that the *B*-parameter increases slowly as the mass of the heavy quark increases, which is the opposite conclusion one would draw from comparing the results in eqs.(64) and (65), with that of the JLQCD collaboration with propagating quarks.

The Hyperfine Splitting,  $M_{B^*} - M_B$ : As a final example of quantities which can be evaluated in lattice simulations, consider the mass difference between the vector and pseudoscalar heavy-light mesons. In the static limit these mesons are degenerate, and their mass difference is of  $O(1/m_Q)$ , where  $m_Q$  is the mass of the heavy quark. The hyperfine splitting is given by the matrix element of the chromomagnetic operator which appears at  $O(1/m_Q)$ in the action. The results of lattice calculations of the hyperfine splitting give values which are considerably lower (by a factor of 2 or so) than the experimental result <sup>45,37,46</sup>. For example in ref.<sup>37</sup> it was found that

$$M_{B^*}^2 - M_B^2 = 0.281 + {}^{15}_{-16} (\text{stat}) + {}^{40}_{-37} (\text{syst}) \,\text{GeV}^2 , \qquad (67)$$

where the systematic error represents the uncertainty in the value of the lattice spacing only. The experimental result for this quantity is  $0.488(6) \text{ GeV}^{247}$ .

It has been observed for a considerable time that the values of the hyperfine splitting in heavy mesons (including heavy quarkonia) are found to be too small in lattice simulations with propagating heavy quarks. It is understood that this physical quantity has particularly large discretisation errors, and indeed

 $<sup>^{</sup>f}$ Thus the JLQCD group quote their results in terms of the matrix element renormalized at 5 GeV in the  $\overline{\text{MS}}$  scheme, and not the renormalization group improved one<sup>44</sup>.

as one "improves" the action, the discrepency between the lattice results and experimental measurement decreases  $^{48,32}$ . It is peculiar however that the result obtained with the HQET is so different from the experimental value. In the HQET the discretisation errors are all of  $O(a\Lambda_{\rm QCD})$ , since there is no dependence on the mass of the heavy quark. Of course quenching may be partly responsible for the discrepency, and in addition the matching factor (between the lattice operator in the HQET and that in QCD) is found to have very large one-loop corrections (the factor, which is 1 at the tree level, is found to be about 1.8 at the one-loop level). This is another example of the necessity of computing these matching factors non-perturbatively.

## 3 Lecture 3 – Renormalons and Power Divergences in Lattice Simulations

In the final lecture I will briefly review the status of a subject which is currently very topical, not just in lattice simulations, but in phenomenological studies of QCD in general. This is the problem of renormalons<sup>50</sup>, which arises when one is interested in computing power corrections to hard scattering and decay processes. For example, in the discussion above this problem would arise if one were to compute the  $O(1/m_Q)$  corrections to the decay constant of a heavy meson. Other important examples include the evaluation of higher twist effects in deep-inelastic structure functions and the contributions of the gluon condensate to quantities which are measured in  $e^+$ - $e^-$  annihilation. The discussion in this lecture will be restricted to those processes for which an operator product expansion exists.

#### 3.1 Overview

I will now present the principal results concerning the appearance and cancellation of renormalon singularities in operator product expansions, using the Heavy Quark Expansion as an illustration. Consider the evaluation of the matrix element of some local QCD operator containing one or more heavy quark fields. We call this operator  $O^{\text{QCD}}$ . For example if we wish to evaluate the leptonic decay constant  $f_B$  as in section 2.2, then  $O^{\text{QCD}}$  would be the axial current  $\bar{b}\gamma^{\mu}\gamma^5 q$ , where q represents the field of the light quark. Using the HQET we expand  $O^{\text{QCD}}$  in inverse powers of the mass of the heavy quark  $(m_Q)$ :

$$O^{\text{QCD}} = C_1(m_Q/\mu) O_1^{\text{HQET}}(\mu) + \frac{1}{m_Q} C_2(m_Q/\mu) O_2^{\text{HQET}}(\mu) + O(1/m_Q^2)$$
(68)

where  $\mu$  is the scale at which the operators of the HQET,  $O_1^{\text{HQET}}$  and  $O_2^{\text{HQET}}$ , are renormalized. We consider here the simple situation for which there is a single operator in each of the first two orders of the expansion, but the discussion below can be easily generalized to the case in which there are more operators.

When evaluating matrix elements of  $O^{\text{QCD}}$  beyond the leading order in the  $1/m_Q$  expansion, in addition to the corresponding higher dimension operators on the r.h.s. of eq.(68), it is also necessary to keep higher order terms in the heavy quark action, i.e. by replacing the Dirac term in the QCD action by

$$\bar{Q}(i\gamma \cdot D - m_Q)Q \to \bar{h}_v(iv \cdot D)h_v + \frac{1}{2m_Q}\bar{h}_v(iD)^2h_v + \frac{c_{\text{mag}}}{2m_Q}\frac{g}{2}\bar{h}_v\sigma_{\alpha\beta}F^{\alpha\beta}h_v + O(1/m_Q^2) , \qquad (69)$$

where Q and  $h_v$  represent the fields of the heavy quark in QCD and the HQET respectively, and v is the quark's four-velocity. In the discussion below we will take the quark to be at rest, and will denote the corresponding heavy quark field by h (without any subscript).  $c_{\text{mag}}$  is a constant determined by matching the effective theory onto the full one (QCD). The corresponding constant for the kinetic term  $(\bar{h}(iD)^2h)$  is equal to one by reparametrization invariance<sup>51,18</sup>. Throughout the discussion below it is implied that the action of the HQET contains sufficiently many terms for the precision of the calculation.

In general the QCD operator  $O^{\text{QCD}}$  also requires renormalization and is defined at some scale M. Unless specifically needed I will suppress the dependence on M in  $O^{\text{QCD}}$  and in the coefficient functions  $C_i$ .

I will now summarize the main points which I wish to make in this lecture, a more detailed account can be found in ref. <sup>52,5,53</sup>:

- If we restrict the calculation to the leading order in  $1/m_Q$ , i.e. if we neglect the  $O(1/m_Q)$  terms, then the perturbation series for the coefficient function  $C_1$  diverges, and is not Borel summable. This is due to a singularity in the Borel transform of the perturbation series, called an *infra-red renormalon*. This implies that there is an ambiguity in the evaluation of  $C_1$ , coming from the different possible ways of defining the sum of the series. This ambiguity is of  $O(1/m_Q)$ .
- Formally therefore, we should not include the  $O(1/m_Q)$  corrections in eq.(68) until we have computed sufficiently many terms in the perturbation series for  $C_1$  to control its divergent behaviour.
- For this talk I will restrict the discussion to problems for which the matrix elements of  $O^{\text{QCD}}$  have no renormalon ambiguities. In general such non-

perturbative effects do exist, and appear on the right hand side of eq.(68) in the matrix elements of the operators of the HQET. They do not affect the coefficient functions.

- In renormalization schemes based on the dimensional regularization of ultraviolet divergences in the HQET, such as the  $\overline{\text{MS}}$  renormalization scheme, the matrix elements of  $O_2^{\text{HQET}}$  are also not Borel summable in perturbation theory, due to an *ultraviolet renormalon* singularity in their Borel transforms. The corresponding ambiguities in the matrix elements of  $O_2^{\text{HQET}}$  cancel those in  $C_1$ . Predictions for physical quantities cannot have any ambiguity, of course, but the matrix elements of higher-dimensional, or higher-twist, operators are, in general, not defined uniquely by the  $\overline{\text{MS}}$  procedure.
- If a hard ultraviolet cut-off is used, such as the lattice spacing in the lattice HQET, then the matrix elements of  $O_2^{\rm HQET}$  do not have ambiguities due to ultraviolet renormalons. Indeed the matrix elements can be computed (unambiguously) in lattice simulations, in contrast to those in the  $\overline{\rm MS}$  scheme, which cannot be computed directly using some non-perturbative technique. This, in turn, implies that the coefficient functions  $C_1$  do not contain ambiguities due to infra-red renormalons. In the lattice theory it is natural to present the discussion in terms of bare operators in the effective theory, defined with the lattice spacing a as the ultraviolet cut-off. I will assume here that  $m_Q a \gg 1$ . Of course if the inverse lattice spacing was much smaller than the heavy quark mass then there would be no need to use the HQET.
- The absence of renormalon ambiguities in  $C_1$  in the lattice theory is due to a cancellation between terms which, in any order of perturbation theory, are of different order in the  $1/m_Q$  expansion, i.e. between terms which behave logarithmically with  $m_Q a$  and non-leading ones of  $O(1/m_Q a)$ .
- In the lattice theory, matrix elements of higher dimensional operators (such as  $O_2^{\rm HQET}$ ) diverge as inverse powers of the lattice spacing, and are hence manifestly unphysical. For example, for the matrix element of the kinetic energy operator,

$$\langle H|\bar{h}\vec{D}^2h|H\rangle \sim O(1/a^2) \tag{70}$$

where H represents the heavy hadron. This can readily be confirmed in perturbation theory.

- The subtraction of the power divergences in perturbation theory introduces renormalon ambiguities. Thus for example, the perturbation series of the terms which diverge quadratically, i.e. those which are  $O(1/a^2)$ , in eq.(70) contains a renormalon ambiguity.
- The perturbation series for the pole mass has a renormalon ambiguity of  $O(\Lambda_{\rm QCD})^{54,55}$ . This is not the case for short-distance definitions of the heavy quark mass, such as

$$\overline{m}_Q \equiv m_Q^{\overline{\text{MS}}}(m_Q^{\overline{\text{MS}}}) \ . \tag{71}$$

• It is possible to compute  $\overline{m}_Q$  (and other short-distance definitions of the mass), using only simulations in the HQET. The quantity which is computed directly in lattice simulations is the bare binding energy,  $\mathcal{E}$  in eq.(35).  $\mathcal{E}$  is also not a physical quantity, diverging linearly with the inverse lattice spacing. It's significance can be deduced by matching QCD and the lattice formulation of the HQET, from which one finds

$$\mathcal{E} = M_P - m_{\text{pole}} + \delta m , \qquad (72)$$

where  $M_P$  is the mass of the pseudoscalar meson<sup>g</sup>,  $m_{\text{pole}}$  is the pole mass of the heavy quark, and  $\delta m$  the perturbative series of linearly divergent terms contributing to the mass renormalization in the effective theory with the action (30)<sup>56</sup>. The perturbation series for  $m_{\text{pole}}$  in terms of  $\overline{m}$ has a renormalon singularity, which is cancelled by that in  $\delta m$ . The linear divergence in  $\delta m$  cancels that in  $\mathcal{E}$ . Thus using eq.(72), the measured value of  $\mathcal{E}$  and perturbation theory, one can obtain  $\overline{m}$ . In ref.<sup>56</sup> it was found in this way that

$$\overline{m}_b = 4.17 \pm 0.05 \pm 0.03 \,\text{GeV} + O(1/m_b) \,. \tag{73}$$

• The presence of renormalons in physical quantities for which there is no Operator Product Expansion, such as the Drell-Yan process or in event shape variables in jet physics, is a subject currently under intensive investigation <sup>57,58</sup>. It is hoped that these studies will provide important phenomenological information about the sub-asymptotic (non-leading twist) behaviour of physical quantities. In lattice QCD there are analogous questions about the presence of ambiguities in perturbation series for quantities which contain power divergences, e.g. is there an ambiguity in the perturbative evaluation of the critical mass when using Wilson fermions?

<sup>&</sup>lt;sup>g</sup>Other hadronic states can also be used equally well to determine  $\overline{m}$ .

## **Final Remarks**

I hope that in these lectures I have managed to convey the exciting possibilities which lattice simulations offer for the computation of non-perturbative strong interaction effects in physical quantities. The evaluation of these quantities is important to progress in particle physics. The applications to *B*-physics which were discussed in the secong lecture, are only a small subset of the phenomelogically relevant quantities which are being computed using "on the lattice" (see for example refs.<sup>1,2,3</sup>). At the same time I have tried to explain the difficulties which remain, of which a reliable formalism and algorithms for the inclusion of light quark loops is, mot probably, the most significant.

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