Introduction to Lattice QCD

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LHCb UK Student Talk

26 March 2020





DEPARTMENT OF MATHEMATICS AND COMPUTER SCIENCE

# Thanks to the organisers for making this possible despite the current situation!

This is...

- my first remote talk
- my first remote audience
- ...so please bare with me.

This is intended to be an <u>accessible introduction</u> - please interrupt and ask questions!

# Outline

#### Motivation

- 2 Setting up Lattice QCD (QFT)
- 3 Challenges in *b*-physics on the lattice
- Example of a Lattice QCD computation (arXiv:1812.08791)
- Status of the field
- 6 Jargon, Literature and Summary

## Section 1

#### Motivation

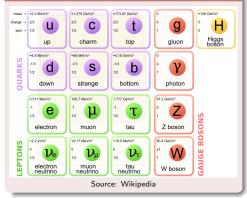
J Tobias Tsang (CP<sup>3</sup>-Origins, SDU) Introduction to Lattice QCD

## Motivation

The SM is very successful, but...

- Matter/Antimatter asymmetry?
- Why hierarchy of masses?
- Why three generations?
- What is dark matter?
- What is dark energy?
- $\cdots$  not the end of the story!

#### The Standard Model

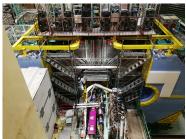


 $\Rightarrow$  Search for New Physics!

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# Search for new physics: (Flavour) Experiments

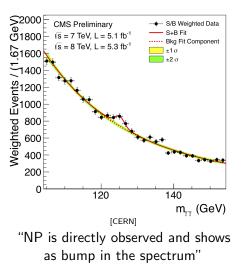




*top*: LHCb at LHC, CERN *left*: Belle II at SuperKEKb, KEK

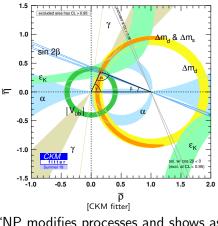
- $\Rightarrow$  Huge experimental efforts!
  - + BESIII and other LHC experiments
- $\Rightarrow$  *B*-factory vs <u>hadron machine</u>
  - "Old" data from BaBar, Belle, Cleo, ...

#### How can we see New Physics?



#### Direct searches

Indirect searches



"NP modifies processes and shows as discrepancy between Exp and The"

# (quark) flavour physics: CKM matrix

#### $experiment \approx \mathrm{CKM} \times nonperturbative \times \mathrm{known} \ \mathrm{factors}$

#### CKM Matrix

- when quarks change flavour
- 3 generations

$$V = egin{pmatrix} V_{ud} & V_{us} & V_{ub} \ V_{cd} & V_{cs} & V_{cb} \ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$$

• in the SM: unitary  $VV^{\dagger} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ 

# (quark) flavour physics: CKM matrix

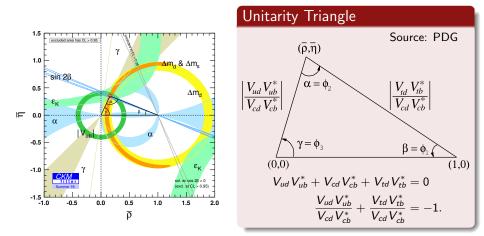
#### $experiment \approx \mathrm{CKM} \times nonperturbative \times \mathrm{known} \ \mathrm{factors}$

CKM Matrix	Unitarity Triangle
<ul> <li>when quarks change flavour</li> </ul>	(ō m) Source: PDG
• 3 generations	(ρ,η)
$V = egin{pmatrix} V_{ud} & V_{us} & V_{ub} \ V_{cd} & V_{cs} & V_{cb} \ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$	$\left  \frac{V_{ud} V_{ub}^*}{V_{cd} V_{cb}^*} \right  \qquad $
in the SM: unitary	$(0,0) \qquad \beta = \phi_1 \qquad (1,0)$
$VV^{\dagger} = egin{pmatrix} 1 & 0 & 0 \ 0 & 1 & 0 \ 0 & 0 & 1 \end{pmatrix}$	$egin{aligned} V_{ud}  V_{ub}^* + V_{cd}  V_{cb}^* + V_{td}  V_{tb}^* &= 0 \ & rac{V_{ud}  V_{ub}^*}{V_{cd}  V_{cb}^*} + rac{V_{td}  V_{tb}^*}{V_{cd}  V_{cb}^*} &= -1. \end{aligned}$

 $\Rightarrow$  Determine CKM matrix elements from many different processes

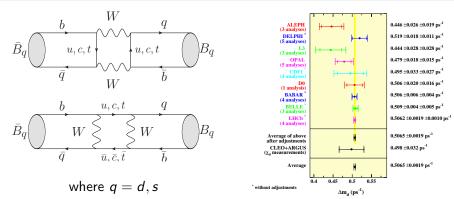
# (quark) flavour physics: CKM matrix

 $experiment \approx \mathrm{CKM} \times nonperturbative \times \mathrm{known} \ \mathrm{factors}$ 



 $\Rightarrow$  Determine CKM matrix elements from many different processes

# Example: Neutral $B_{(s)}$ meson mixing

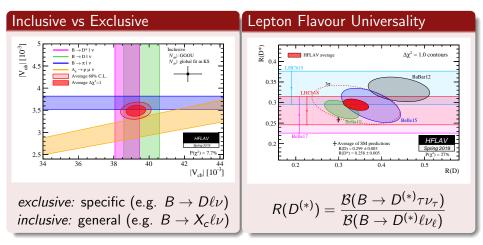


Neutral mesons oscillate: Mass eigenstate  $\neq$  flavour eigenstate  $\Delta m_d = 0.5065(19) {
m ps}^{-1}$  $\Delta m_s = 17.757(21) {
m ps}^{-1}$  [HFLAV]

#### below percent level

 $\Delta m_q \propto |V_{tb}^* V_{tq}| \times \text{nonperturbative} \times \text{known factors}$ 

## Indirect searches: tensions?



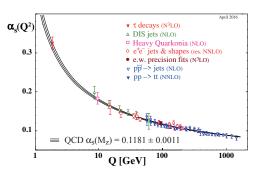
Most stringent test if **EXP and THEO uncertainties are comparable**!

 $\Rightarrow$  More experimental data soon - need to sharpen theory predictions!

#### Section 2

### Setting up Lattice QCD (QFT)

# Theory predictions for non-perturbative physics



At *low energy scales*: perturbative methods <u>fail</u>. Require non-perturbative methods, e.g.

- Effective theories
- 'AdS/CFT-like' correspondences
- Sum rules
- Lattice QFT



- Lattice QCD simulations provide first principle precision predictions for phenomenology
- Calculations need to be improved for observables where the error is dominated by **non-perturbative physics**...

#### Formulating LQCD I: Minkowski to Euclidean

Recall the Path Integral in Minkowski space-time

$$\mathcal{Z} = \int \mathcal{D}[\psi, \bar{\psi}] \mathcal{D}[U] e^{i \left(S_G[U] + S_F[\psi, \bar{\psi}, U]\right)}$$
$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi, \bar{\psi}] \mathcal{D}[U] \mathcal{O}[\psi, \bar{\psi}, U] e^{i \left(S_G[U] + S_F[\psi, \bar{\psi}, U]\right)}$$

Highly oscillatory, infinite dimensional integral...

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Highly oscillatory, infinite dimensional integral...  $\Rightarrow$  Wick rotating to Euclidean (i.e. imaginary) time  $(t \rightarrow i\tau)$ ...

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$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi, \bar{\psi}] \mathcal{D}[U] \mathcal{O}[\psi, \bar{\psi}, U] e^{-(S_G[U] + S_F[\psi, \bar{\psi}, U])}$$

Exponentially decaying, infinite dimensional integral...

# Formulating LQCD II: Interpretation as a probability weight

Abusing notation<sup>1</sup>, we write the fermion action as

$$S_{F}[\psi,\overline{\psi},U] = \int \mathrm{d}^{4}x \sum_{f=1}^{N_{f}} \overline{\psi} D_{f}[U] \psi$$

 $\mathcal{S}_{\mathcal{F}}$  is quadratic in the fields and  $\psi,\overline{\psi}$  are Grassmannian, so

$$\int \mathcal{D}[\psi,\bar{\psi}]e^{-\int \mathrm{d}^4 x \overline{\psi}(D_f[U])\psi} = \det\left(D_f[U]\right)$$

Now

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}[\psi, \bar{\psi}] \, \mathcal{D}[U] \, e^{-\left(S_G[U] + S_F[\psi, \bar{\psi}, U]\right)} \\ &= \int \mathcal{D}[U] \, \left[\prod_{n=1}^{N_f} \det\left(D_f[U]\right)\right] e^{-S_G[U]} \end{aligned}$$

<sup>1</sup>Dirac operator for flavour f:  $D_f = \gamma_\mu D_\mu + m_f$  where  $D_\mu$  is the covariant derivative

# Formulating LQCD II: Interpretation as a probability weight

$$\mathcal{Z} = \int \mathcal{D}[U] \underbrace{\left[\prod_{n=1}^{N_f} \det\left(D_f[U]\right)\right] e^{-S_G[U]}}_{\text{probability weight}}$$

Assuming  $\left|\prod_{n=1}^{N_f} \det(D_f[U])\right| > 0$  we can interpret this as a **probability** weight and sample this probability distribution.<sup>2</sup>

- A collection of *configurations* which samples this probability distribution is called an *ensemble*.
- Neglecting the fermionic vacuum bubbles (determinant factors in Z) is called the *quenched approximation*.
- Accounting for fermionic vacuum bubbles from two, mass-degenerate flavours only, i.e. det  $D_u = \det D_d \equiv \det D_l$  is called " $N_f = 2$ ".

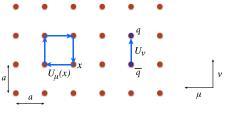
<sup>2</sup>Assuming  $\gamma_5$  hermiticity ( $\gamma_5 D \gamma_5 = D^{\dagger}$ ) we can show that det D is real (det  $D^* = \det D^{\dagger} = \det \gamma_5 D \gamma_5 = \det D$ )

# Formulating LQCD III: Make finite dimensional

We still have the issue of an infinite dimensional integral...

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi, \bar{\psi}] \mathcal{D}[U] \mathcal{O}[\psi, \overline{\psi}, U] e^{-\left[S_{\mathcal{G}}[U] + S_{\mathcal{F}}[\psi, \bar{\psi}, U]\right]}$$

Now we introduce the lattice for make the PI finite dimensional:



- Finite lattice spacing a
   ⇒ UV regulator
- Finite Box of length  $L^3 \times T$  $\Rightarrow$  IR regulator
- $\int \rightarrow \sum$ ,  $\partial \rightarrow$ finite differences
- Choose boundary conditions.

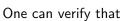
PDG

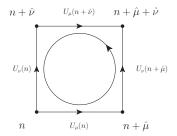
#### $\Rightarrow$ The Path Integral is now (large but) <u>finite dimensional</u>.

 $\Rightarrow$  Need to discretise the action ( $S_G$  and  $S_F$ ) and any operators  $\mathcal{O}_{\cdots}$ 

## Formulating LQCD IVa: Discretising the gauge action

- Gauge fields A<sub>μ</sub> enter through link variables, i.e. U<sub>μ</sub>(n) is on the link from n to n + μ̂. They are related to the gauge field by U<sub>μ</sub>(n) = e<sup>iaA<sub>μ</sub>(n)</sup>.
- A plaquette U<sub>μν</sub>(n) is the oriented product of link-fields as depicted to the right.





$$\begin{split} S_G[A] &= \frac{1}{2g^2} \int \mathrm{d}^4 x \operatorname{tr} \left( F_{\mu\nu}(x) F_{\mu\nu}(x) \right) \\ &= \frac{a^4}{2g^2} \left( \sum_{n \in \Lambda} \sum_{\mu < \nu} \mathcal{R} \left[ \operatorname{tr} \left( \mathbbm{1} - U_{\mu\nu}(n) \right) \right] + O(a^2) \right) \end{split}$$

This reproduces the correct **<u>continuum limit</u>**, i.e. behaviour as  $a \rightarrow 0$ .

• When naively discretising the Dirac operator, the propagator has  $2^4 = 16$  poles, i.e. 16 copies of the desired particle ("doublers")

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Note: We are free to add higher dimensional operators to the action by multiplying the appropriate powers of *a*.

$$S_{\mathrm{eff}} = a^4 \sum_{x} \left[ \mathcal{L}_0(x) + a \mathcal{L}_1(x) + a^2 \mathcal{L}_2(x) + \cdots \right]$$

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- Adding a dimension-5 operator, called the Wilson term, adds a mass x <sup>2</sup>/<sub>a</sub> to the unwanted poles, i.e. they disappear in the continuum limit. ⇒ simulate single fermion of mass m!
- but this term explicitly breaks chiral symmetry...

## ASIDE: Lattice QCD and chiral symmetry

... this turns out to be more than just bad luck:

The **Nielsen-Ninomiya theorem** states that it is impossible to simultaneously achieve

- a doubler free theory
- an ultra-local theory
- Chiral symmetry ( $\gamma_5 D = D\gamma_5$ )
- the correct continuum limit

Overcome by modifying the above to the Ginsparg-Wilson equation

$$D\gamma_5 + \gamma_5 D = aD\gamma_5 D$$

i.e. replacing  $\gamma_5$  by  $\hat{\gamma}_5 = \gamma_5(\mathbb{1} - aD)$ .

So one has to make a choice about the fermion action - MANY choices:

- Naive Wilson fermions (have doublers)
- Wilson-like fermions (no chiral symmetry)
- Ginsparg-Wilson-type fermions: Overlap, Domain Wall (not ultra-local)
- Staggered (involves rooting of the determinant, so not-local)
- Many more choices, e.g. inspired by effective theories to solve particular problems: NRQCD (non-relativistic QCD), HQET, static quarks, relativistic heavy quarks (RHQ), ···

*"Improvement"*: one can tune and add higher dimensional operators to cancel the leading discretisation effects by smartly choosing terms in

$$S_{ ext{eff}} = a^4 \sum_{x} \left[ \mathcal{L}_0(x) + a \mathcal{L}_1(x) + a^2 \mathcal{L}_2(x) + \cdots \right]$$

 $\Rightarrow$  **UNIVERSALITY**: physical predictions need to agree in the CL.

# Formulating LQCD V: Correlation functions

Operators induce <u>all states</u> with the correct **quantum numbers**:

$$\begin{split} \frac{1}{Z} \int \mathcal{D}[U] \prod_{n=1}^{N_f} \det\left(D_f[U]\right) \, e^{-S_G[U]} \sum_{\mathbf{x}} \operatorname{tr}\left(\left[\gamma_5 S_d(\mathbf{0}, 0 | \mathbf{x}, t)\gamma_5 S_u(\mathbf{x}, t | \mathbf{0}, 0)\right]\right) \\ &= \frac{1}{Z} \int \mathcal{D}[U] \prod_{n=1}^{N_f} \det\left(D_f[U]\right) e^{-S_G[U]} \sum_{\mathbf{x}} \overline{u}(\mathbf{x}, t)\gamma_5 \overline{d}(\mathbf{x}, t) \overline{d}(\mathbf{0}, 0)\gamma_5 u(\mathbf{0}, 0) \\ &= C_2(t)|_{\mathbf{p}=0} = \sum_{\mathbf{x}} \left\langle 0 \right| \mathcal{T}[\overline{u}\gamma_5 d](\mathbf{x}, t) \, [\overline{d}\gamma_5 u]^{\dagger}(\mathbf{0}, 0) \left| 0 \right\rangle \\ &= \sum_{\mathbf{x}} \sum_n \frac{1}{2m_n} \left\langle 0 \right| [\overline{d}\gamma_5 u](\mathbf{x}, t) \left| n \right\rangle \left\langle n \right| [\overline{d}\gamma_5 u]^{\dagger}(\mathbf{0}, 0) \left| 0 \right\rangle \\ &= \sum_n \sum_{\mathbf{x}} \frac{1}{2m_n} \left\langle 0 \right| e^{Ht} [\overline{d}\gamma_5 u](\mathbf{0}, 0) e^{-Ht} \left| n \right\rangle \left\langle n \right| [\overline{d}\gamma_5 u]^{\dagger}(\mathbf{0}, 0) \left| 0 \right\rangle \\ &= \sum_n \frac{1}{2m_n} \left| \left\langle 0 \right| \overline{d}\gamma_5 u \left| n(\mathbf{p} = \mathbf{0}) \right\rangle \right|^2 e^{-m_n t} \end{split}$$

- We compute and contract the propagators S on each configuration.
- We extract masses and matrix elements by fitting to the last line.

A lattice QCD computation starts from **first principles**, i.e. the **action**. So the parameters that are *inputs* to a lattice QCD computation are the bare **coupling constant** g and the bare **quark masses**  $m_f$ .

$$\begin{split} S_{\rm QCD}[\psi,\overline{\psi},U] &= S_G[U] + S_F[\psi,\overline{\psi},U] \\ &= \int d^4x \, \frac{1}{2g^2} {\rm Tr} \left[F_{\mu\nu}F_{\mu\nu}\right] + \sum_{N_f} \overline{\psi}_f \left(\gamma_\mu D_\mu + m_f\right) \psi_f \end{split}$$

So we <u>do not know the lattice spacing of the quark masses a priori</u>, these are determined from the scale-setting. To make contact with "the real world", we need to sacrifice as many predictions as we have parameters.

### EXAMPLE: scale setting (rough idea)

Consider a (set of)  $N_f = 2 + 1$  ensemble(s).

- need to determine 3 parameters:  $m_l (= m_u = m_d)$ ,  $m_s$  and a
- need to sacrifice 3 predictions: e.g.  $m_{\pi}$ ,  $m_K$  and  $m_{\Omega}$

Note that the output of a lattice computation is always dimensionless, i.e. we only obtain numbers such as  $am_{\pi}$  from the simulation.

**1** Vary the quark masses  $m_l$  and  $m_s$  until

$$\left(rac{am_{\pi}}{am_{\Omega}}
ight)_{
m lat} \equiv \left(rac{m_{\pi}}{m_{\Omega}}
ight)_{
m PDG} \qquad ext{and} \qquad \left(rac{am_{K}}{am_{\Omega}}
ight)_{
m lat} \equiv \left(rac{m_{K}}{m_{\Omega}}
ight)_{
m PDG}$$

2 Require  $(m_{\Omega})_{\text{lat}} = (m_{\Omega})_{\text{PDG}}$ , i.e.

$$a^{-1} = rac{(m_\Omega)_{
m PDG}}{(am_\Omega)_{
m lat}}$$

# Size of the numerical problem

Using  $N_{\rm spin} = 4$ ,  $N_{\rm colour} = 3$  and defining  $|\Lambda| = (X/a)^3 \times (T/a)$ 

- Gauge fields  $\rightarrow$  *link variables*  $U_{\mu}(n)$ : SU(3) matrix linking sites:  $9 \times |\Lambda|$  complex entries.
- Fermion fields turn vectors of size  $4\times 3\times |\Lambda|$
- Operators  $\rightarrow$  matrices. E.g. Dirac operator:  $(4 \times 3 \times |\Lambda|)^2$  entries.



(former) BG/Q in Edinburgh

**Small volume** : L = 16a, T = 32a :  $2.5 \times 10^{12}$  entries **State of the art** : L = 96a, T = 196a :  $4.2 \times 10^{18}$  entries

Propagators are the inverse of the Dirac operator...

...clearly not possible to do by hand or on your laptop

# A Lattice Computation

Lattice vs Continuum			
We simulate:	We want:		
<ul> <li>at finite lattice spacing a</li> </ul>	• <i>a</i> = 0		
• in finite volume $L^3$	• $L = \infty$		
<ul> <li>lattice regularised</li> </ul>	<ul> <li>some continuum scheme</li> </ul>		
<ul> <li>Some bare input quark masses</li> </ul>	• $m_l = m_l^{\rm phys}$		
am <sub>l</sub> , am <sub>s</sub> , am <sub>h</sub>	• $m_s = m_s^{\rm phys}$		
In general: $m_\pi  eq m_\pi^{ m phys}$	• $m_h=m_c^{ m phys}, m_b^{ m phys}$		
Need to control all Particle			

 $\Rightarrow$  Need to control all limits!

 $\rightarrow$  particularly simultaneously control FV and discretisation  $\Rightarrow$  Decide on a fermion action (suitable to your problem): Wilson, Staggered, Twisted Mass, **Domain Wall fermions**,  $\cdots$ 

#### Section 3

#### Challenges in *b*-physics on the lattice

#### Multiple scale problem on the lattice: back of the envelope

Control effects of IR (finite volume) and UV (discretisation) regulators:

$$m_{\pi}L \gtrsim 4$$
  $a^{-1} \gg$  Mass scale of interest  
 $\bullet \bullet \bullet \star \bullet \bullet$   
 $10^0 \ 10^1 \ 10^2 \ 10^3 \ 10^4 \ 10^5 \ 10^6$   
 $m_q [\text{MeV}]$ 

For  $m_{\pi} = m_{\pi}^{\mathrm{phys}} \sim 140 \,\mathrm{MeV}$  and  $\overline{m_b}(m_b) \approx 4.2 \,\mathrm{GeV}$ :

 $L \gtrsim 5.6 \, {\rm fm}$   $a^{-1} \gg 4.2 \, {\rm GeV} \approx (0.05 \, {\rm fm})^{-1}$ 

Requires  $N \equiv L/a \gg 120 \Rightarrow N^3 \times (2N) \gg 4 \times 10^8$  lattice sites.

**VERY EXPENSIVE** to satisfy both constraints simultaneously... ... needs to be repeated for different values of *a*.

## How to simulate the *b*-quark?

For now choose between:

Effective action for b • Can tune to m <sub>b</sub> • comes with systematic which are hard to estimate/reduce	tic errors	<ul> <li>e Theoretically cleaner and systematically improvable</li> <li>e Need to control extrapolation in heavy quark mass</li> </ul>		
Different properties:				
<ul> <li>computational cost</li> </ul>	• tuning erro	rs • cut off effects		
<ul> <li>chirality</li> </ul>	systematic	errors • renormalisation		

#### How to simulate the *b*-quark?

For now choose between:

Effective action for b		Relativistic action for b		
<ul> <li>Can tune to m<sub>b</sub></li> <li>comes with systematic which are hard to estimate/reduce</li> </ul>	tic errors	<ul> <li>Theoretically cleaner and systematically improvable</li> <li>Need to control extrapolation in heavy quark mass</li> </ul>	on	
Different properties:				
<ul> <li>computational cost</li> </ul>	• tuning e	errors • cut off effects		
<ul> <li>chirality</li> </ul>	systema	atic errors • renormalisation		

#### BUT SOON:

Huge efforts in the community to produce very fine lattice spacings:

 $\Rightarrow$  Direct simulation of  $\approx m_b^{\rm phys}$  will become possible!

#### Signal-to-noise estimates

- The signal decays with the lowest lying energy in the spectrum:  $e^{-E_0t}$ .
- The variance decays with the lightest combination of states with the correct quantum numbers that can be built from the square of the operator. The noise (statistical error) is the square root of the variance.

#### Signal-to-noise estimates

- The signal decays with the lowest lying energy in the spectrum:  $e^{-E_0t}$ .
- The variance decays with the lightest combination of states with the correct quantum numbers that can be built from the square of the operator. The noise (statistical error) is the square root of the variance.

Consider a *B* meson, i.e.  $\mathcal{O} = \overline{b}\gamma_5 u$ : From the "square" of the operator we can build two *B*-mesons or a  $\pi$  and a  $\eta_b$ . From the PDG we find:

 $m_{\pi} \approx 0.140 \,\mathrm{GeV}$   $m_B \approx 5.3 \,\mathrm{GeV}$   $m_{\eta_b} \approx 9.4 \,\mathrm{GeV}$ 

So  $(m_{\pi} + m_{\eta_b})/2 \approx 4.77 \,\mathrm{GeV} \approx 0.9 m_B$ 

 $\Rightarrow$  The noise decays slower than the signal.

 $\Rightarrow$  The noise-to-signal ratio grows exponentially with  $e^{+0.1m_Bt}$ 

## Signal extraction and excited state contamination

Assume you have an operator O that induces a ground state  $|P_0\rangle$  with energy  $m_0$  and first excited state  $|P_1\rangle$  with energy  $m_1$ .

$$C(t) = \sum_{n} \frac{|\langle 0|\mathcal{O}|n\rangle|^2}{2E_n} e^{-E_n t}$$
  
$$\approx \frac{|\langle 0|\mathcal{O}|P_0\rangle|^2}{2E_0} e^{-E_0 t} \times \left(1 + \frac{E_0}{E_1} \frac{|\langle 0|\mathcal{O}|P_1\rangle|^2}{|\langle 0|\mathcal{O}|P_0\rangle|^2} e^{-(E_1 - E_0)t}\right)$$

For heavy mesons there are many excited states which might lie close together making it hard to unambiguously isolate the ground state.  $\Rightarrow$  Can only extract the ground state at "late times", i.e. fit for larger values of *t*.

⇒ BUT Signal-to-noise problem from above!

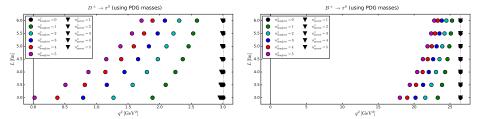
# Semi-leptonic decays I: $q^2$ -coverage

$$rac{d\Gamma(P
ightarrow D\ell 
u_\ell)}{dq^2}pprox \left|V_{q_2q_1}
ight|^2 imes \left[\left|f_+(q^2)
ight|^2\mathcal{K}_1+\left|f_0(q^2)
ight|^2\mathcal{K}_2
ight]$$

For a semi-leptonic decay we are interested in  $f(q^2)$  for

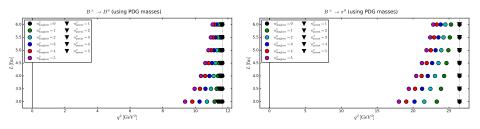
$$q^2 = (E_P - E_D)^2 - (\mathbf{p}_P - \mathbf{p}_D)^2 \in [0, (m_P - m_D)^2]$$

In a finite volume, momenta are discretised:  $\mathbf{p} = \frac{2\pi}{L} (n_x, n_y, n_z)$ .



# Semi-leptonic decays II: q<sup>2</sup>-coverage

$$q^2 = (E_P - E_D)^2 - (\mathbf{p}_P - \mathbf{p}_D)^2 \in [0, (m_P - m_D)^2]$$



- Lattice is easiest near  $q_{\max}^2$ , experiment easiest near  $q^2 = 0$ .
- Covering  $q^2$  becomes harder as
  - $m_P m_D$  becomes larger
  - $m_P, m_D$  become heavier  $(E \approx m)$
  - Volume increases (but large V needed for physical pions...)
- Noise increases as  $n^2 = n_x^2 + n + y^2 + n_z^2$  increases.
- Discretisation errors increase as *n*<sup>2</sup> increases.

Section 4

# Example of a Lattice QCD computation (arXiv:1812.08791)

# Work-flow of a Lattice QCD computation

- Settle on the desired ensemble properties (number of flavours in the sea, fermion discretisation, gauge discretisation).
- Generate multiple gauge ensembles for desired choices of  $(a^{-1}, V, m_q)$  to allow for all necessary inter/extrapolations.
  - "Set the scale", i.e. determine parameters of your ensemble (lattice spacing and quark masses).
- Settle on a measurement strategy (valence quark masses, valence fermion actions, included operators and currents, source types and positions, contractions).
- Generate correlation functions and extract observables (masses, energies, matrix elements) from them.
- § Extrapolate data to the "physical point", i.e.  $a o 0, \ V o \infty, \ m_q o m_q^{\rm phys}, \ \ldots$
- Full statistical and systematic error analysis.

# Example of a Lattice QCD computation (arXiv:1812.08791)

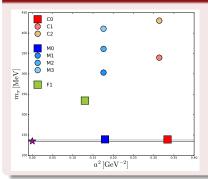
[1812.08791]

Edinburgh - Southampton - Boulder - BNL (RBC/UKQCD)

Peter Boyle, Luigi Del Debbio, Nicolas Garron, Andreas Jüttner, Amarjit Soni, JTT, Oliver Witzel

# EXAMPLE - Steps 1-3: RBC/UKQCD's ensembles

#### ensembles (steps 1 and 2)

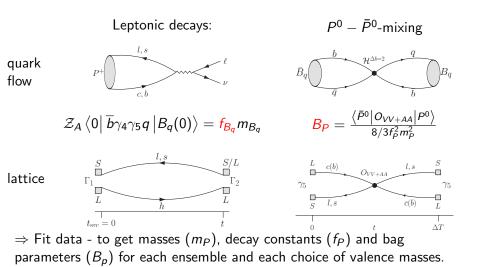


- $N_f = 2 + 1$
- Iwasaki gauge action
- Domain Wall Fermion action
- 2 ensembles with physical pion masses [PRD 93 (2016) 074505]
- 3 Lattice spacings [JHEP 12 (2017) 008]
- Heavier  $m_{\pi}$  ensembles guide small chiral extrapolation of F1

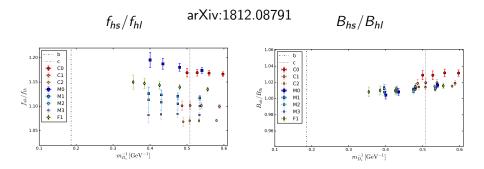
#### measurement strategy (steps 3) - arXiv:1812.08791

- Keep light and strange quark like in the sea
- Simulate multiple c(b)-like quarks with suitably chosen DWFs
- Decide to measure decay constants and  $B_{(s)} \bar{B}_{(s)}$  mixing

#### EXAMPLE - Steps 4: Correlators - arXiv:1812.08791



#### EXAMPLE - Steps 5: back to the continuum



#### Data from correlator fits

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#### EXAMPLE - Steps 5: back to the continuum

arXiv:1812.08791  $f_{hs}/f_{hl}$  $B_{hs}/B_{hl}$ 1.20 1.02 1.01  $B_{sh}/B_{lh}$  $f_{sh}/f_{lh}$  $B_{B_c}/B$  $f_R/f_1$ 1.1 0.99 0.98 1.05 0.97 0.96 0.1 0.5  $m_{D_{\star}}^{-1}$  [GeV<sup>-1</sup>]  $m_{D_{*}}^{-1}$  [GeV<sup>-1</sup>]

Global fit to  $m_{\pi}$ , a and  $m_H$  behaviour

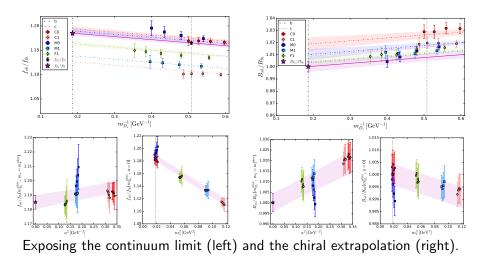
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#### EXAMPLE - Steps 5: back to the continuum

 $f_{hs}/f_{hl}$ 

arXiv:1812.08791

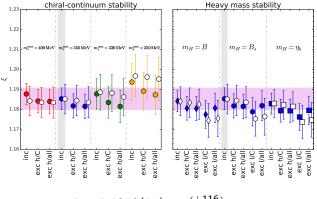
 $B_{hs}/B_{hl}$ 



Introduction to Lattice QCD

## EXAMPLE - Steps 6: Error budget I (1812.04981)

- Global fits all correlated with satisfying *p*-values.
- sys error: includes chiral-CL (left), heavy mass (right), H.O. terms,  $m_u \neq m_d$  and FV.



$$\xi = 1.1853(54)_{\text{stat}} \begin{pmatrix} +116\\ -156 \end{pmatrix}_{\text{sys}}$$

# EXAMPLE - step 6: Error budget II (1812.04981)

Experimental precision on  $\Delta m_s \sim 0.1\%$  and  $\Delta m_d \sim 0.4\%$ . Theoretical precision on  $\xi \sim 1.3\%$ 

	$f_{D_s}/f_D$		$f_{B_s}/f_B$		ξ		$B_{B_s}/B_{B_d}$	
	absolute	relative	absolute	relative	absolute	relative	absolute	relative
central	1.1652		1.1852		1.1853		1.0002	
stat	0.0035	0.30%	0.0048	0.40%	0.0054	0.46%	0.0043	0.43%
fit chiral-CL	$+0.0112 \\ -0.0031$	$^{+0.96}_{-0.26}$ %	$^{+0.0110}_{-0.0045}$	$^{+0.93}_{-0.38}\%$	+0.0084 -0.0038	$^{+0.71}_{-0.32}$ %	+0.0020 -0.0044	$^{+0.20}_{-0.44}\%$
fit heavy mass	$^{+0.0003}_{-0.0000}$	$^{+0.02}_{-0.00}\%$	$^{+0.0000}_{-0.0081}$	$^{+0.00}_{-0.69}\%$	$^{+0.0000}_{-0.0091}$	$^{+0.00}_{-0.77}\%$	$^{+0.0012}_{-0.0031}$	$^{+0.12}_{-0.31}\%$
H.O. heavy	0.0000	0.00%	0.0054	0.45%	0.0049	0.41%	0.0021	0.21%
H.O. disc.	0.0009	0.07%	0.0009	0.07%	0.0021	0.18%	0.0016	0.16%
$m_u \neq m_d$	0.0009	0.08%	0.0009	0.07%	0.0010	0.08%	0.0001	0.01%
finite size	0.0021	0.18%	0.0021	0.18%	0.0021	0.18%	0.0018	0.18%
total systematic	+0.0114 -0.0039	+0.98 % -0.34 %	+0.0125 -0.0137	$^{+1.06}_{-1.16}\%$	+0.0102 -0.0146	+0.86 % -1.24	+0.0041 -0.0070	$^{+0.41}_{-0.70}\%$
total sys+stat	$^{+0.0120}_{-0.0052}$	$^{+1.03}_{-0.45}\%$	$^{+0.0134}_{-0.0145}$	$^{+1.13}_{-1.22}\%$	$^{+0.0116}_{-0.0156}$	$^{+0.97}_{-1.32}\%$	$^{+0.0060}_{-0.0082}$	$^{+0.60}_{-0.82}\%$

 $\Rightarrow$  Systematically Improvable with finer lattices at (near) physical  $m_{\pi}$ .

#### Section 5

#### Status of the field

## What we can do well

I.e. full calculations from multiple groups and different formulations.

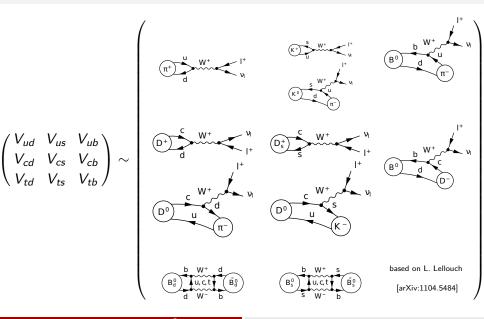
- $m_q 
  ightarrow m_q^{
  m phys}$ , e.g. "chiral extrapolation"
- $a \rightarrow 0$ , i.e. the continuum limit has been taken
- $V 
  ightarrow \infty$ , i.e. infinite volume limit has been taken or accounted for

#### mature calculations

(Mostly) single hadron "stable states", mostly mesons

- Quark masses
- Spectrum i.e. extracting masses and energies
- Leptonic decay constants ( $f_{\pi}$ ,  $f_{K}$ ,  $f_{D_s}$ ,  $f_{B_s}$ , ...)
- ullet Semi-leptonic form factors (mostly PS final state) near  $q^2_{\rm max}$
- Short-distance matrix elements of OPE's (e.g.  $B_{(s)} \overline{B}_{(s)}$  mixing).
- Determination of LECs (we often simulate at  $m_\pi > m_\pi^{
  m phys})$

#### What we can do well



J Tobias Tsang (CP<sup>3</sup>-Origins, SDU)

Introduction to Lattice QCD

## Some more things we can do

#### advanced or advancing, but fewer complete calculations

- Hadronic vacuum polarisation (g-2)
- Scattering of <u>two</u> hadrons in the final state mature field but costly:  $\Rightarrow$  Information is gained from FV  $\Rightarrow$  many volumes  $\equiv$  \$£ $\in$ ...
- Possible to use this to treat vector final states, i.e. B → K<sup>\*</sup>(→ Kπ), but only if decays to only 2 hadrons
- Including isospin breaking effect into simulations:
  - $m_u \neq m_d$
  - $\alpha_{QED} \neq 0$
- baryons (signal to noise problems)
- Hadronic light-by-light scattering
- Testing strongly coupled BSM theories (e.g. composite Higgs)

# Many more topics

#### "Lattice" is a <u>BIG FIELD</u> with many topics I have not touched upon...

LATTIC The 38th International Symposium on Lattice Field Theory (Lattice 2020)									
3-8 August 2020 Hörsaalzentrum Poppelsdorf GropeBerin Imezore									
Overview Important dates   deadlines	The International Symposium on Lattice Field Theory is an annual conference that attracts scientists from around the world. Originally started as a place for physicists to discuss their recent								
Travel and Transportation	developments in lattice gauge theory, nowadays the conference is the largest of its type and has grown to include areas like algorithms and machine architectures, code development, chiral symmetry, physics beyond the standard model, and strongly interacting phenomena in low- dimensions.								
Venue Financial Support Registration Information	The 38th Lattice conference will take place in Bonn, Germany, from August 3 to August 8 2020. The scientific programme of this conference will include planary talks and parallel sessions on the following topics:								
Conditions Conditions Conference Registration Indico Registration	Algorithms and Machines     Applications Beyond QCD     Oriral Symmetry								
Call for Abstracts Excursions	Hadron Spectroscopy and Interactions     Hadron Succurve     GCD at nonzero Temperature and Density								
Cologne - cathedral and old town	Physics Beyond the Standard Model     Standard Model Parameters and Renormalisation     Theoretical Developments     Vacuum Structure and Confinement								
Lava-Dome Mendig and Volcano Nuseum	vacuum suructure and commernen     vacuum suructure and commernen     vacuum suructure and commernen     Code Development								

- Algorithms and Machines
- Applications Beyond QCD
- Chiral Symmetry
- Hadron Spectroscopy and Interactions
- Hadron Structure
- QCD at nonzero Temperature and Density
- Physics Beyond the Standard Model
- Standard Model Parameters and Renormalisation
- Theoretical Developments
- Vacuum Structure and Confinement
- Weak Decays and Matrix Elements
- Code Development

Relevant for particle physicists (theorists, phenomenologists and experimentalist) but also computer science, applied mathematics, algorithm developments, high performance computing, statistics, statistical mechanics, condensed matter,...

## Section 6

## Jargon, Literature and Summary

37 / 42 J Tobias Tsang (CP<sup>3</sup>-Origins, SDU)

Introduction to Lattice QCD

## Literature I: Text books and lecture notes

Many great lecture notes and textbooks - some examples below:

- "Quantum Chromodynamics on the Lattice: An Introductory Presentation" - Gattringer and Lang, 2010
- "*Lattice methods for quantum chromodynamics*" DeGrand and Detar, 2006
- "Quarks, gluons and lattices", M. Creutz, 1985.
- "Modern perspectives in lattice QCD: Quantum field theory and high performance computing" - L. Lellouch, R. Sommer, B. Svetitsky, A. Vladikas and L. F. Cugliandolo, eds., proceedings for Les Houches Summer School in Theoretical Physics 2009) (many chapters on the arXiv)
- hep-lat/9802029 and references within (Advanced lattice QCD M, Luescher) (Part of the proceedings for Les Houches Summer School in Theoretical Physics 1997)

# Literature II: FLAG - Flavour Lattice Averaging Group

Vest and Vest

Navigation

In any (research) community it is hard to assess results from the outside.

The Flavour Lattice Averaging Group (FLAG) aims to

- Summarise lattice results
- Assess their quality
- Provide averages of different results

The 201	G Re		
Figures for version	The 2019 edition of version can be obt		

FLAG Review 2019

The 2019 edition of the FLAG review can be downloaded here. The version dated March 4, 2020 is the one accepted for publication in EPUC. The EPUC version can be obtained from here. The separate sections can be downloaded as separate pdf rifes following the links in the table of contents below, or via the menu in the sidebar. Clicking

The latest figures can be downloaded in eps, pdf and png format, together with a bib-file containing the bibter-entries for the calculations which contribute to the FLAG averages and estimates. The downloads are available via the meru in the sidebar.

In the notes we compile detailed information on the simulations used to calculate the quantities discussed in the review. Here we provide the complete tables, in contrast to the paper version of the review which contains this information only for results that have appeared since FLAG 16.

The original complete 2015/2016 review is still accessible from EPJC. The 2016/2017 updates are available from here. The 2013/2014 review is accessible here or from EPJC.

Contents
1. Introduction
1. FLAG composition, guidelines and rules
2. Citation policy
3. General issues
4. References
2. Quality criteria
3. Quark masses
4. V <sub>id</sub> and V <sub>in</sub>
5. Low-energy constants
6. Kaon mixing
7. D-meson decay constants and form factors
8. B-meson decay constants, mixing parameters, and form factors
9. The strong coupling $\alpha_s$
10. Nucleon matrix elements
11. Glossary
12. Notes

on the FLAG logo in the upper left corner links back to this main pape.

#### FLAG-webpage

 $\Rightarrow$  This is a very useful and handy tool, BUT...

...please cite the original papers and not just FLAG.

... be aware that more recent results might not yet be included.

# Jargon I

• Ensemble, configuration, trajectory, measurement, correlator An <u>ensemble</u> is a collection of representative gauge fields with the same input parameters

A **trajectory** is an individual step in the (hybrid) Monte Carlo chain **configuration** is an element of the ensemble. Configurations are "de-correlated" from each other, e.g. only take every *N*th trajectory. A **measurement** is an observable evaluated on a specific configuration.

A <u>correlator</u> or <u>correlation function</u> is the ensemble (i.e. gauge) average of a measurement.

- Continuum Limit (CL):  $\lim_{a\to 0} \mathcal{O}(a, m_q, V, ...)$
- O(a)-improved: Discretisation effects of O(a) are absent.
- Infinite Volume Limit (IV):  $\lim_{L\to\infty} \mathcal{O}(a, m_q, V, ...)$

# Jargon II

• Sea vs valence:

Sea quarks or dynamical fermions: These are included in the ensemble. For each choice you need a new ensemble. Valence quarks: The quarks from which operators are constructed. They can - but do not have to - agree with the sea quarks (see below).

• Number of flavours: (IN THE SEA)

 $N_f = 0 = quenched = pure gauge$ : No vacuum bubbles are included in the ensemble

 $N_f = 2$ : Vacuum bubbles from two degenerate light (u, d) quarks are included.

 $N_f = 2 + 1(+1)$ : Vacuum bubbles from two degenerate light (u, d) quarks + a strange quark (+ a charm quark) are included.

• Unitary vs partially quenched

uni *Unitary* data points have the same parameters in valence and sea pq *Partially quenched* data points differ between valence and sea.

# Summary

I hope I have convinced you that Lattice QCD

- provides a <u>first principles</u> and <u>systematically improvable</u> method to compute non-perturbative observables.
- requires large computational resources, several steps of data analysis and <u>human time</u> (Sound familiar...?).

I hope you have gained some insight into how LQCD works - if anything is unclear **please ask**!

- If you need lattice input for a particular process, or
- If there are particular analysis choices that would help you (momentum ranges, choice of bins, ...),

please email me.