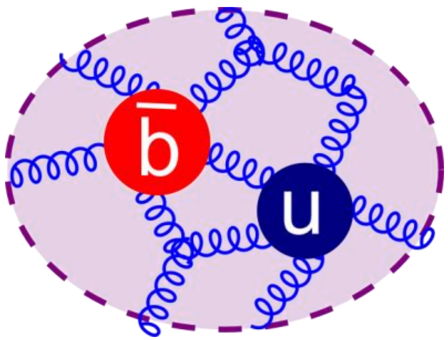
Understanding the Universe with Lattice QCD

Sophie Hollitt, KMI Topics 11-04-2018

Outline

- Part 1: What is Lattice QCD?
  - Why is QCD important?
  - How does it work?
    - Building the lattice
    - Collecting results
- Part 2: Understanding the Universe with Lattice
  - Recent research in lattice and upcoming talks at KMI
  - B physics in lattice QCD
  - Symmetry breaking of the B decay constant



Why is QCD important?

- The Strong Force is one of the four fundamental forces of nature, and helps form hadronic matter.
  - Hadrons (such as protons and neutrons) and electrons make up nearly all of the visible matter in the Universe
  - 99% of the mass of a proton is due to Strong interactions!
- Quantum Chromodynamics (QCD) is the study of the Strong Force at the individual particle level.
  - High energy and high density QCD can tell us more about the conditions inside neutron stars, or the conditions of the early Universe (quark-gluon plasma)
  - Low energy QCD can tell us about how protons, neutrons, and other hadrons are formed from quarks

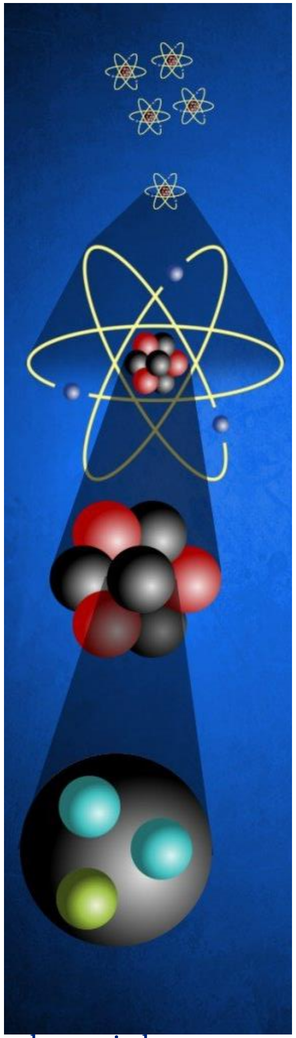
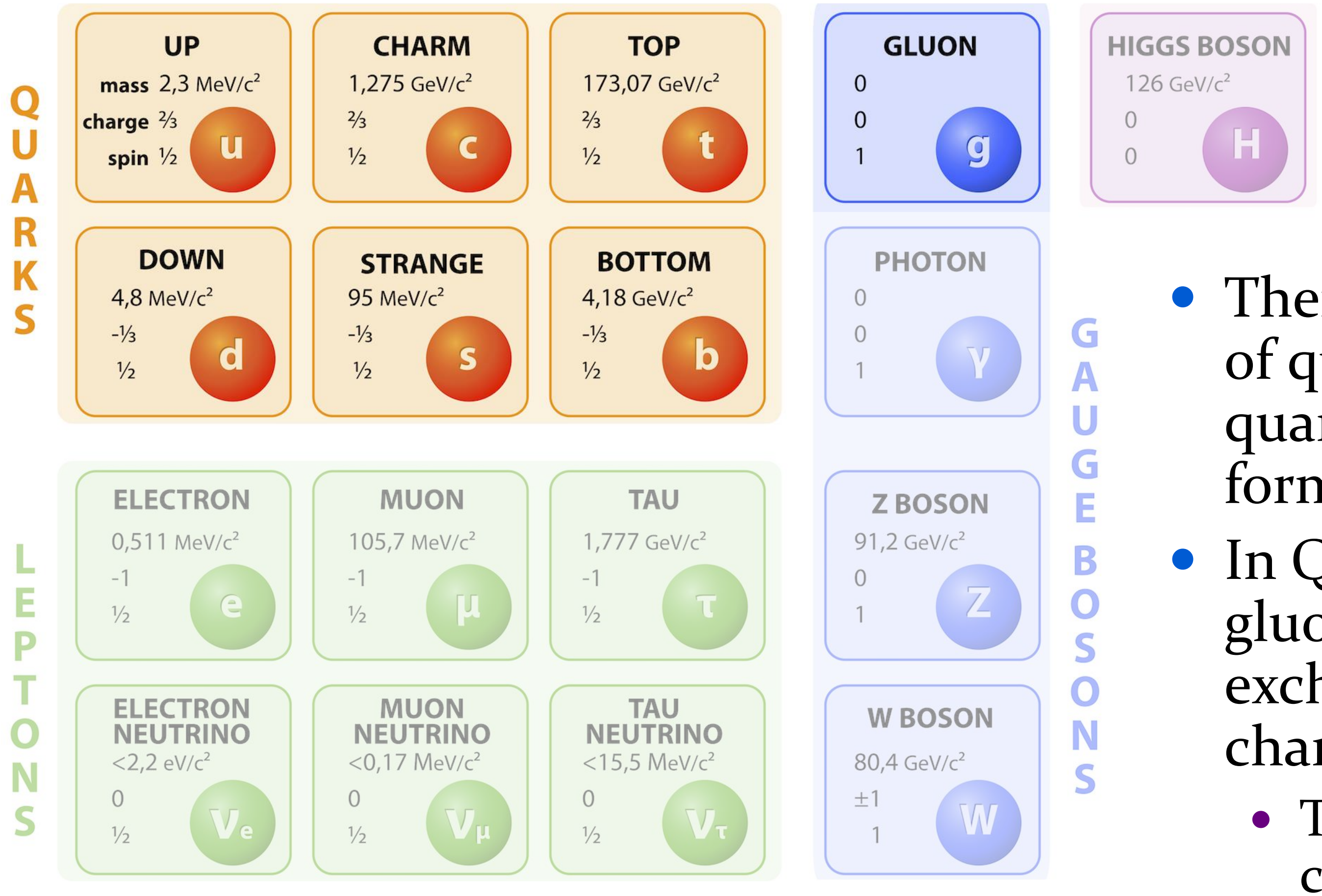


Image: https://steemit.com/science/@veteranz/string-theory-i-the-great-conflict

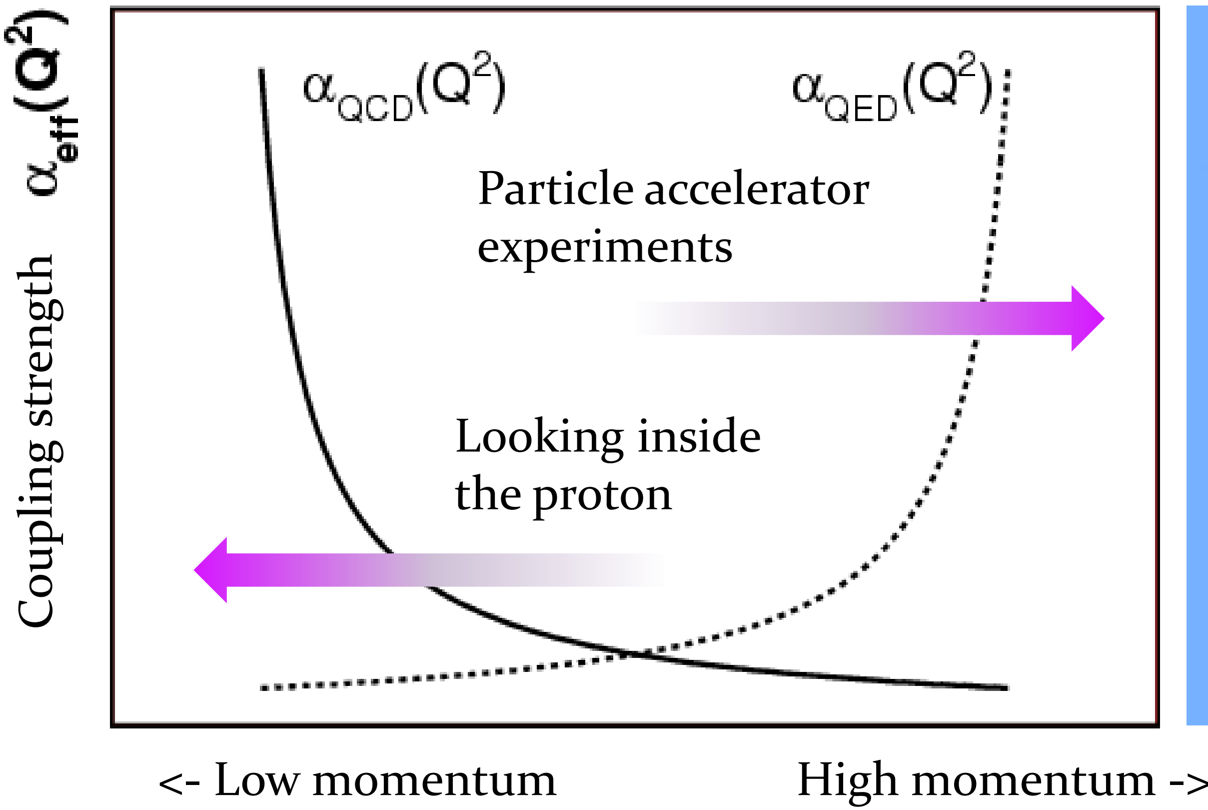
QCD in the Standard Model

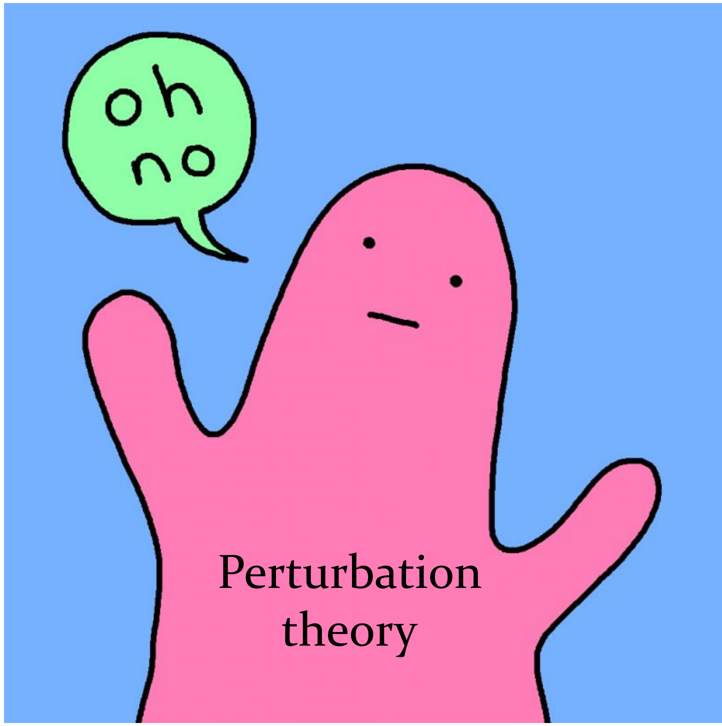


- There are six flavours of quarks, but the top quark is too heavy to form hadrons
- In QCD, quarks and gluons carry and exchange colour charges:
  - There are three colours and three anti-colours

Is colour charge like EM charge?

- No! While electromagnetism is weak at low momentum transfer, this is where the Strong force has the most effect.
  - We can't use perturbation theory for QCD



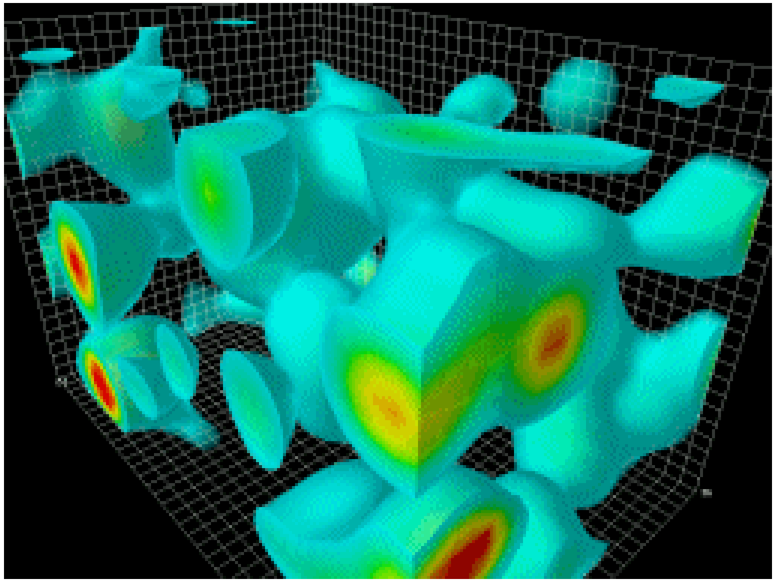


https://www-cdf.fnal.gov/~group/WORK/DISS_PAGE/diss_page.htm

http://webcomicname.com

What do we know about QCD?

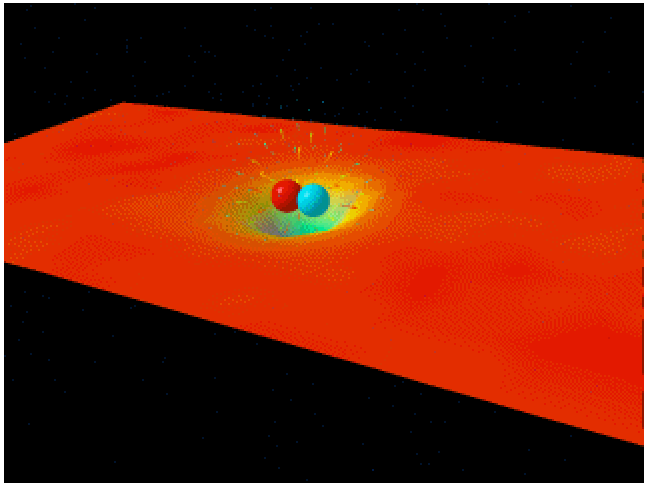
- Gluons interact with quarks, but also other gluons
  - This means that the QCD vacuum is never empty, because gluons can radiate other gluons
  - This gluon self-interaction is what makes QCD complicated



Simulations: http://www.physics.adelaide.edu.au/cssm/lattice/

What do we know about QCD?

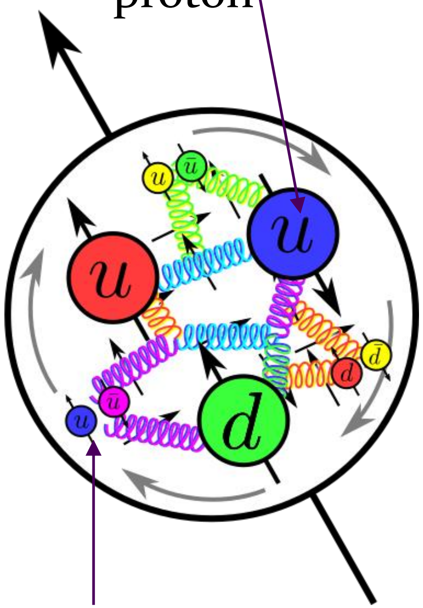
- The vacuum is also full of quarks and antiquarks
  - The Strong Force between two quarks is constant as the distance between them increases
  - The constant force means the energy in the link increases linearly with distance.
  - At some point, there is so much energy in the gluons linking the quarks that it takes less energy to form a quark-antiquark pair in the middle and break the link
- This is why we do not see individual quarks in nature!



Simulations: http://www.physics.adelaide.edu.au/cssm/lattice/

What is lattice QCD?

“valence” quark in the proton



Extra quark contributions from vacuum

Image: A. Chambers (UofA,2017)

- Lattice is a non-perturbative tool for helping us to simulate the vacuum, or hadrons (like the proton) with QCD.
  - Hadrons are made of quarks: we say mesons have 2 and baryons have 3
  - …but hadrons also include quark contributions from the vacuum, and these are crucial to their properties
- Lattice simulations require a large amount of computing power to create sets of different vacuum configurations, and to calculate properties of hadrons on these configurations

Building lattice QCD

Process 1: Creating the lattice

- Generating vacuum configurations
- 1. Discretisation
- 2. Creating the lattice
- 3. Making integration efficient

Process 2: Physics on the lattice

- Calculating hadron properties
- 1. Adding quarks to the lattice
- 2. Inverting large matrices
- 3. Gathering results

- The path integral is the sum of all the possible paths a particle could take between two points, weighted by the probability of the path.
- To measure some observable property of the QCD vacuum with operator $\mathscr{O}$:

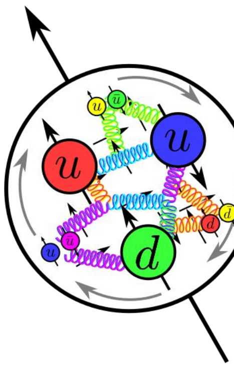
PATHS:
Integration over all possible gluon fields A and quark fields Ψ

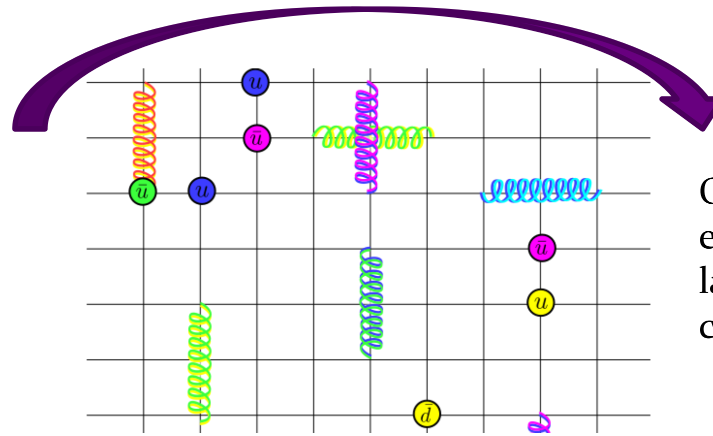
WEIGHTING:
The action S depends on the QCD Lagrangian equation over all spacetime, and encodes particle interactions

$$\langle \mathscr{O} \rangle = \frac{\int \mathrm{D}\Psi \mathrm{D}\overline{\Psi} \mathrm{D}A \, \mathscr{O} \exp(iS)}{\int \mathrm{D}\Psi \mathrm{D}\overline{\Psi} \mathrm{D}A \, \exp(iS)}$$

NORMALISATION

- Instead of integrating over continuous space, we divide space and time into a grid/lattice



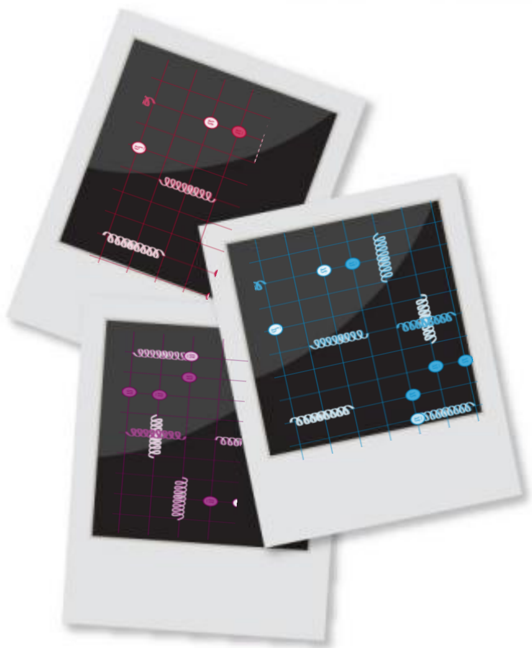


Opposite edges of lattice are connected

↔ spacing *a*

- We represent vacuum quarks and gluons on the lattice by:
  - Putting quarks on the corners of the grid
  - Adding gluons along the lines of the grid
- This is only one possible arrangement of quarks and gluons: and we need to integrate over many!

Images: A. Chambers (UofA,2017)



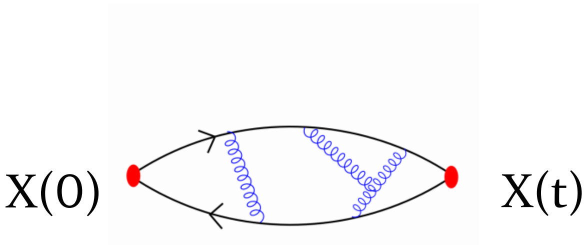
- We want to repeat the same calculation on many different random “snapshots” of the vacuum (lattice configurations) to complete the integration over all possible paths/particle fields.
- This is called Monte Carlo integration
- But generating vacuum configurations is very computationally expensive!
  - Lots of lattice physicists work in collaborations that share configurations.
  - Some collaborations make some of their configurations available to anyone! (PACS in Japan)

- If we generate all kinds of configurations equally and then weight them by the action, we might be using our computing space to store a configuration that doesn't contribute to the result.
- Instead, we generate configurations using a Markov Chain and choose to save them according to their expected weighting.
  1. We calculate $P = \exp(-S)$, where S is the action for this configuration.
  2. We use a threshold on the probability, to decide if the configuration should be accepted and stored or not.
  3. The Markov Chain is used to generate a new configuration from the last accepted one by changing the configuration a little bit.
- Now, the integral for our observable will be a simple sum of the accepted configurations instead of a weighted sum.

Depending on the properties we want to study, there are different ways to add hadrons to the lattice

Two point function:

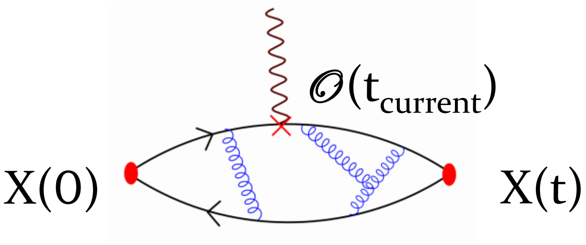
Properties at constant momentum



- Ground state mass
- Energy of excited states
- Decay constants

Three point function:

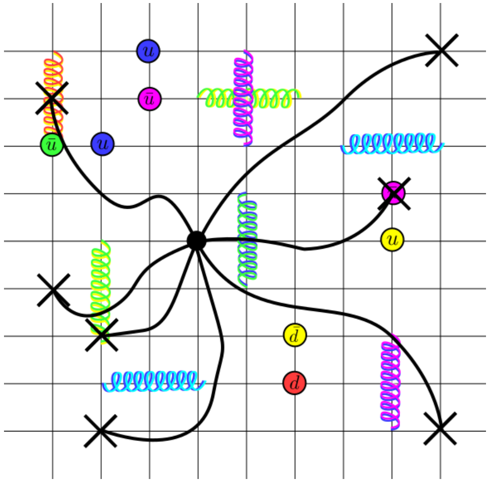
Properties with different initial and final states



- Form factor
- Weak decays (change flavour/mass of one quark)

- For a two point function, we control:
  - The equations for the quarks (the quark action)
    - We often choose actions that remove errors that come from the edges of the lattice, and include other terms to cancel all errors of order *a*
  - The mass of the quarks we add
    - There is no electric charge in pure QCD, the flavour of the quarks is controlled by their mass
    - Lighter quarks require more computation time than heavier quarks, so most calculations have heavier quarks than is physical
- To look at the properties of the hadron, we need to calculate quark propagators from a fixed source (where the particle is created) to a sink (where it is destroyed).

Photograph: Eggers & Villermaux (2008)



- The source is fixed, and we calculate the quark propagator for every possible sink position (space and time) on the lattice.
- This is often called a "point-to-all" propagator

- We calculate the point-to-all propagators because:
  - By Fourier theory, a particle with well defined momentum will be spread across multiple positions.
  - The time dependence of a hadronic state can tell us about its energy
  - If we calculate more propagators, our results have more statistics and less error

Image: A. Chambers (UofA,2017)

- We get the point-to-all propagator by inverting the large matrix that represents the quark action across all lattice sites x,y for quarks Ψ with gluon links Uμ

$$\mathcal{S}_{\mathrm{F}}^{Latt}[\psi, \overline{\psi}, U_\mu] = \sum_{x,y} \overline{\psi}_i^a(x)\, M_{ij}^{ab}(x,y)\, \psi_j^b(y)\,.$$

- For a typical calculation, we would use
  - 32^3 x 64 lattice sites (time axis is larger)
  - 3 colours and 4 spin indices
- That's a 2,5165,824 x 2,516,5824 matrix for each quark!
  - Fortunately, most values are zero
  - Our group in Adelaide uses GPUs to perform these inversions

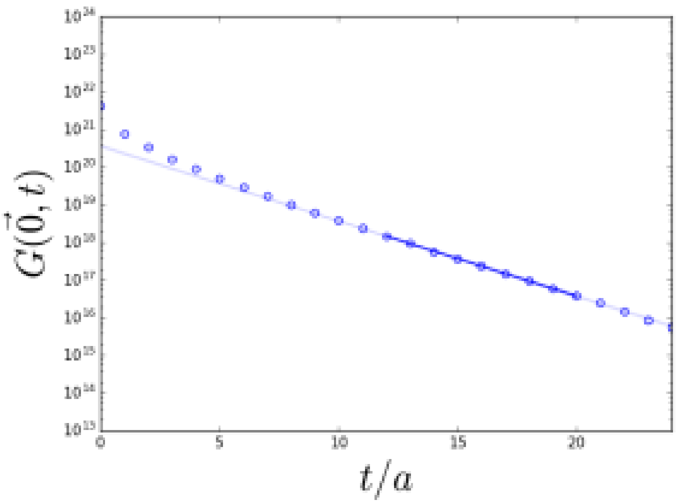
- As an example, let's follow the process to measure the mass of the proton, assuming we already have the appropriate point-to-all propagator.

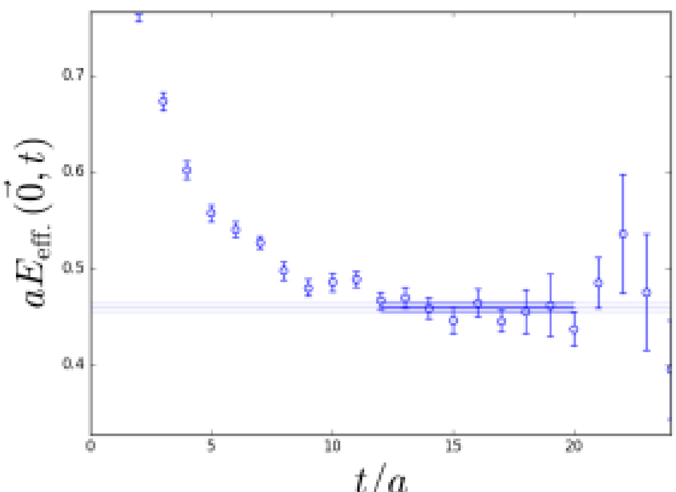
1. The mass is the energy of the proton when momentum is zero, so we Fourier project the point-to-all propagator to collect all the possible hadrons with zero momentum.

$$\underbrace{G(\mathbf{p};t)}_{\text{Correlation function}} = \int d\mathbf{x}\, e^{-i\mathbf{p}\cdot\mathbf{x}} \underbrace{\langle \chi'(\mathbf{x},t)\chi(0) \rangle}_{\text{Point-to-all-propagator}}$$

   - This collects *all* states with zero momentum that contain the right quarks, including heavier excited states of the proton

2. Each single state has a different exponential time dependence according to its energy. At large time, the sum of exponentials in our result looks like the single exp(-E_o t) for the ground state, which we can fit!





- It is hard to see visually if we have chosen a late enough starting time for our fit to make sure we only have the ground state, and it's hard to see whether or not we are fitting to lattice noise
- We define the effective mass in terms of the difference between two neighbouring times

$$E_{\text{eff.}}(\mathbf{p};t) = \frac{1}{a}\ln\left|\frac{G(\mathbf{p};t)}{G(\mathbf{p};t+a)}\right|$$

- Then we have a single state when the effective mass plot forms a plateau (is flat)
- We now know the proton mass for this set of configurations!

Example graphs: A. Chambers (UofA,2017)

- The last step is to repeat the calculation for different sets of lattice configurations
  - With different quark masses, and
  - With different lattice spacings/lattice sizes
- This lets us extrapolate to the physical point, check for lattice discretisation errors, and make predictions of the QCD properties of physical particles
- Computing power and storage have been improving rapidly. It's now possible to make simulations at the physical quark masses, to have a very large lattice, or to have a very small spacing between lattice points.

Summary of Part 1: Lattice QCD

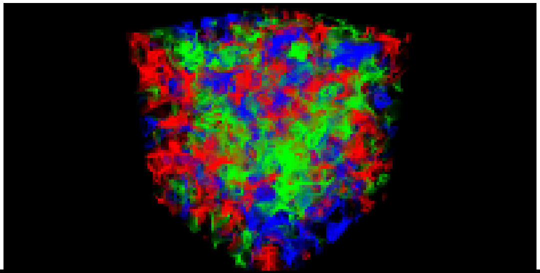
- Lattice is important for studying low energy QCD interactions (such as inside of protons and neutrons), where perturbation theory doesn't work
- We change a continuous path integral, into a Monte Carlo sum over configurations of vacuum quarks and gluons on a grid
- Configurations are generated according to their weighting to save computational time
- Calculating quark propagators for our hadrons requires inverting large matrices efficiently
- We collect results by fitting to data from multiple configurations, and at multiple lattice sizes

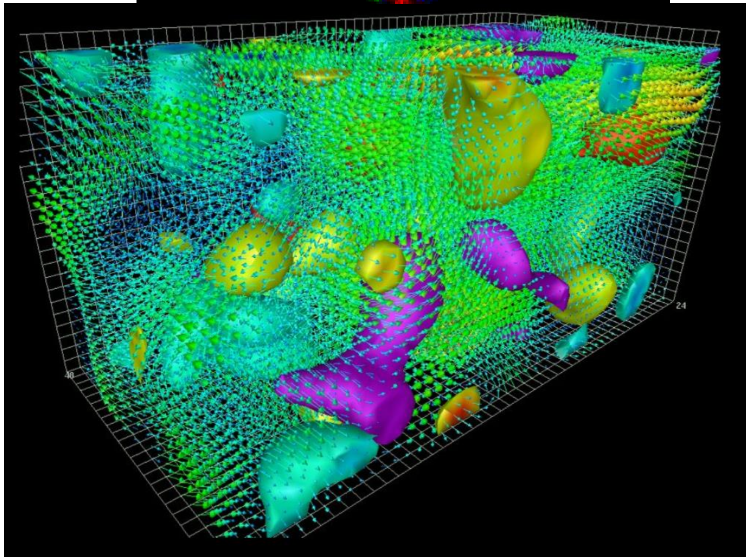
Part 2: What can we research with lattice QCD?

What can we research with lattice?

This is lattice research that I think is fun, from colleagues, collaborators, and friends (not a full review of the field!)

- Simulations of high temperature QCD, where hadrons break apart [F. Stokes, University of Adelaide]
- With lots of computing power, we can now simulate small atoms on the lattice [Search for P. Shanahan & W. Detmold, JLab]
- QCD+QED simulations include interactions with photons as part of the lattice [J. Charvetto, PhD student, University of Adelaide]



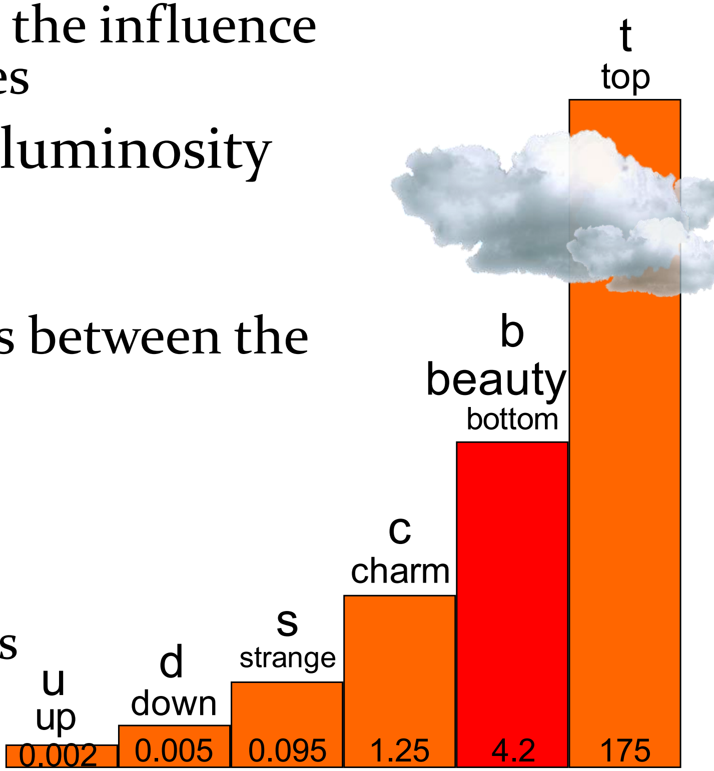


What can we research with lattice?

- Isolating excited states of protons and neutrons on the lattice, to help determine the quark structure of resonances in experiment:
    - See theory seminar by Finn Stokes, 16th April
- The nature of hadrons, quark-hadron duality, and forming a method to calculate inclusive B decay rates:
    - See KMI Colloquium by Shoji Hashimoto, 25th April
- QCD properties in Weak decays of *b* quarks, relevant to flavour physics experiments at Belle II
    - This is my work!
    - I am also a part-time experimentalist in the Belle II Collaboration, but today I will focus on my lattice research

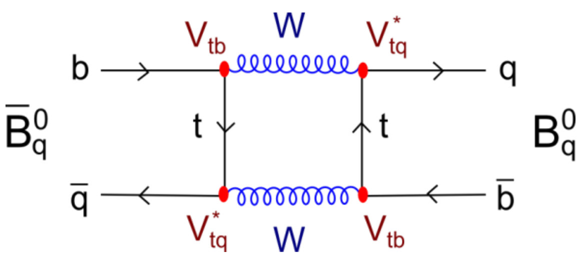
Why *b* quarks on the lattice?

- Flavour physics is the study of the properties of the different types of quarks and leptons, and the couplings between them.
  - The bottom quark is the heaviest quark still able to form hadrons, and can decay into the heaviest lepton (tau)
  - Studies of these heavy particles could reveal the influence of other heavy non-Standard-Model particles
- We're currently moving into an era of high-luminosity experiments in flavour physics
  - decreasing statistical error
  - searching for smaller, more subtle anomalies between the SM and reality.
- Belle II is coming online very soon!
- Need to:
  - reduce error in theoretical calculations to match reduced statistical and systematic errors
  - Make sure we understand all of the QCD contributions



Why *b* quarks on the lattice?

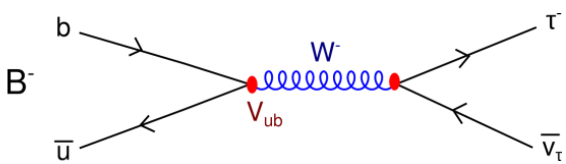
- My work focuses on calculations of f_B and f_{Bs}, the B meson decay constants.
- These constants are an important part of calculating the branching ratio of rare decay channels, and are also used in the calculation of CKM matrix elements.
  - These elements govern quark mixing in the Standard Model
  - If the matrix is not unitary, or the matrix elements seem to have different values for different B decay products, either we don't understand QCD and leptons very well, or there are new undiscovered particle interactions altering the results.



From B^0-$\bar{B}^0$ oscillations

$$\begin{bmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{bmatrix}$$

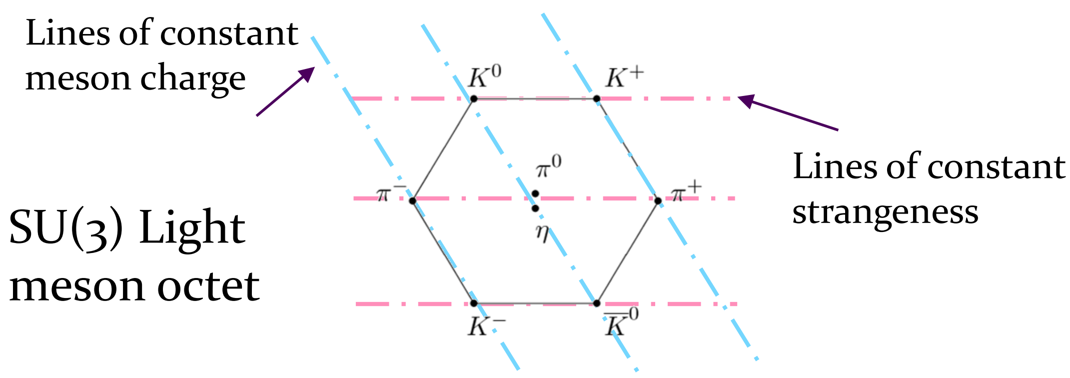
From leptonic and semileptonic B decays



$$\mathrm{Br}(B \to \tau\nu)_{\mathrm{SM}} = \frac{G_F^2 |V_{ub}|^2}{8\pi} \tau_B f_B^2 m_\tau^2 m_B \left(1 - \frac{m_\tau^2}{m_B^2}\right)^2$$

The B meson and light flavour

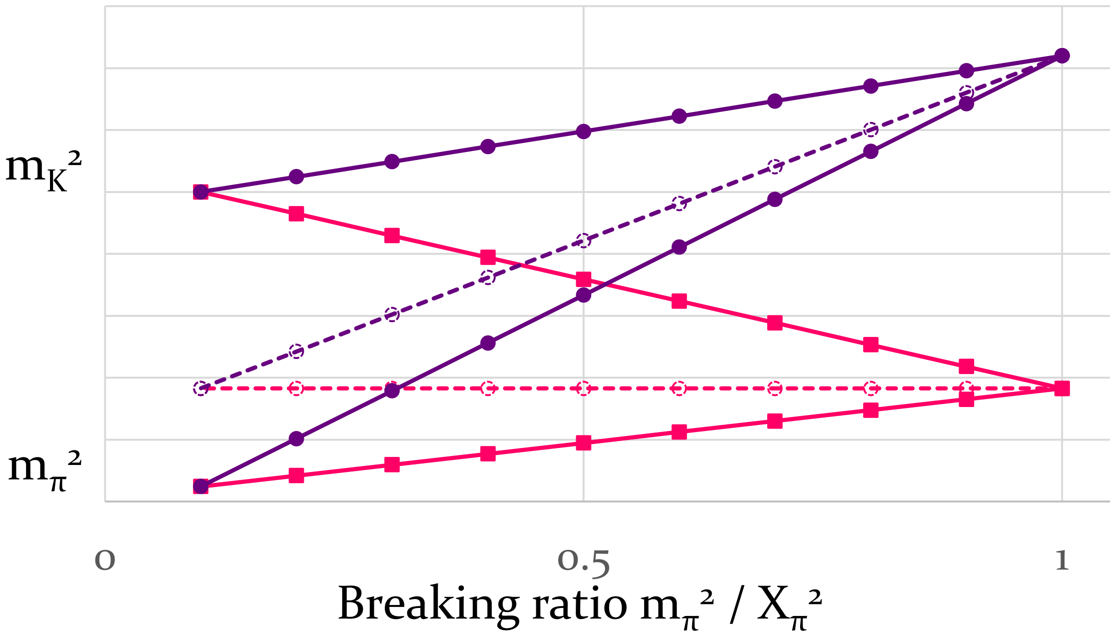
- B mesons consists of one bottom quark (or antiquark), paired with one lighter antiquark (or quark).
  - Recall: in pure QCD, quarks and antiquarks are the same because we have no electromagnetic charges
  - We are interested in whether these lighter quarks are u, d, or s flavour. (The b+s meson is usually labelled B_s)
- Quark flavour has an (approximate) SU(3) symmetry between the up, down, and strange quarks, that is broken by their different masses.



I want to calculate the B decay constants f_B and f_{Bs} on the lattice while directly controlling for SU(3) breaking effects!

Choosing light and strange quarks

- We choose to study SU(3) breaking in a controlled way, by keeping the average mass of these three lightest quarks constant.
  - Lattice configurations for this method are produced by the QCDSF Collaboration. These configurations are simplified with $m_u = m_d$, called m_{light}



m_s = constant

The kaon is light + strange, so its mass still changes when m_s is constant

SU(3) breaking effects and effects from simulating a heavier vacuum occur together

$$\overline{m} = 1/3\ (2m_l + m_s)$$

The average quark mass in the vacuum is constant

Generating *b*-quarks

- As *b* quarks are so heavy, they aren't included in our vacuum lattice configurations, and they require a slightly different quark action to avoid discretisation errors.
  - This lets us make our own choice about whether the *b* quark mass should stay constant, or shift to keep the average B meson mass constant
  - We choose to adjust the b quark to keep the average B mass constant
- We use an anisotropic, clover-improved action based on the Fermilab action, and then tune the free parameters to physical quantities for the B meson.

$$S_{lat} = a^4 \sum_{x,x'} \overline{\psi}(x') \left(m_0 + \gamma_0 D_0 + \zeta \vec{\gamma} \cdot \vec{D} - \frac{a}{2}(D^0)^2 - \frac{a}{2}\zeta(\vec{D})^2 + \sum_{\mu,\nu} \frac{ia}{4} c_P \sigma_{\mu\nu} F_{\mu\nu} \right)_{x,x'} \psi(x)$$ [1]

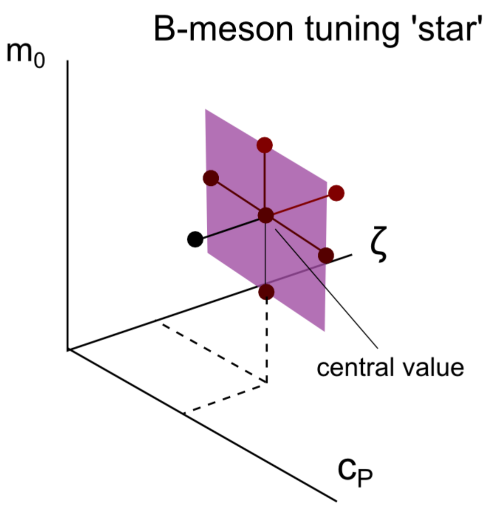
bare mass → spin-averaged meson mass

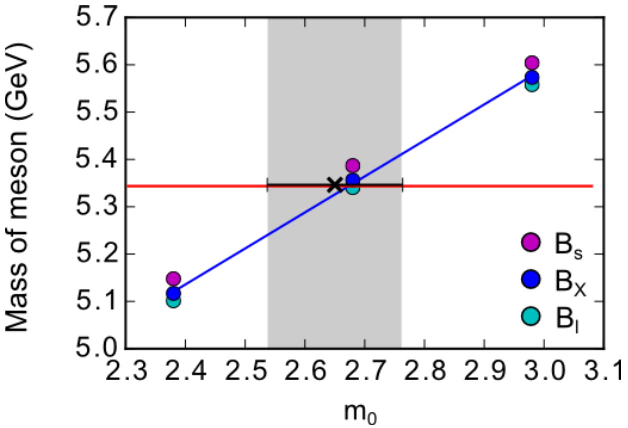
anisotropy → dispersion relation

clover coefficient → hyperfine splitting between B* and B

1 Aoki, Y et al (2012). "Nonperturbative tuning of an improved relativistic heavy-quark action with application to bottom spectroscopy." *Physical Review D, 86*(11), 116003. doi:10.1103/PhysRevD.86.116003

Generating b-quarks





METHOD:

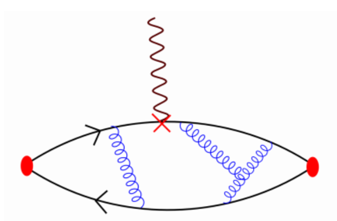
1. On every set of configurations, generate one "central" b-quark and six other b-quarks in a "parameter star" by changing our three free variables.
2. Make a B_{light} and $B_{strange}$ meson for each b quark
3. Calculate the average B meson, $B_X = (2/3)\ B_l + (1/3)\ B_s$ for each of our seven b-quarks.
4. Compare the calculated B_X mesons to the physical B_X meson, and find the set of parameters matching the physical B.

Calculating the decay constant f_{Bq}

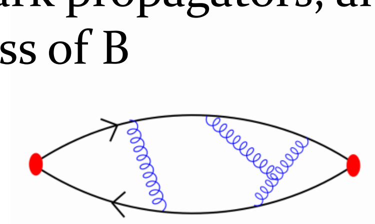
- Once we have chosen the appropriate quarks, the decay constant is calculated mostly using two point functions

$$f_B = \frac{\hbar c}{a} Z_\Phi \left[\Phi_B^0 + c_A \Phi_B^1\right]$$

Renormalisation factor:
Ratio of 2 point and 3 point functions with constant coefficient ρ=1



Lattice decay constant:
2 point functions with different operators in the quark propagators, and mass of B



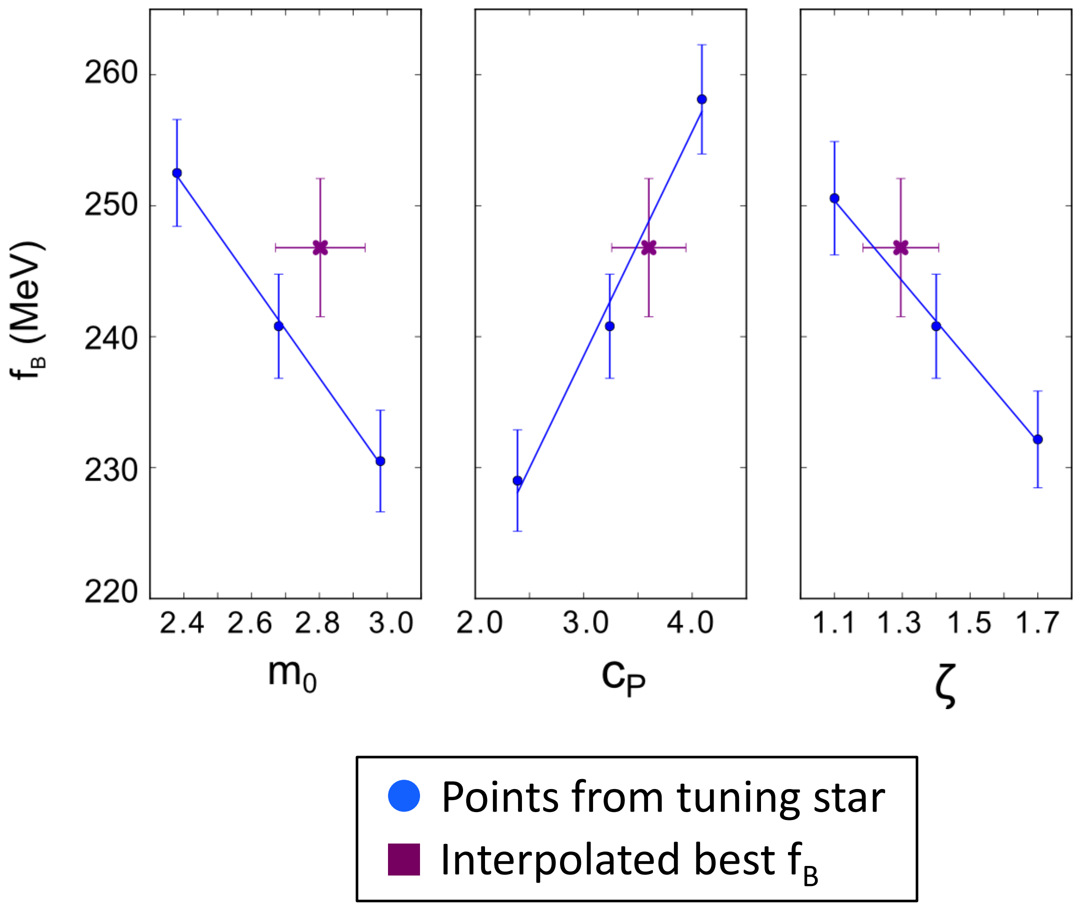
Improvement term:
2 point correlators & coefficient c_A

Currently take c_A=0, Exact value can be calculated using perturbative QCD

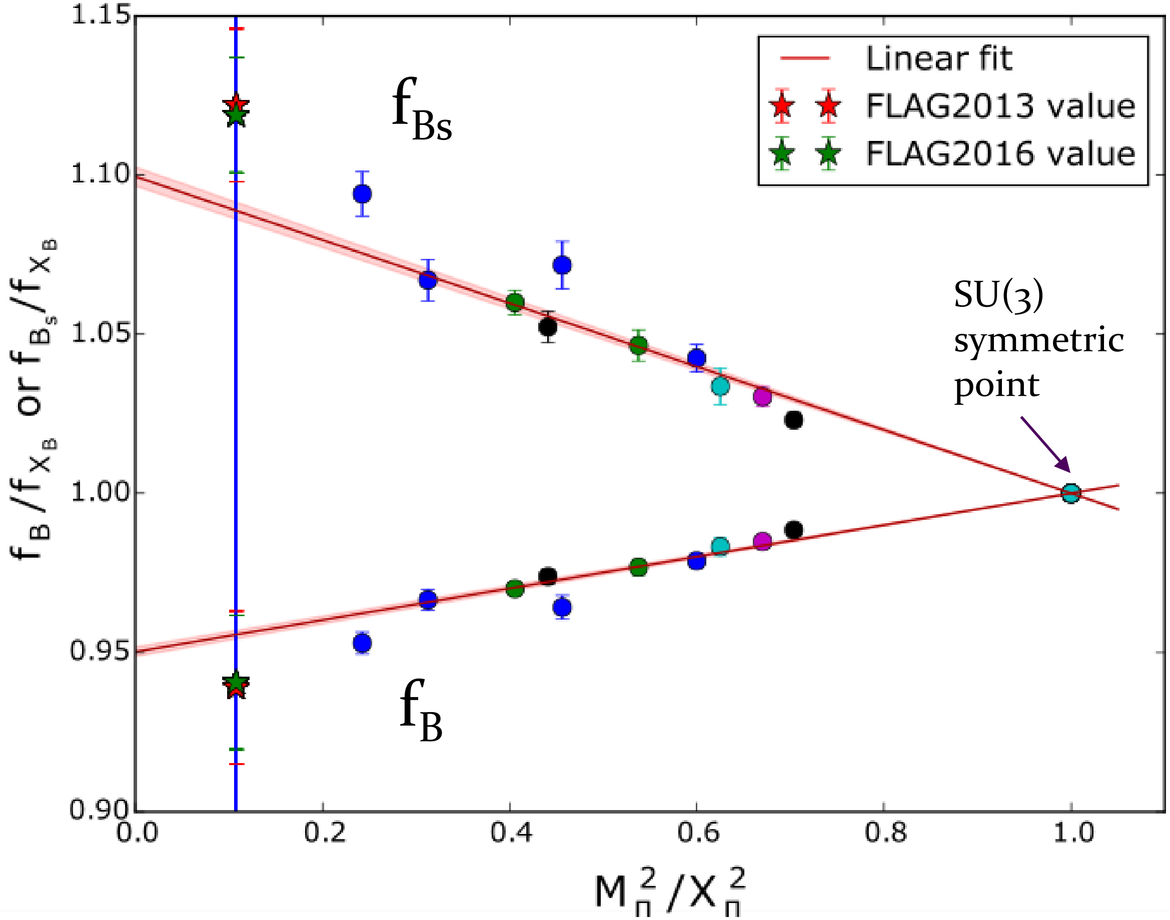
Calculating the decay constant f_{Bq}

1. Calculate Φ_B and Φ_{Bs} for each of the *b*-quarks in the tuning "star"
2. For each set of lattice configurations, find tuning parameters that match physical properties of the B_X meson as required
3. Use these parameters to interpolate to a "best" Φ_B and thus calculate "best" f_B
4. Repeat at other light quark masses and lattice spacings!

f_B at symmetric point $m_l = m_s$

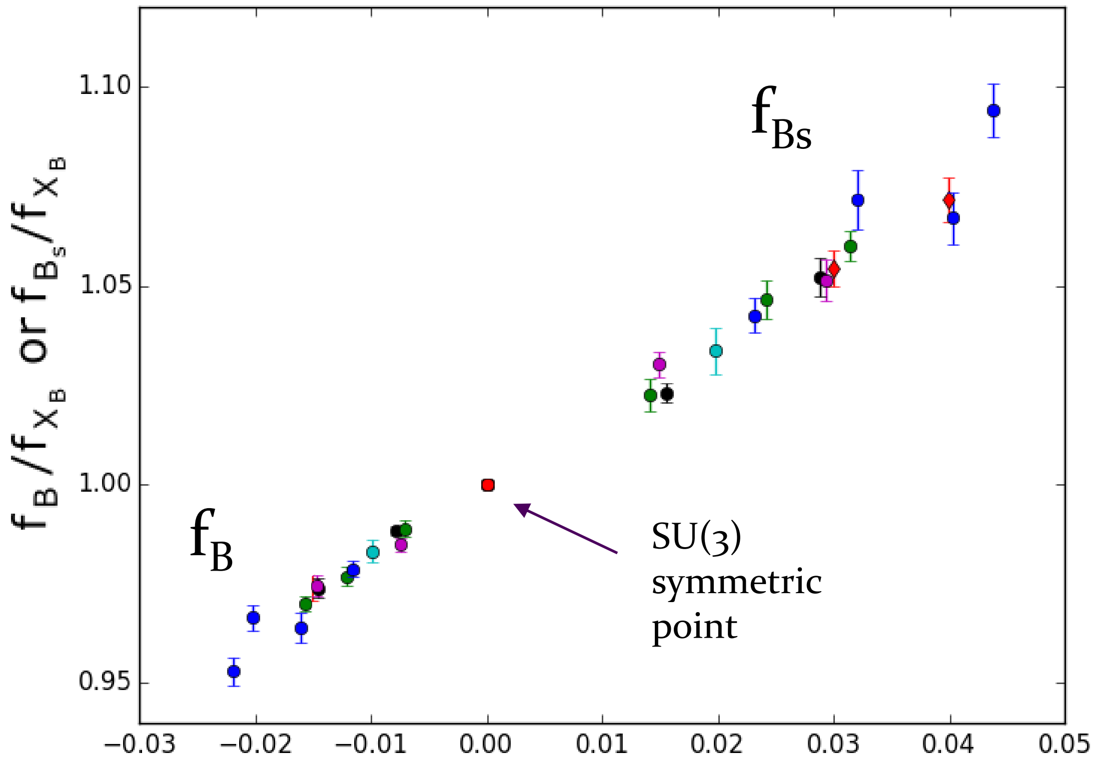


SU(3) breaking of f_{Bq}



- On each configuration, calculate f_{Bl} and f_{Bs} and the average f_{Bx} to cancel most systematic errors from calculation method
- BLUE configurations have a systematic error in the SU(3) breaking encoded in the vacuum, so we need a more careful approach

Toward physical f_B and f_{Bs}



δm_q
(change in quark mass from SU(3) symmetric point)

- Arrange all f_B and f_{Bs} according to the mass of the lighter quark in the B meson, relative to the SU(3) symmetric point
- Make fits to theory expectation of SU(3) breaking for f_B, for each lattice spacing
  - Currently in progress
- Extrapolate from finite lattice spacing to continuum QCD

Summary

- We can use lattice QCD to improve our understanding of the theory of QCD directly, or calculate results suitable for use by experiments probing QCD and flavour.
  - Please see further KMI seminars on lattice in the next few weeks!
- My lattice research is focused on:
  - The decay constants f_B and f_{Bs} for the B meson, relevant to rare decays B and calculations of CKM matrix elements
  - Breaking the SU(3) symmetry of up, down, and strange quarks in a systematic way
- I am close to having my own lattice prediction of the physical f_B and f_{Bs} to add to the global average.

Thank you!
I hope you have learned something new about lattice!