Higgs-Maxwell Meeting, February 2024

50 years of Lattice QCD

Christine Davies,
University of Glasgow,
HPQCD collaboration

TOPICS

- Early days of lattice QCD

- 50 years later … a small selection of results

- Example of ongoing work - the anomalous magnetic moment of the muon

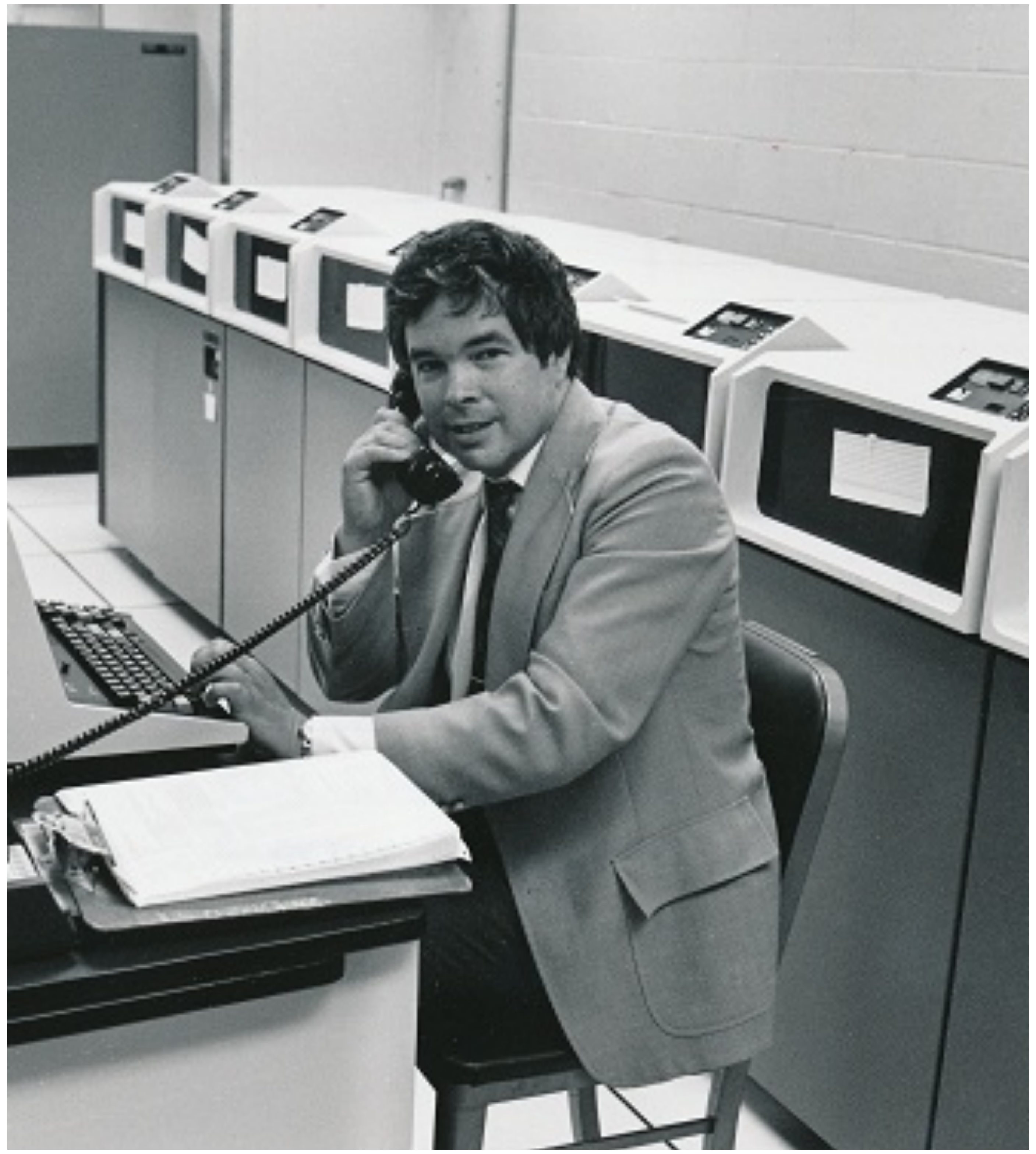
- Future ?

PHYSICAL REVIEW D VOLUME 10, NUMBER 8 15 OCTOBER 1974

Confinement of quarks*

Kenneth G. Wilson
Laboratory of Nuclear Studies, Cornell University, Ithaca, New York 14850
(Received 12 June 1974)

A mechanism for total confinement of quarks, similar to that of Schwinger, is defined which requires the existence of Abelian or non-Abelian gauge fields. It is shown how to quantize a gauge field theory on a discrete lattice in Euclidean space-time, preserving exact gauge invariance and treating the gauge fields as angular variables (which makes a gauge-fixing term unnecessary). The lattice gauge theory has a computable strong-coupling limit; in this limit the binding mechanism applies and there are no free quarks. There is unfortunately no Lorentz (or Euclidean) invariance in the strong-coupling limit. The strong-coupling expansion involves sums over all quark paths and sums over all surfaces (on the lattice) joining quark paths. This structure is reminiscent of relativistic string models of hadrons.



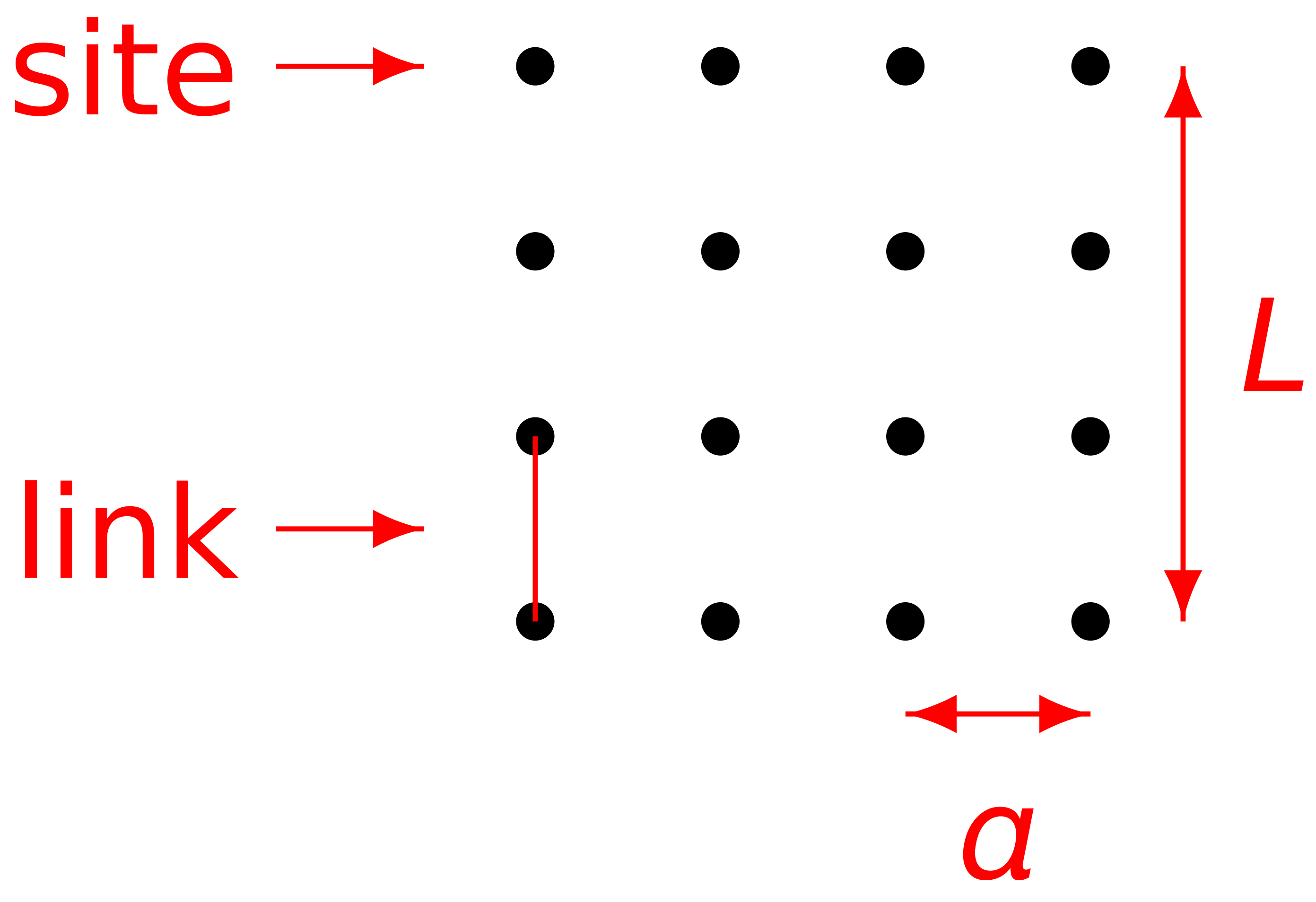
Ken Wilson 1936 - 2013, Nobel prize 1982, for the Renormalisation Group

The origins of lattice gauge theory, hep-lat/0412043 explains:

1973, exciting discovery of asymptotic freedom … eager jump in … recent work in statistical mechanics meant that a lattice version of QCD seemed easier to work with …

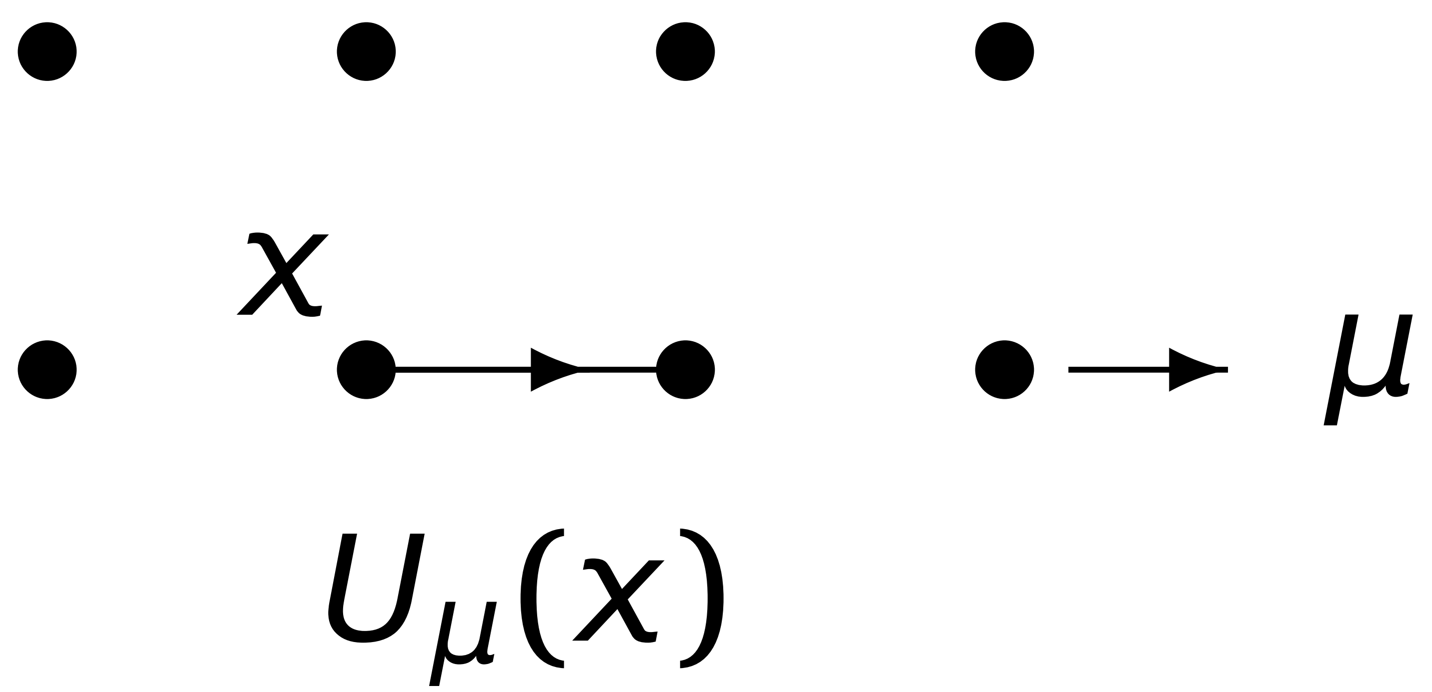
Elements of lattice QCD

- Theory is defined on a Euclidean space-time lattice



- Gluon fields live on the links joining lattice points and are elements of the gauge group i.e. SU(3) matrices rather than elements of the Lie algebra

$$U_\mu(x) = e^{-igA_\mu(x+a/2)}$$



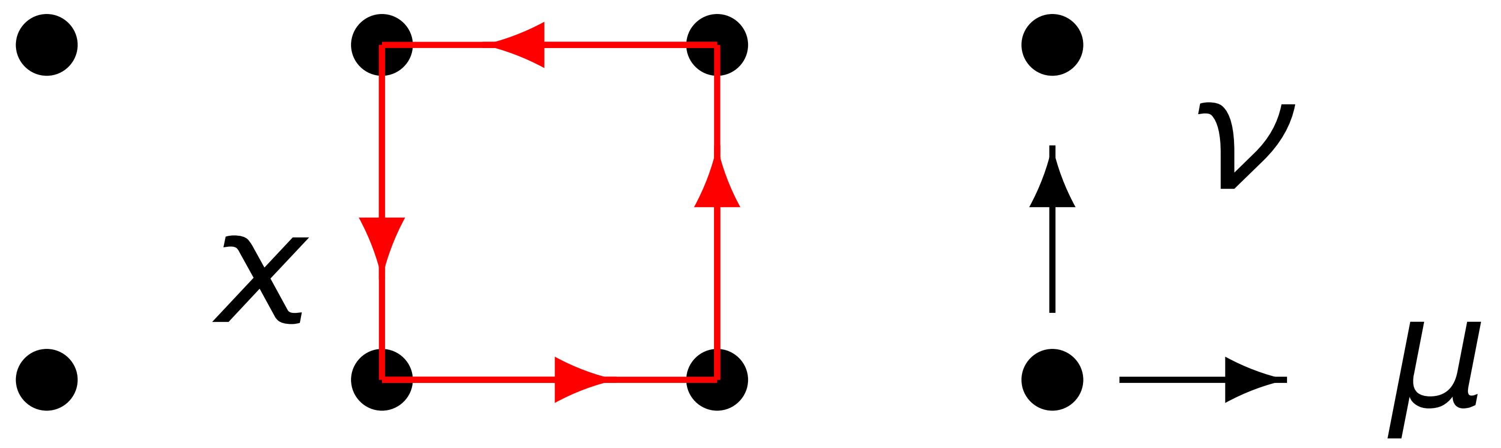
- Solving QCD via the Feynman path integral becomes a multi-dimensional integral

$$\int \mathcal{D}A_\mu \ldots e^{-\int L dt} \rightarrow \int \prod_{x_j \in \text{grid}} dU_\mu(x_j) \ldots e^{-a \sum L_j}$$

action, S

Wilson's gluon action

$$S^{\text{lattice}}_{\text{gluon}} = \frac{6}{g^2(\pi/a)} \sum_{x,\mu>\nu} (1 - P_{\mu\nu}(x))$$



$P_{\mu\nu}(x)$

where

$$P_{\mu\nu} \equiv \frac{1}{3}\text{ReTr}\left(U_\mu(x)U_\nu(x+a\hat{\mu})U^\dagger_\mu(x+a\hat{\mu}+a\hat{\nu})U^\dagger_\nu(x)\right)$$

(plaquette)

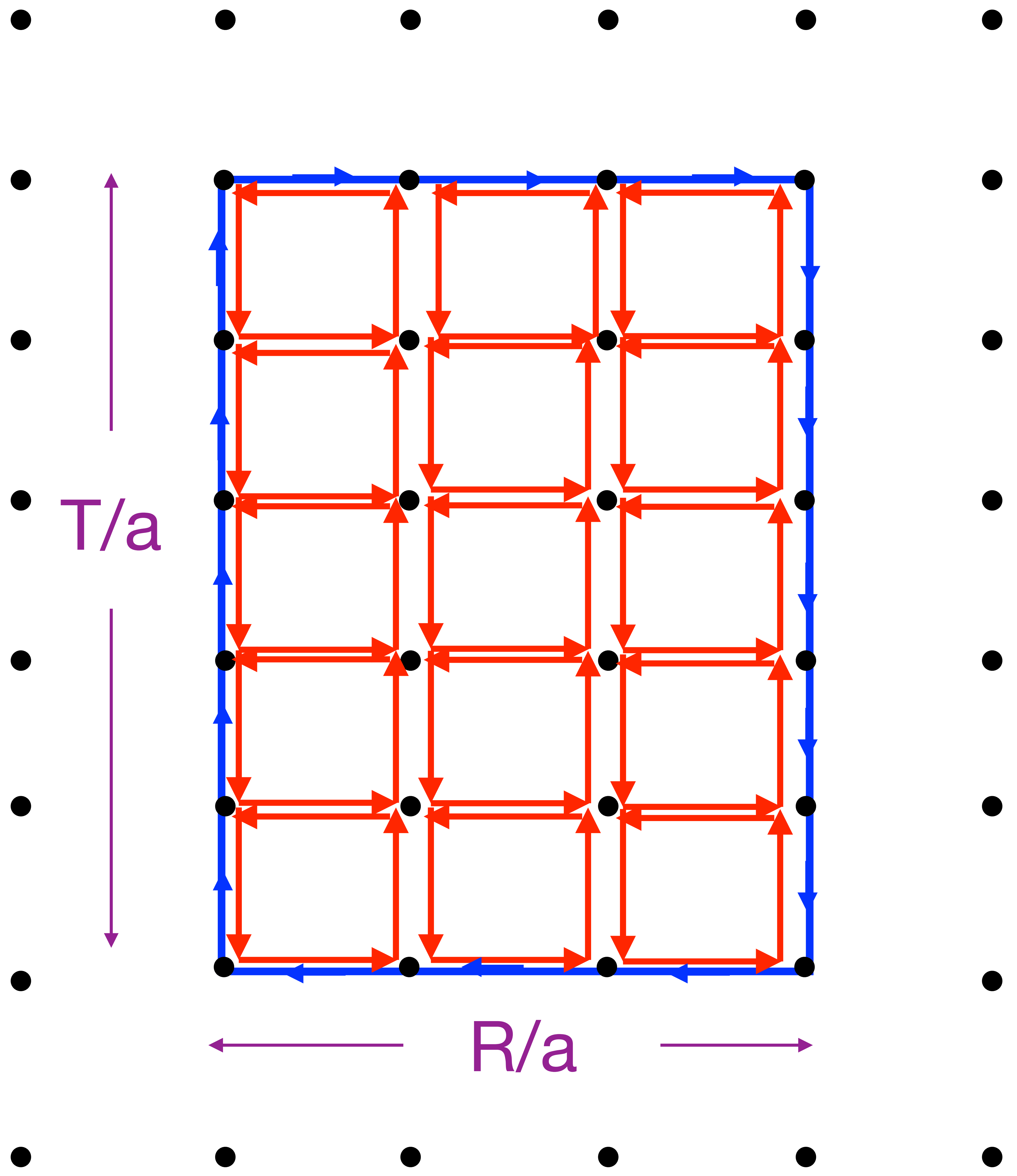
- The theory is locally gauge-invariant at NON-ZERO lattice spacing i.e. NO gauge-fixing is needed.

- For small *a*

$$S^{\text{lattice}}_{\text{gluon}} \to \left(S^{\text{cont}}_{\text{gluon}} = \int d^4x \sum_{\mu>\nu} \text{Tr}F^2_{\mu\nu} \right) + \mathcal{O}(a^2)$$

Discretisation errors

Theory shows colour confinement in strong coupling (large g²) limit



Expectation value of RxT Wilson loop

$$\frac{1}{Z}\int \prod_{x_j \in \text{grid}} dU_\mu(x_j)\ \Box\ e^{-\beta \sum (1 - \Box)}$$

$\beta \equiv \dfrac{6}{g^2}$

For small β (large g²), expand exponential and use

$$\int dU\, U^{ab} = 0 \qquad \int dU\, U^{ab} (U^\dagger)^{cd} = \frac{1}{3}\delta_{ad}\delta_{bc}$$

We must 'tile' the loop with plaquettes at leading-order

$$\langle\ \Box\ \rangle \propto \beta^{RT} \equiv e^{-\ln(g^2) RT}$$

'Area Law'

We also have $\langle\ \Box\ \rangle = e^{-V(R)T}$

so $V(R) = KR$ ➡ confinement!

BUT large $g(\pi/a)$ implies large a - we want the continuum limit, $a \to 0$, for phenomenology

➡ numerical integration of path integral instead - this needs Monte Carlo/ importance sampling methods.

M. Creutz, Monte Carlo study of quantised SU(2) gauge theory, Phys. Rev. D21 (1980) 2308; used 4^4 to 10^4 lattices, measuring Wilson loops from 5 (!) equilibrated gluon field configurations. (Could be done on your phone today)

➡ possible to reach weak coupling regime. Can then measure other quantities in terms of string tension, i.e. use string tension to determine lattice spacing. $\sqrt{K} \approx 440\,\mathrm{MeV}$

Big computing challenge, however!

Strong coupling

$-\ln(\beta/4)$

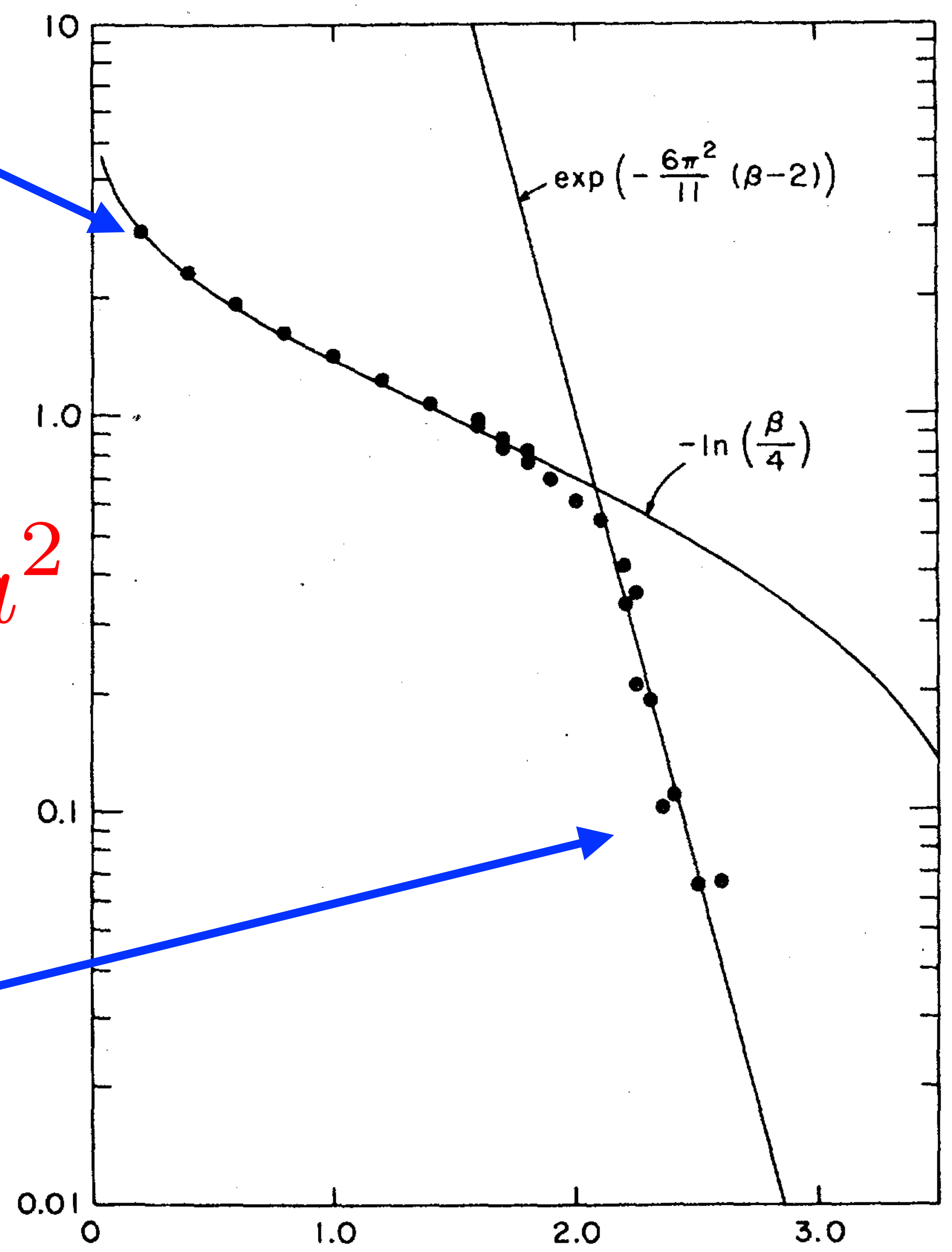
'String tension' in lattice units

Ka^2

Weak coupling

$$g^2(\pi/a) \propto \frac{1}{\ln(A/a)}$$

➡ $a^2 = A^2 e^{-C\beta}$

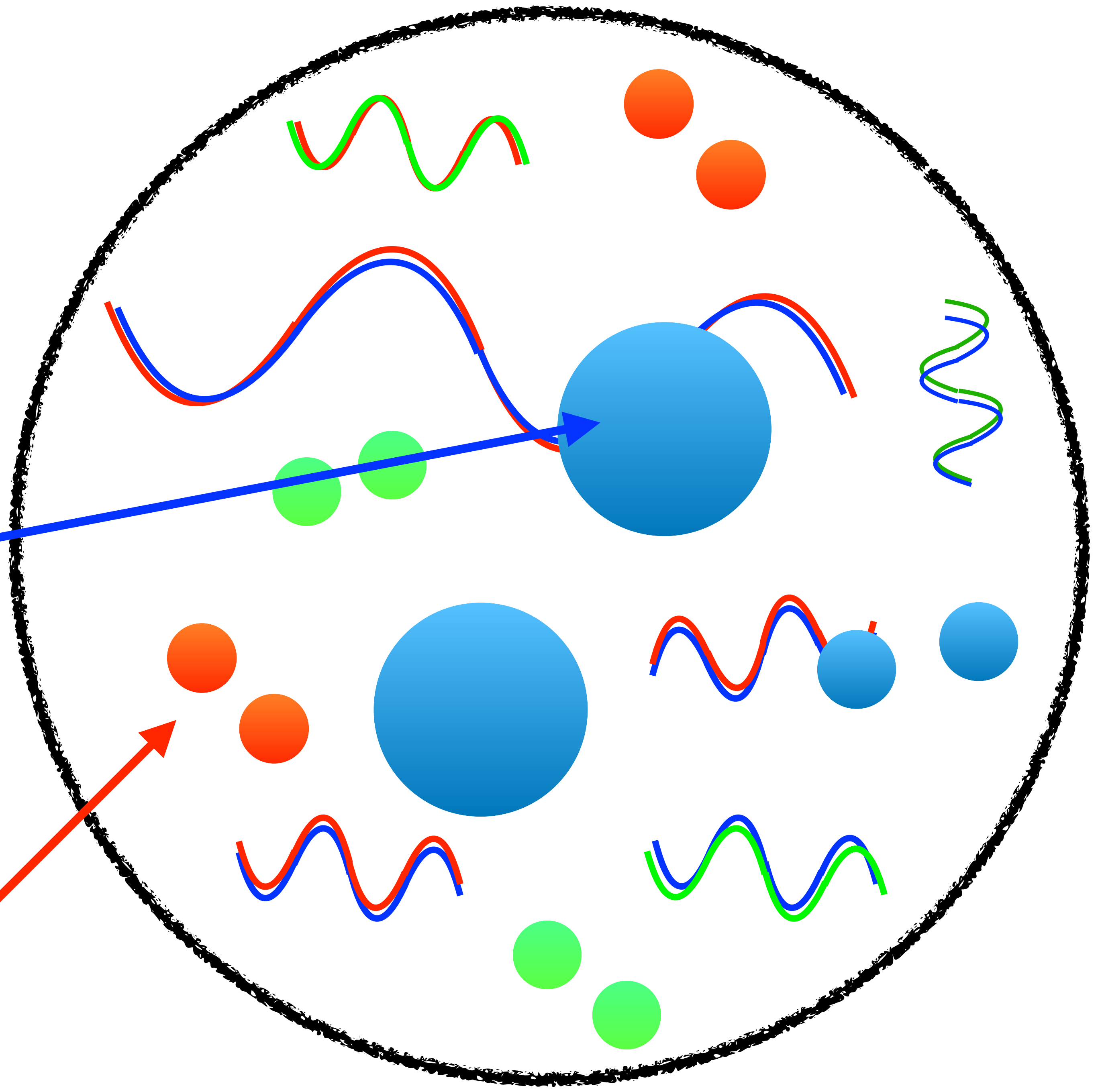


$$\beta = \frac{4}{g^2(\pi/a)}$$ ← for SU(2)

Including quarks

Dirac matrix

$$S_q = \overline{\psi}(\gamma \cdot D[U] + m)\psi$$



Valence quarks: construct hadron correlator by solving Dirac equation on background gluon field and combining quark propagators, expensive for small m

Sea quarks: include Det(Dirac matrix) in importance sampling of gluon fields, extremely expensive for small m.

S. Duane, A. Kennedy, B.Pendleton, D.Roweth, , Hybrid Monte Carlo, Phys. Lett. B195 (1987) 216.

Quenched approximation, 1980s and 1990s - ignore determinant.

Slow-going …

Key progress was made in improving the discretisation of QCD (adding terms to cancel discretisation errors), particularly for quarks.

Smaller discretisation errors means larger a values can be used. Cost (~$1/a^8$) much reduced.

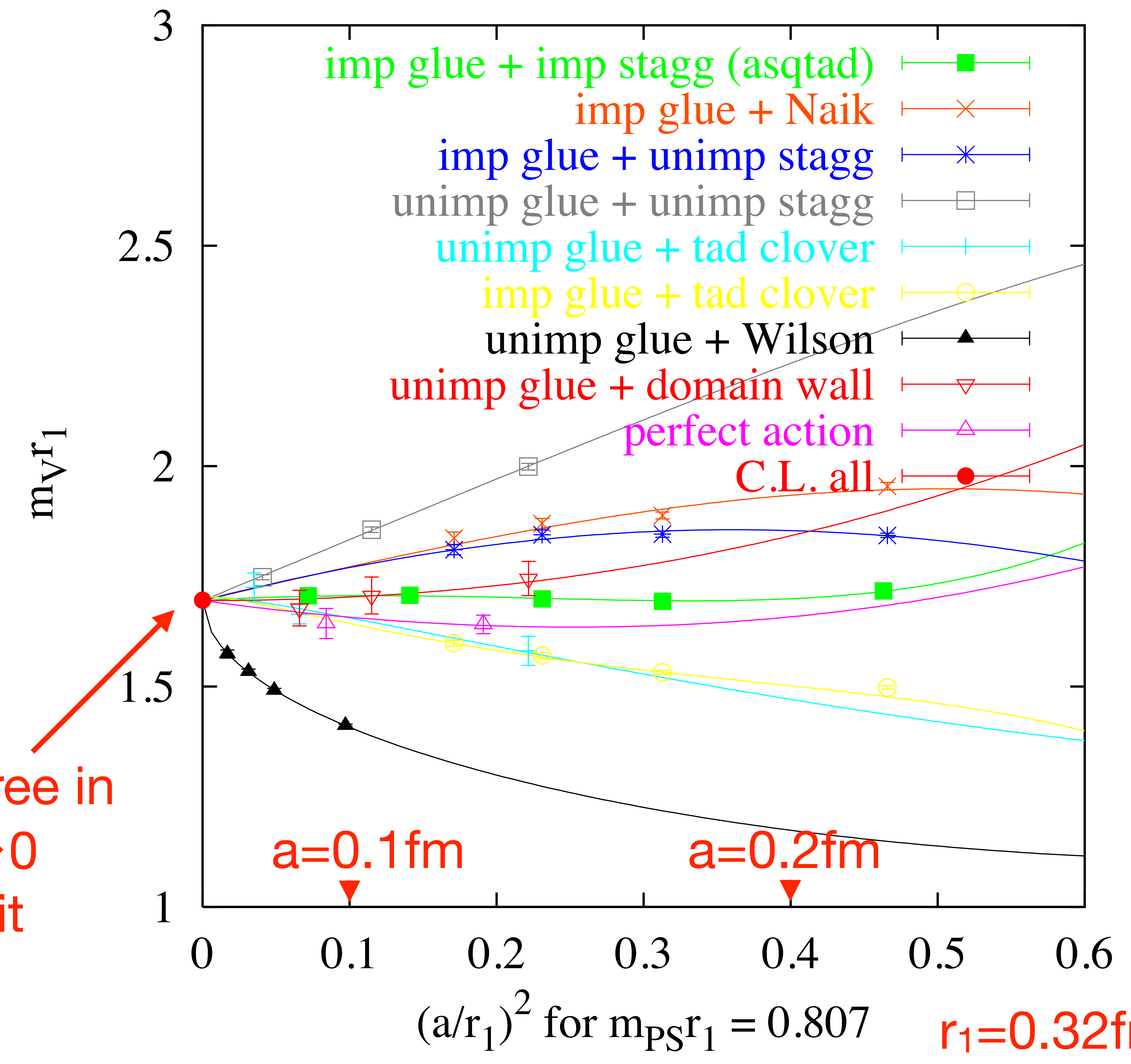
➡ This makes the inclusion of sea quarks possible with u/d quark masses that are small enough.

How small is small enough?

By early 2000s it was possible to include u, d, s in sea with $m_u=m_d=m_l$ and m_l/m_s down to 0.2

(real world m_l/m_s~0.04 now reachable)

agree in a→0 limit



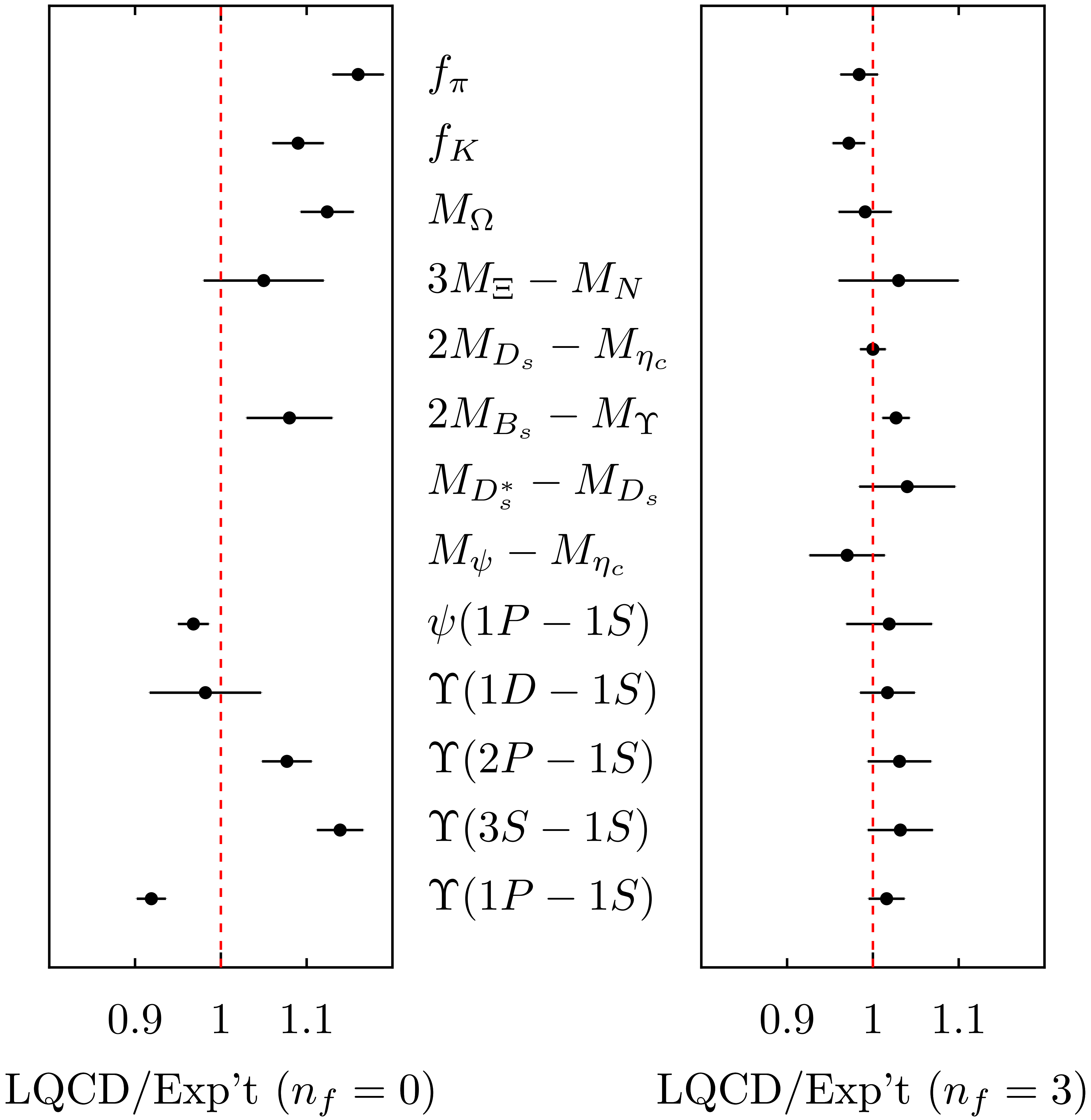
r_1=0.32fm

C. Davies, P.Lepage, F. Niedermayer, D. Toussaint, hep-lat/0409039.

Including sea quarks

Quenched approx: no sea quarks

With u, d and s sea quarks



Ratio of lattice QCD/experiment - correct answer is 1

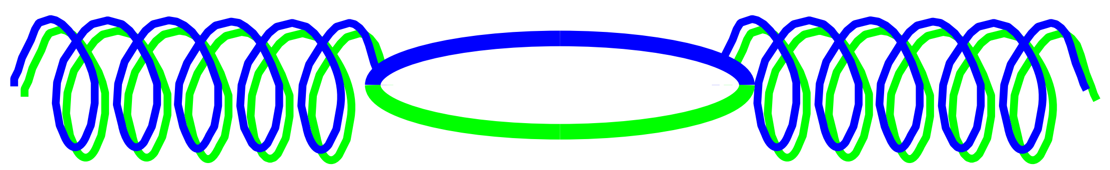
- focus on gold-plated quantities
- must fix parameters of QCD i.e. lattice spacing and quark masses. Here used

$$\Upsilon(2S - 1S), M_\pi, M_K, M_{\eta_c}, M_{\eta_b}$$

No further free parameters!

- plot shows that sea quarks give correct answers across a wide range of hadrons; quenched approx. fails at 10-20% level.

Quenched approx. inconsistent because of missing

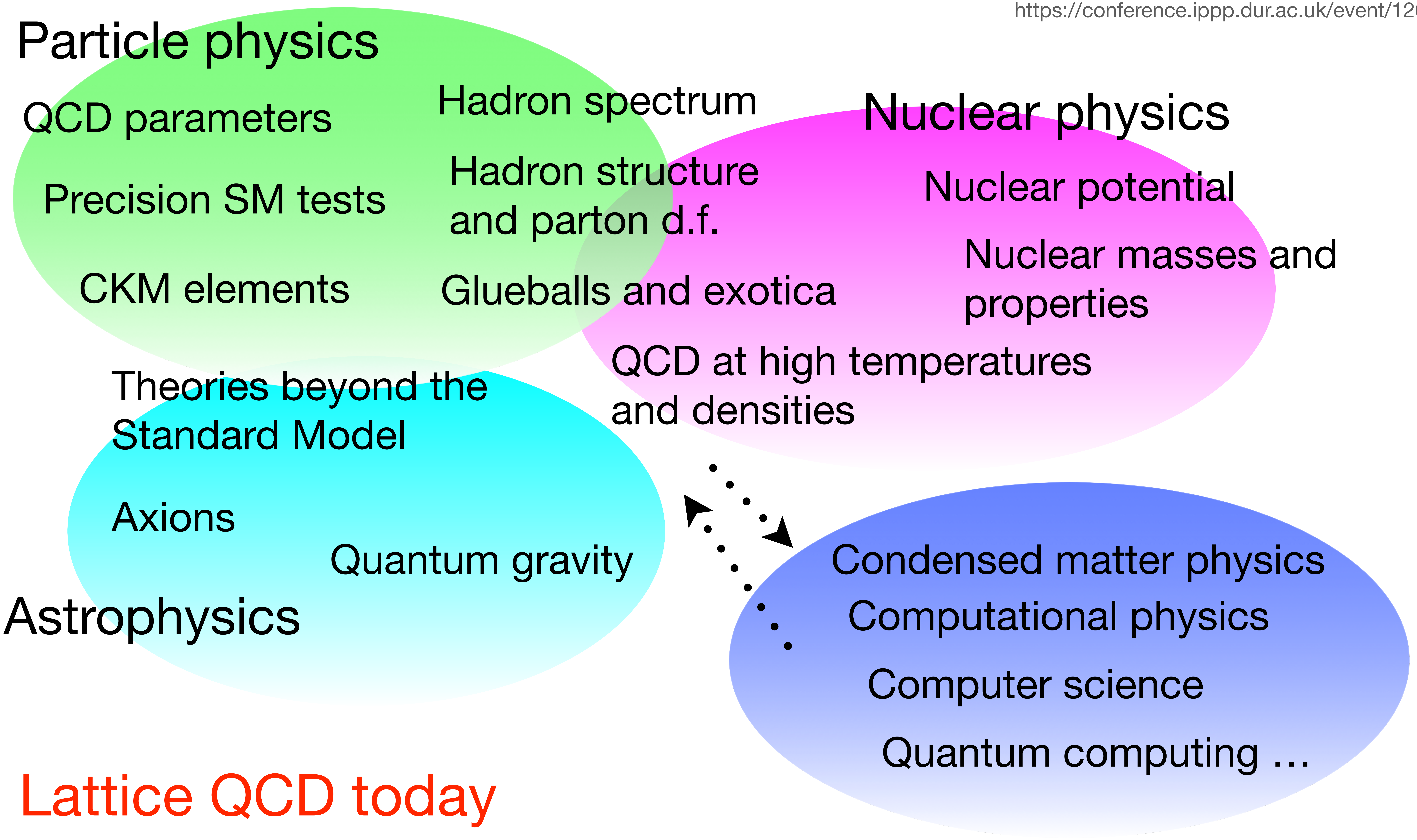


No QED included here but <1% effects

C. Davies et al, HPQCD/Fermilab/MILC, PRL92:022001 (2004), with updates from HPQCD, PRD72:212001 (2005)

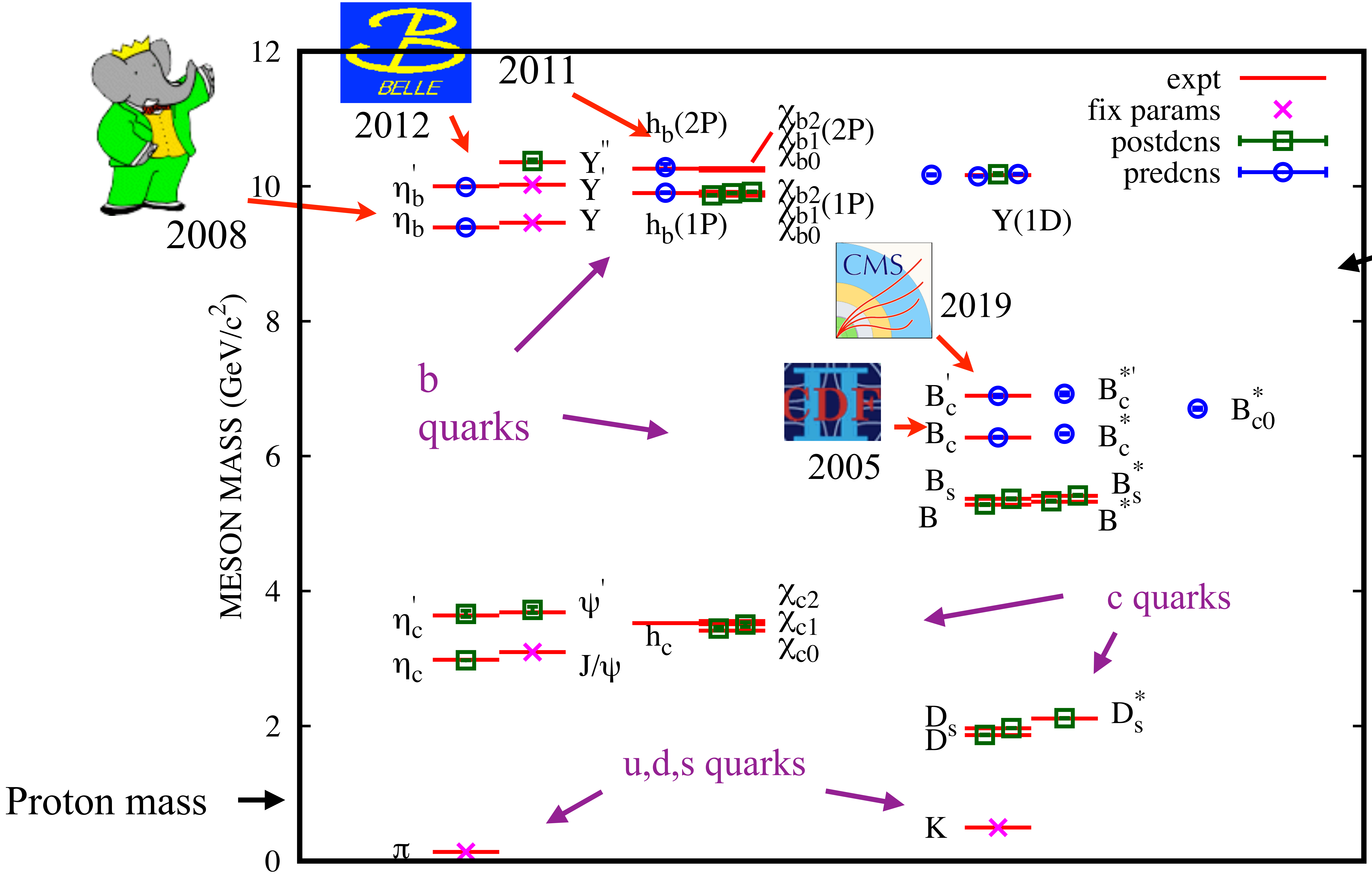
Lattice 2024 in Liverpool!

https://conference.ippp.dur.ac.uk/event/1265/overview



Lattice QCD today

The masses of mesons from lattice QCD

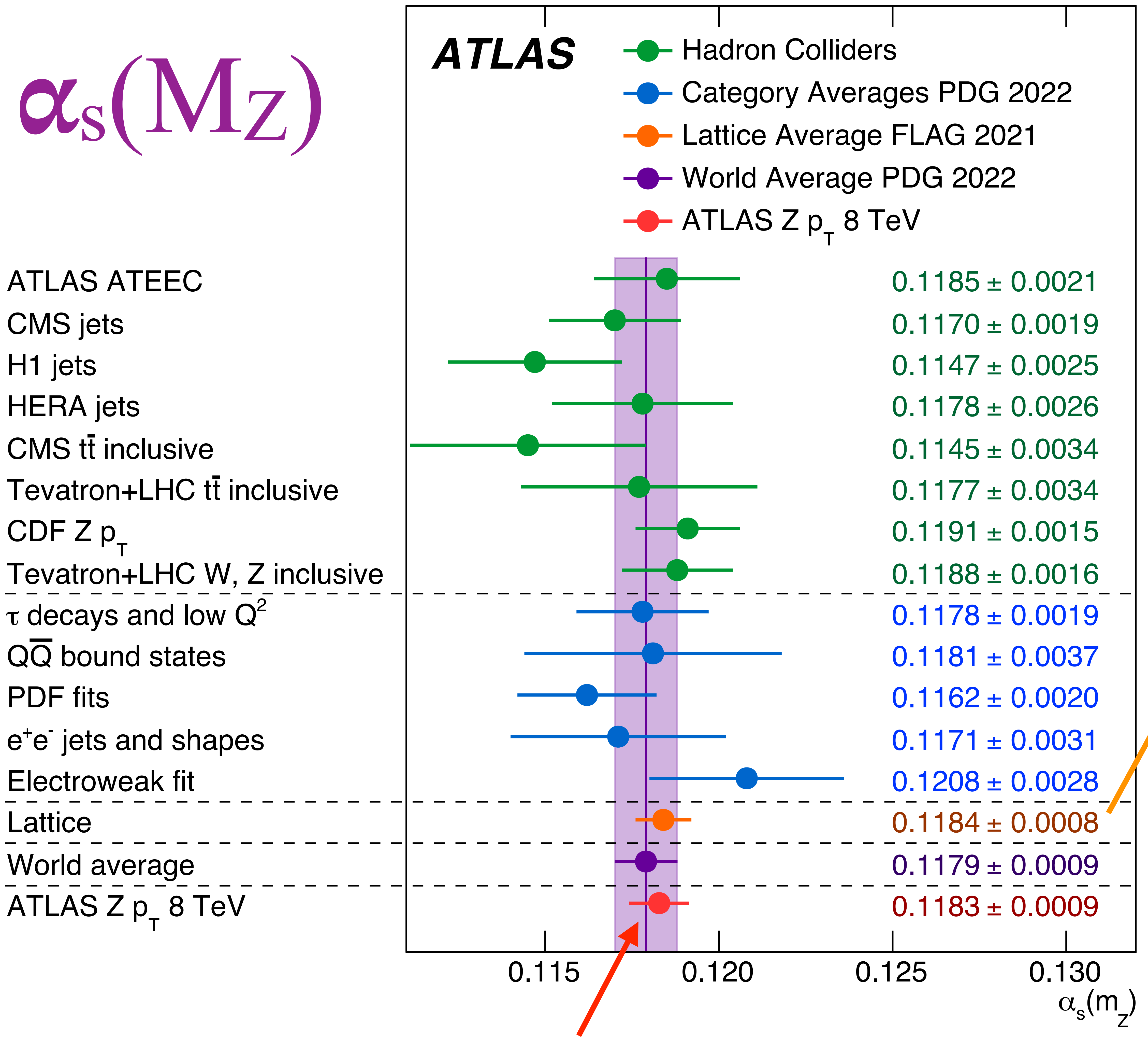


These are mesons that have relatively long lifetime and a well-determined mass from experiment.

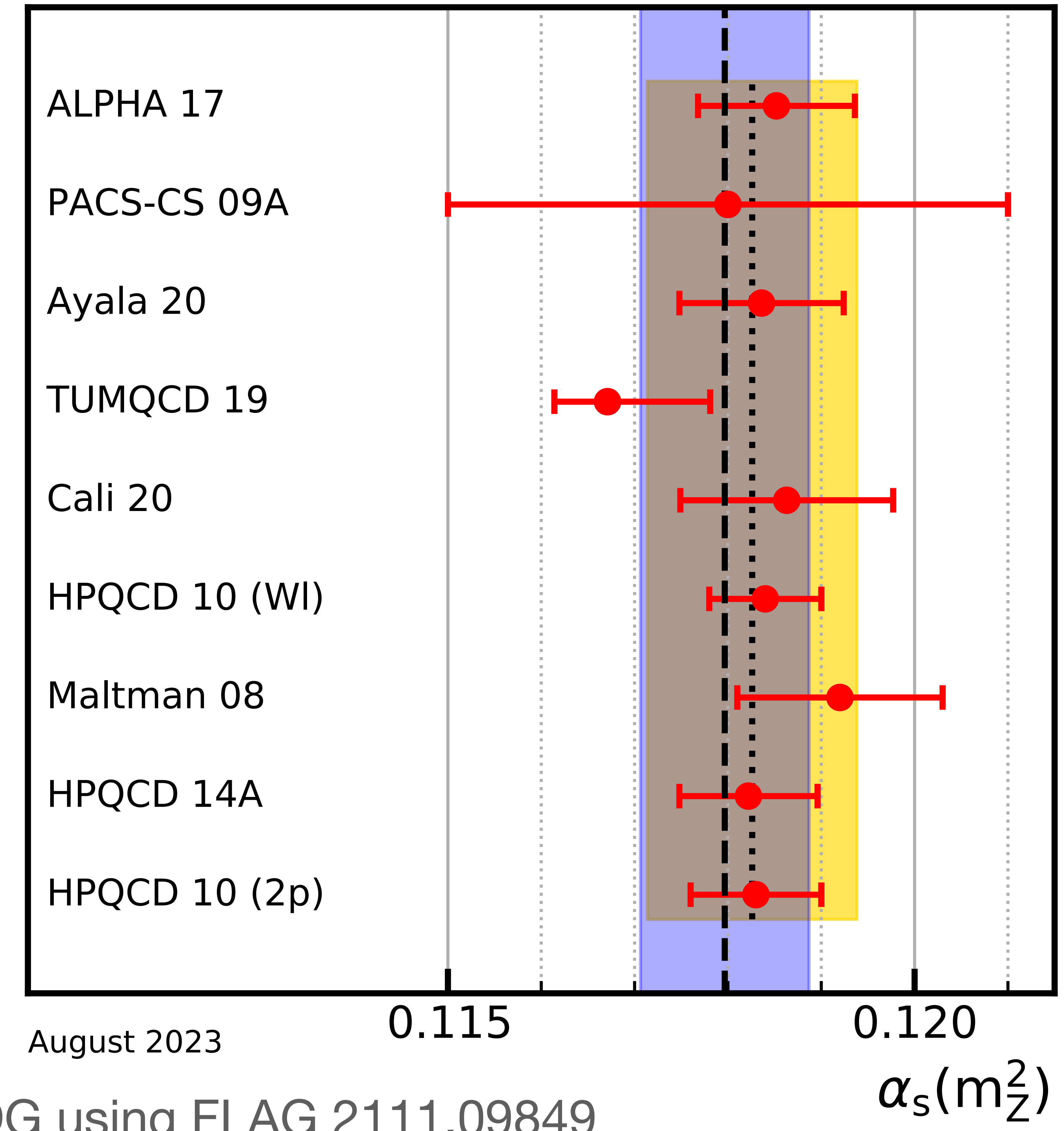
Agreement is good to very high (few MeV) accuracy. Now including QED effects to reduce uncertainties further …

QCD parameters - α_s

$\alpha_s(M_Z)$



Lattice QCD: measure a quantity on the lattice and compare to $O(\alpha_s^3)$ QCD perturbation theory



Step-scaling

Heavy quark potential

Light x-space correlators

Wilson loops

Heavy correlator time-moments

PDG using FLAG 2111.09849

ATLAS compared p_T distribution of Z bosons to $O(\alpha_s^3)$ QCD perturbation theory

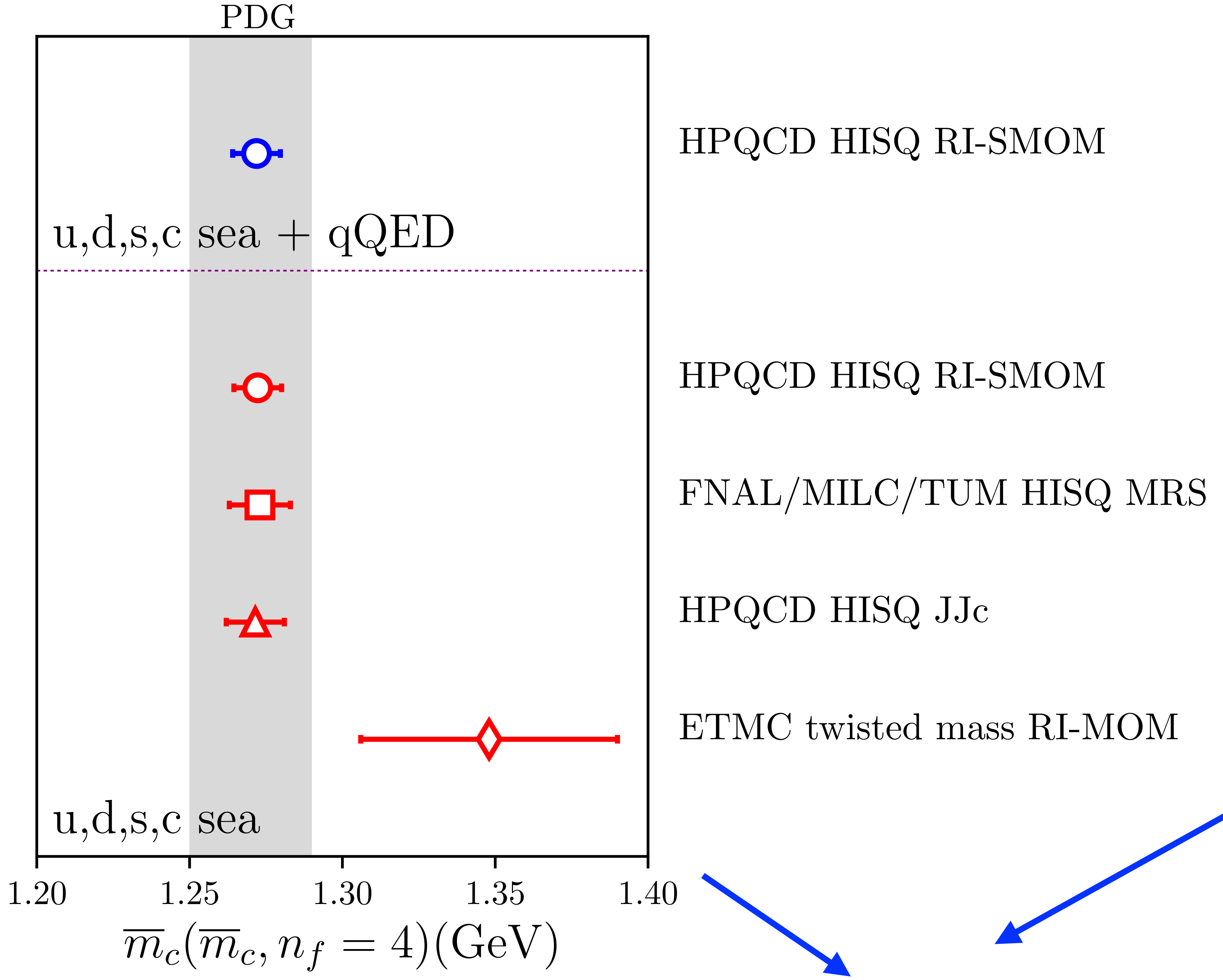
Lots of different lattice QCD approaches - results agree well

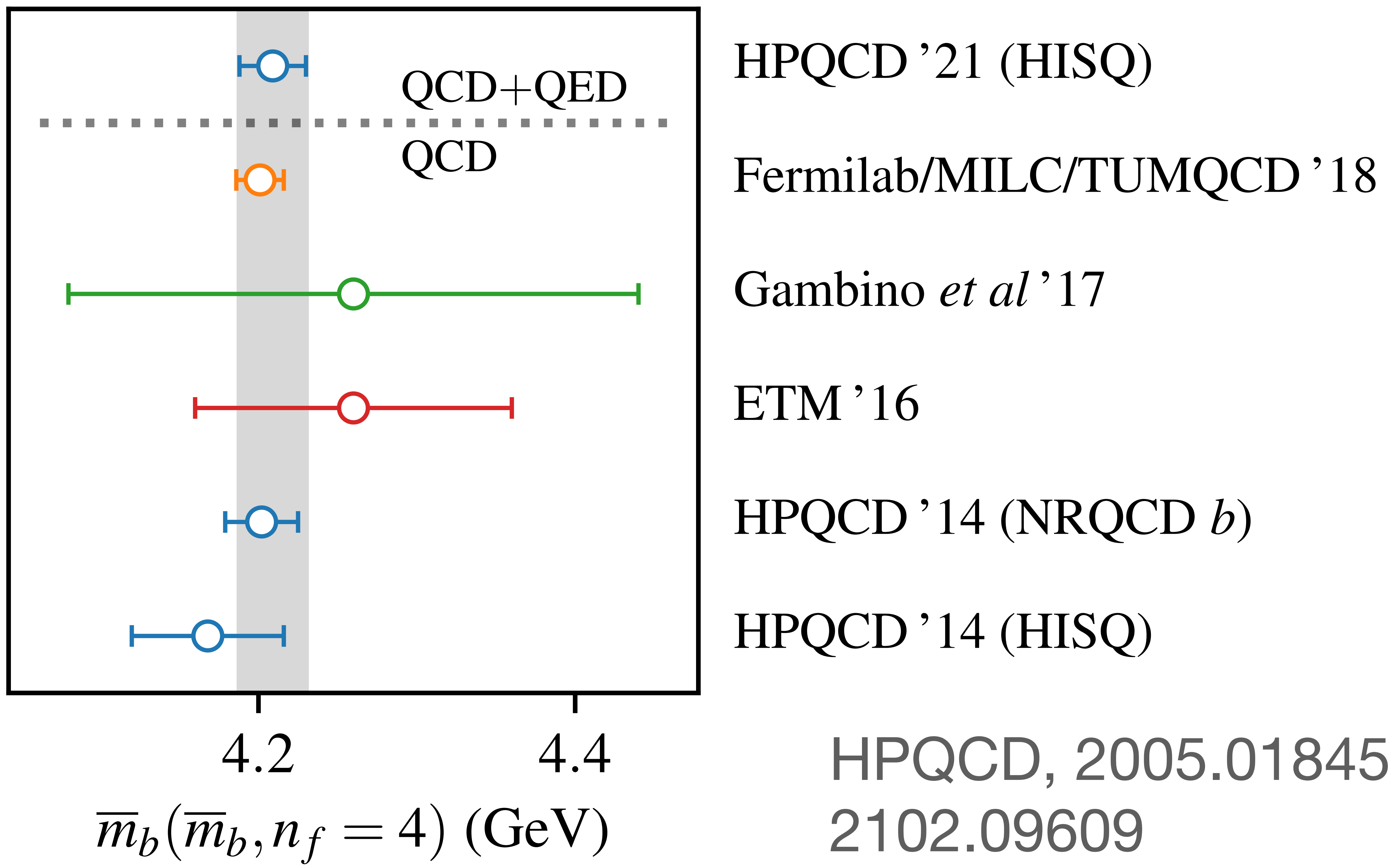
In good agreement!

ATLAS, 2309.12986

QCD parameters - quark masses

Multiple lattice methods agree well - now including effects from electric charge of valence quarks





HPQCD, 2005.01845, 2102.09609

Ratio more accurate than individual masses: $$\left.\frac{\overline{m}_b(3\,\mathrm{GeV}, n_f = 4)}{\overline{m}_c(3\,\mathrm{GeV}, n_f = 4)}\right|_{\mathrm{QCD+QED}} = 4.586(12)$$

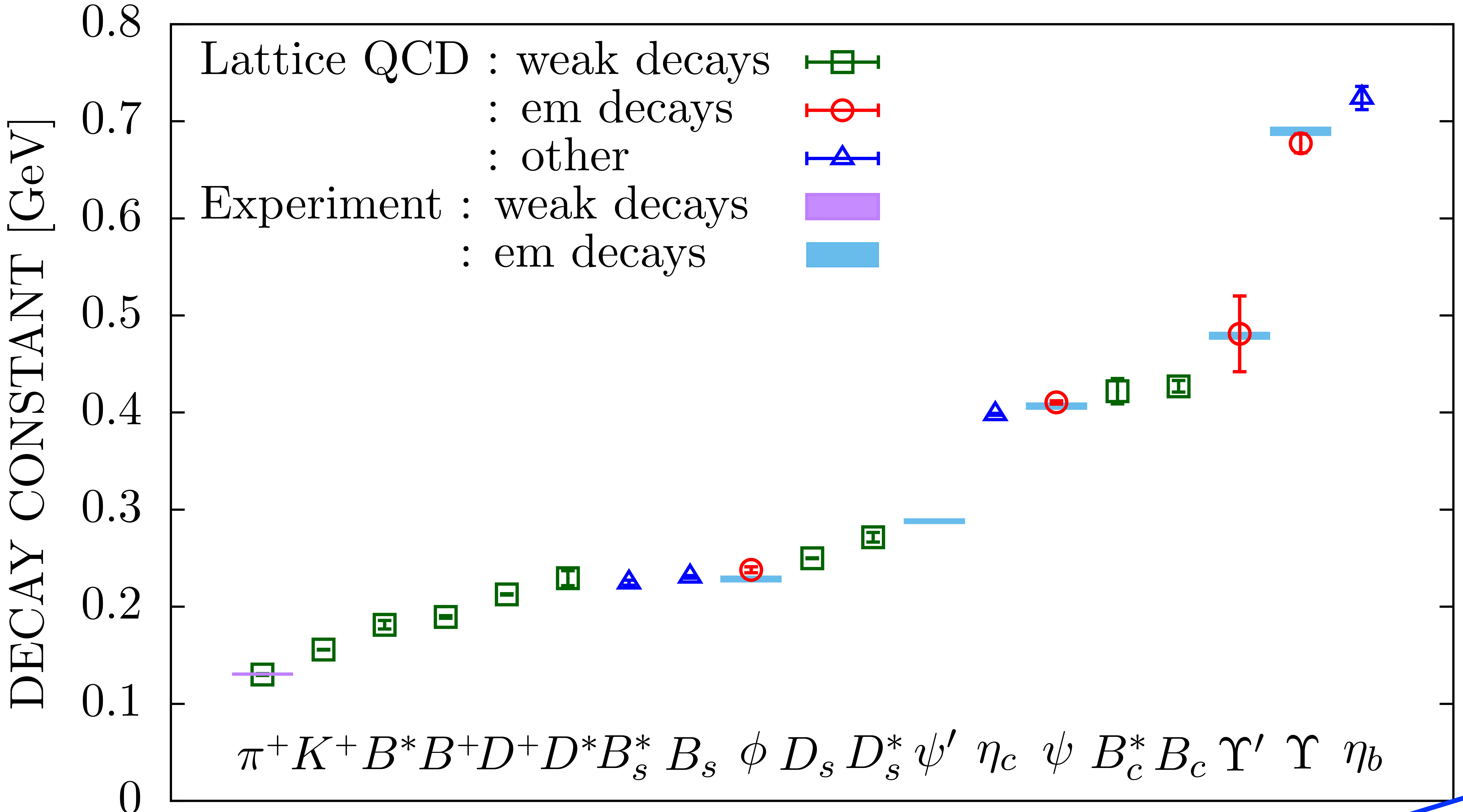
0.3% accurate

$$\left.\frac{\Gamma(H \to b\bar{b})}{\Gamma(H \to c\bar{c})}\right|_{\mathrm{SM}} = \frac{\overline{m}_b^2(M_H)}{\overline{m}_c^2(M_H)}\frac{(1 + r_b)}{(1 + r_c)}$$

calculable to 0.9%

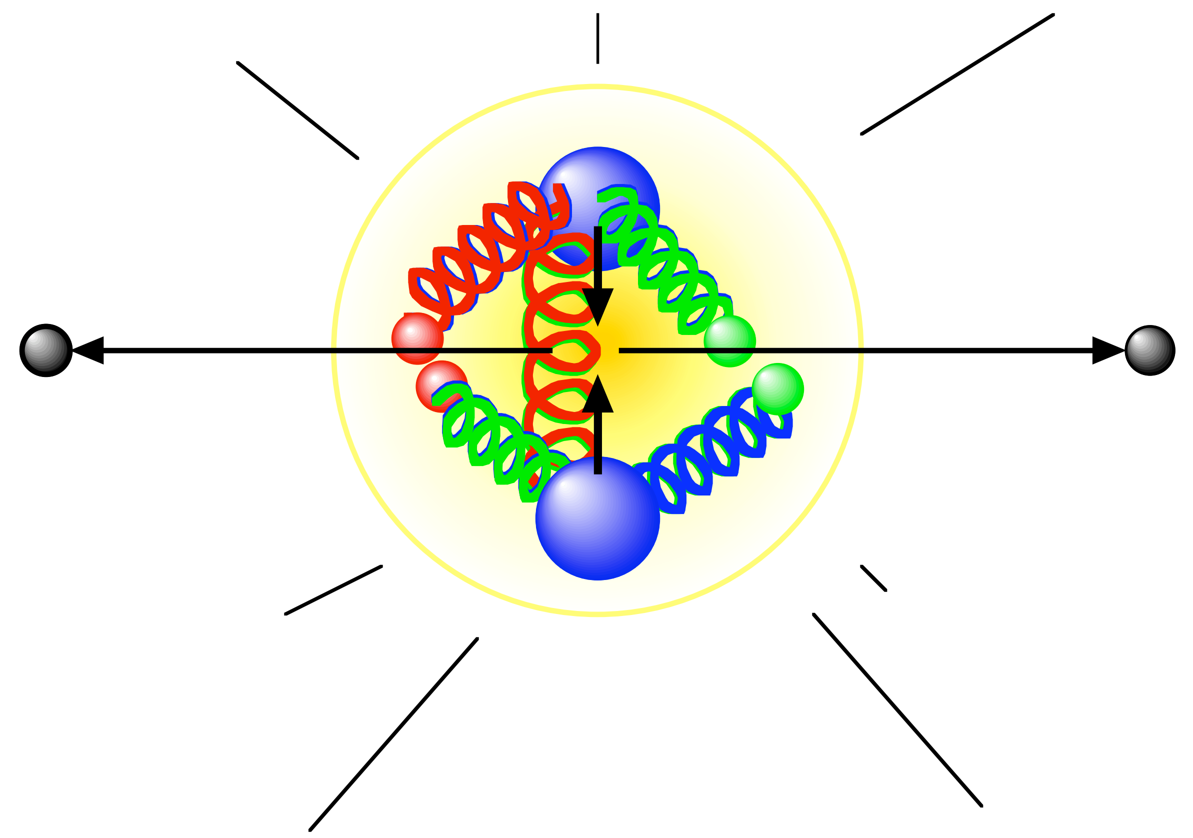
(LHC HiggsWG give 6%)

Meson weak and electromagnetic decay rates



C. Davies in *50yrs of QCD*, 2212.11107

Uncertainty <1% from lattice QCD:
e.g: 0.4% f_ψ, 0.2% f_K/f_π



Annihilation rate to γ or W determined by hadronic parameter called decay constant, f.

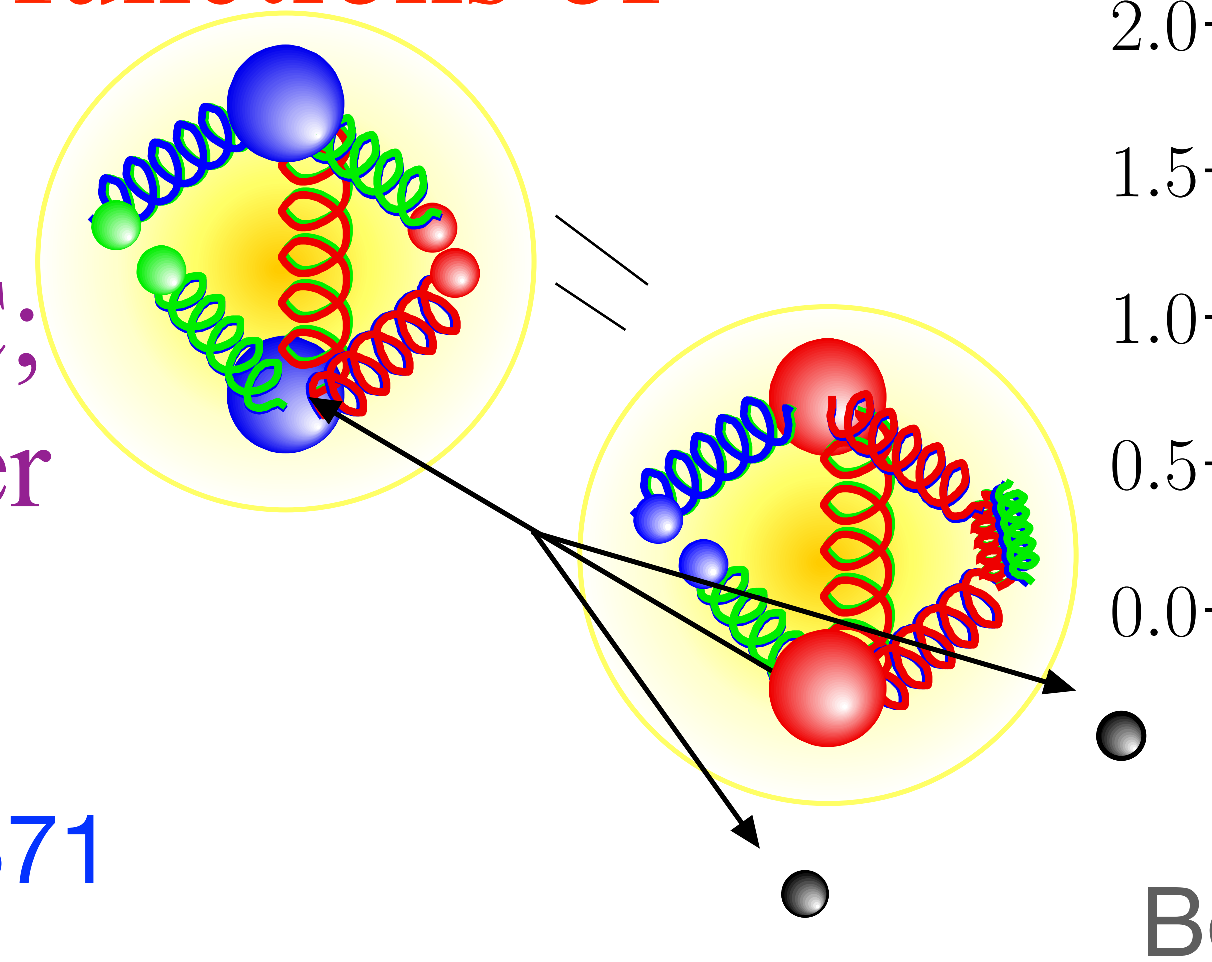
$$\Gamma = f^2 \times (\text{kin. factors}) \times (\text{CKM}^2 \text{ or } e_q^2)$$

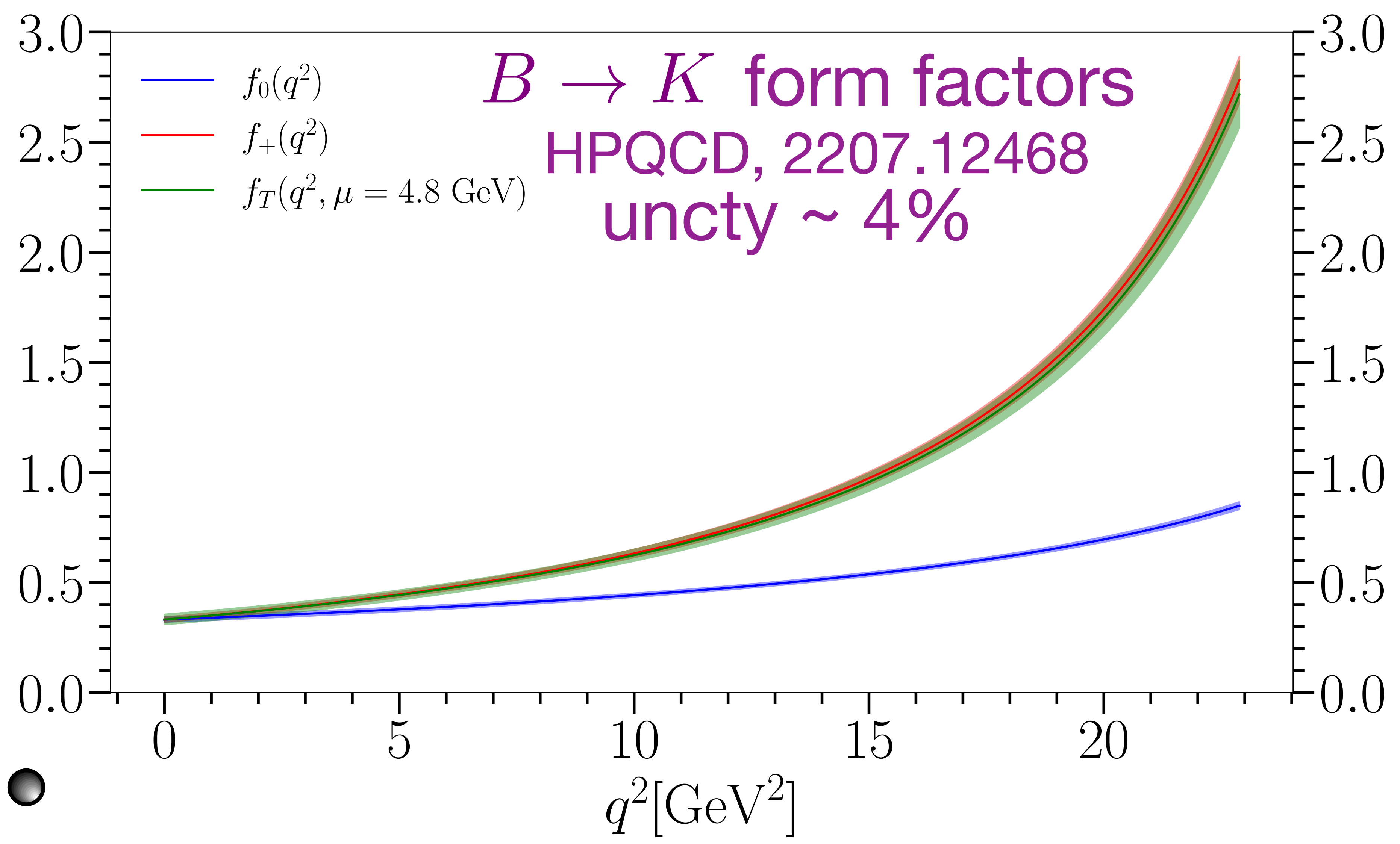
Comparison to expt. tests SM and/ or gives CKM elements

Meson semileptonic decay rates

Rate determined by form factors, functions of (4-momentum transfer)² = q^2

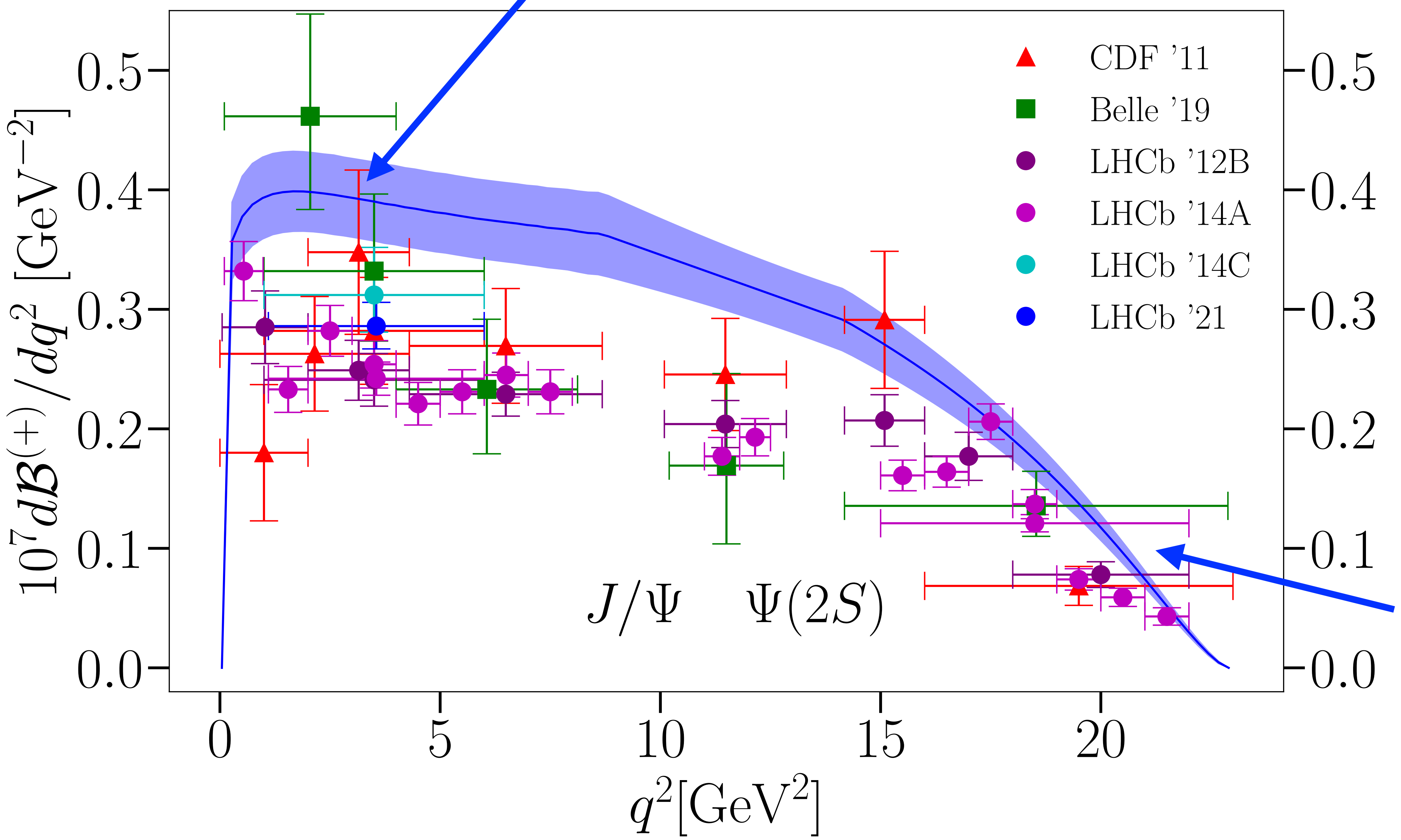
B→K decay proceeds via b→s FCNC; 3 form factors. Can now calculate over full q^2 range with lattice QCD.





$B \to K \ell^+ \ell^-$

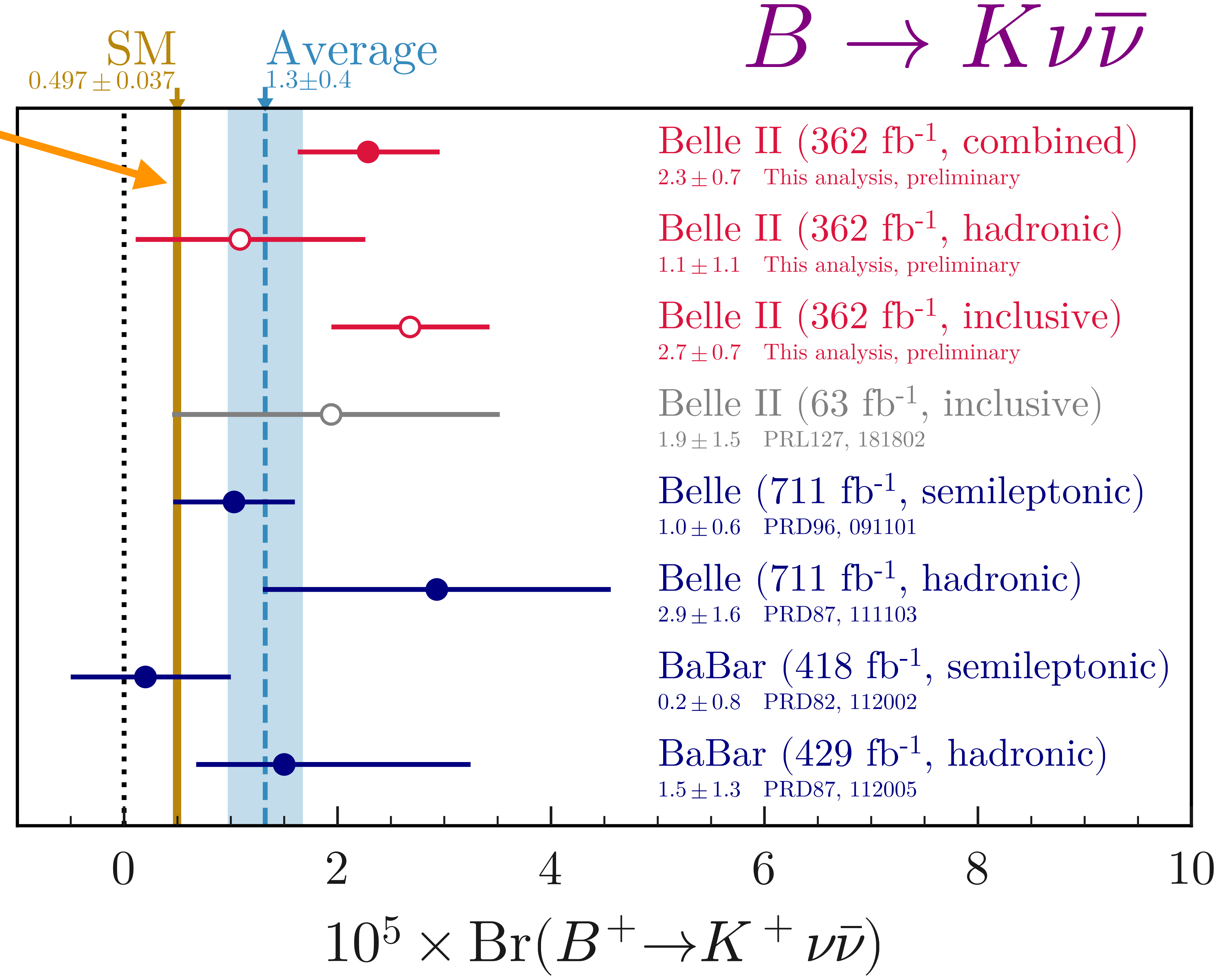
HPQCD, 2207.13371



LHCb 14A in 4σ tension with SM= HPQCD, 2207.13371

Belle II, 2311.14647 - 3.5σ evidence for $B \to K \nu \bar{\nu}$

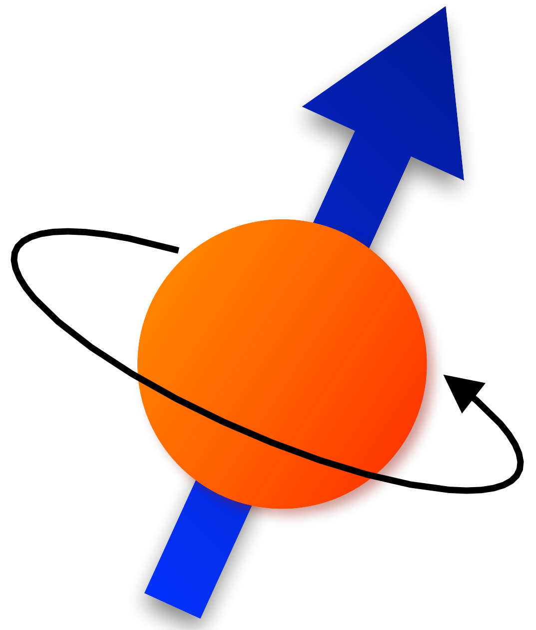
Belle II result in 2.7σ tension with SM= HPQCD, 2207.13371



Current hot topic - anomalous magnetic moment of the muon

The muon, μ, has electric charge and spin and therefore a magnetic moment

$$\vec{\mu} = g\left(\frac{e}{2m}\right)\vec{S}$$



Naive value of g=2 (from Dirac equation) in absence of any interactions

BUT μ interacts with a host of virtual particles generated by vacuum energy fluctuations.

Anomalous magnetic moment $$a_\mu = \frac{g-2}{2}$$

Accurate comparison of theory and experiment provides stringent test of the Standard Model

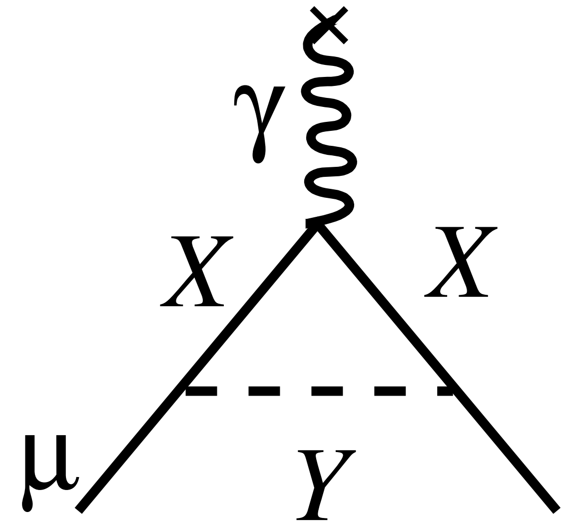
Current status

$$10^{11}a_\mu = 116592055(24)$$

Experiment - Muon g-2@FNAL PRL131:161802 (2023); runs1-3.

$$10^{11}a_\mu = 116591810(43)$$

Theory white paper: Phys. Rep. 887:1 (2020)



New physics?

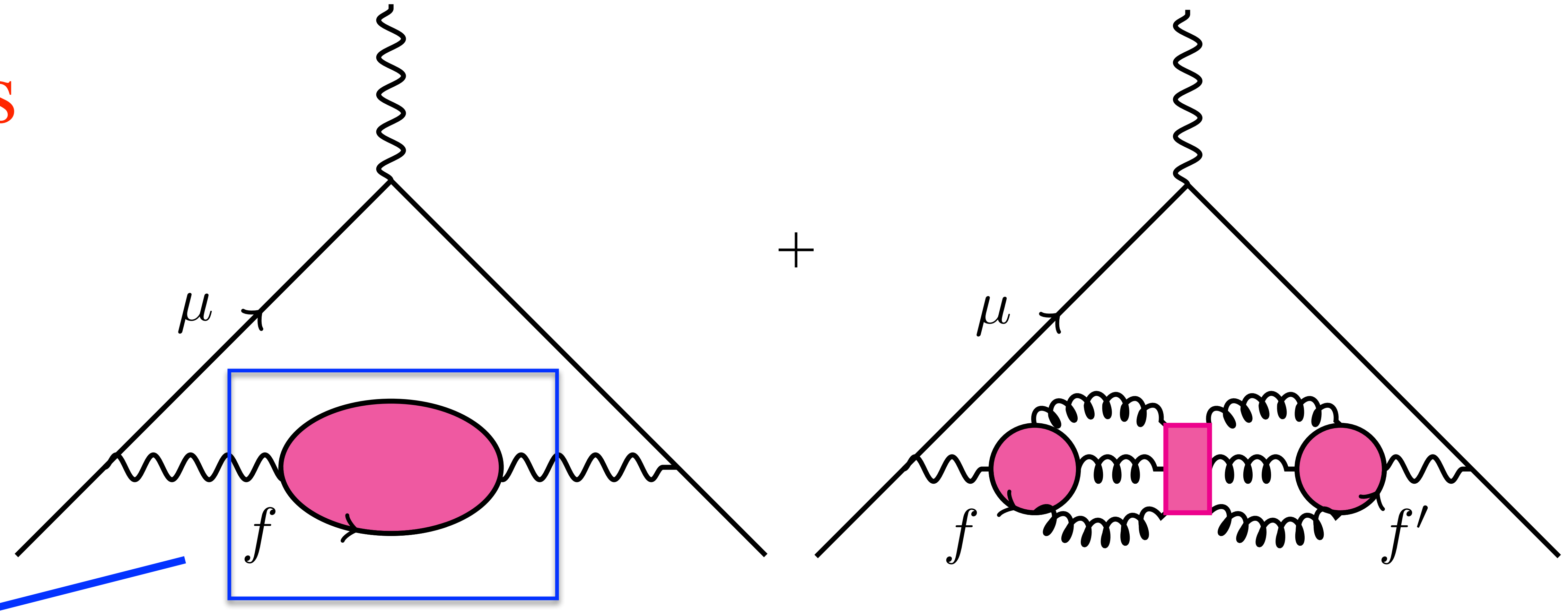
Difference $= 245(49) \times 10^{-11}$

5σ !

but QCD contributions need more work ....

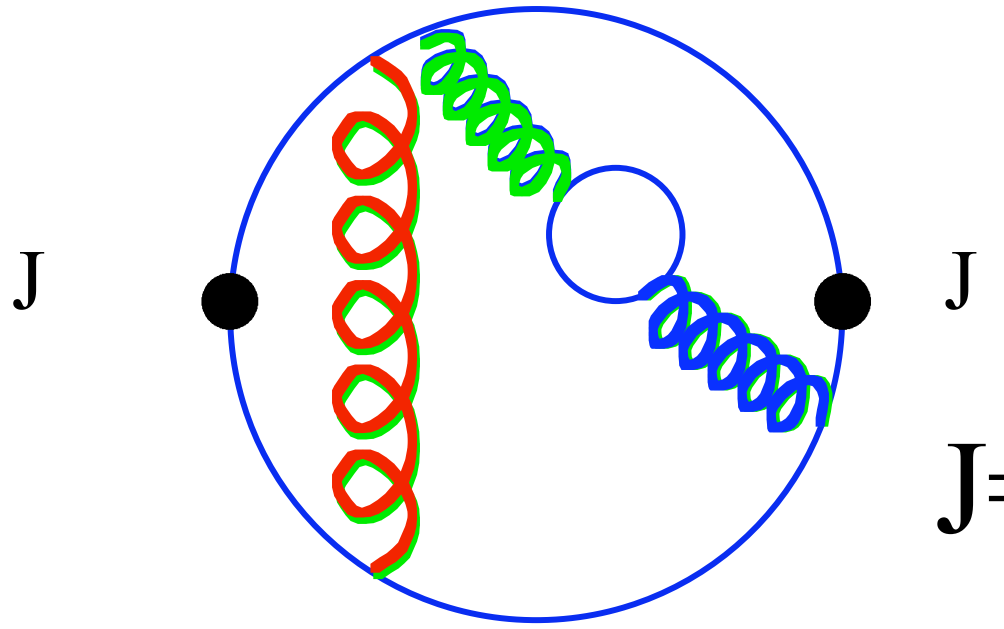
QCD contributions to a_μ start at α^2_{QED}, nonperturbative in QCD

LO Hadronic vacuum polarisation (HVP) dominates uncertainty in SM result. Largest non-QED piece: ≈7000×10^{-11}



How to calculate a_μ^{HVP} ?

Key ingredient is central quark bubble connected to a photon at either side



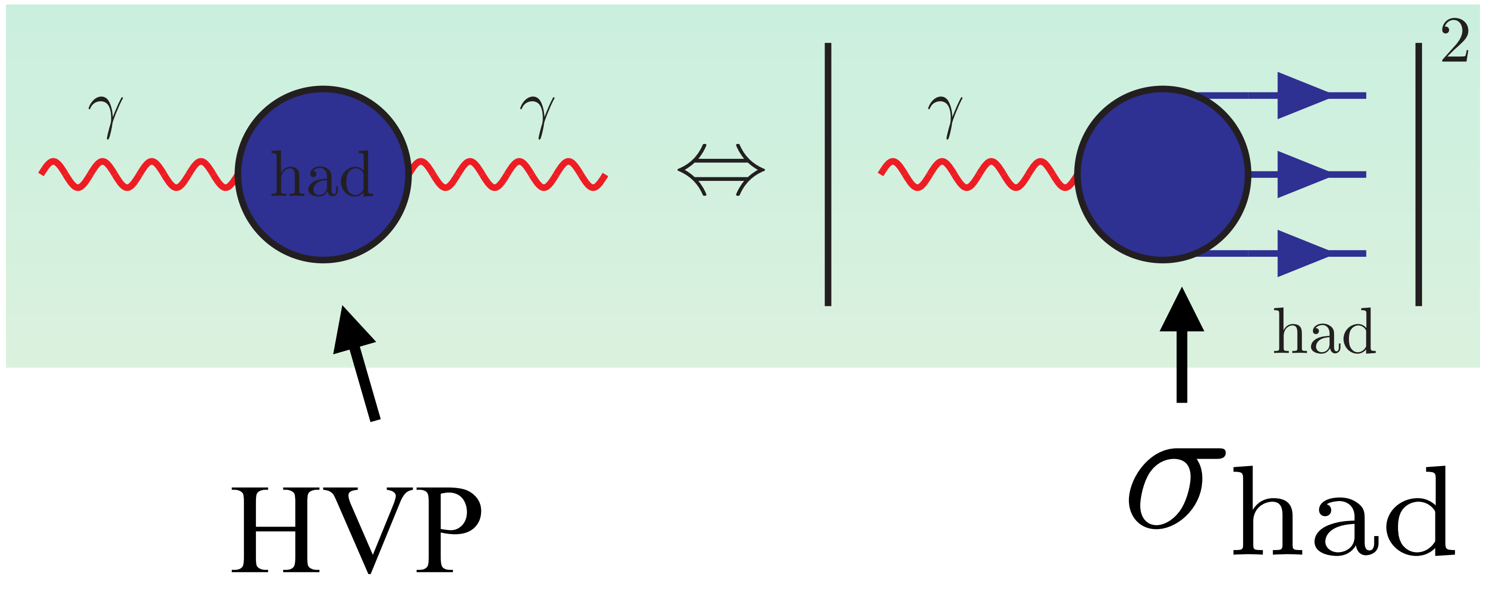
J=vector current

$= e_f \overline{\psi}_f \gamma_\mu \psi_f$ couples quark, of flavour f, to photons

Two methods

1) Use optical theorem to relate HVP to $\sigma(e^+e^- \longrightarrow \gamma^* \longrightarrow$ hadrons) and use experimental data

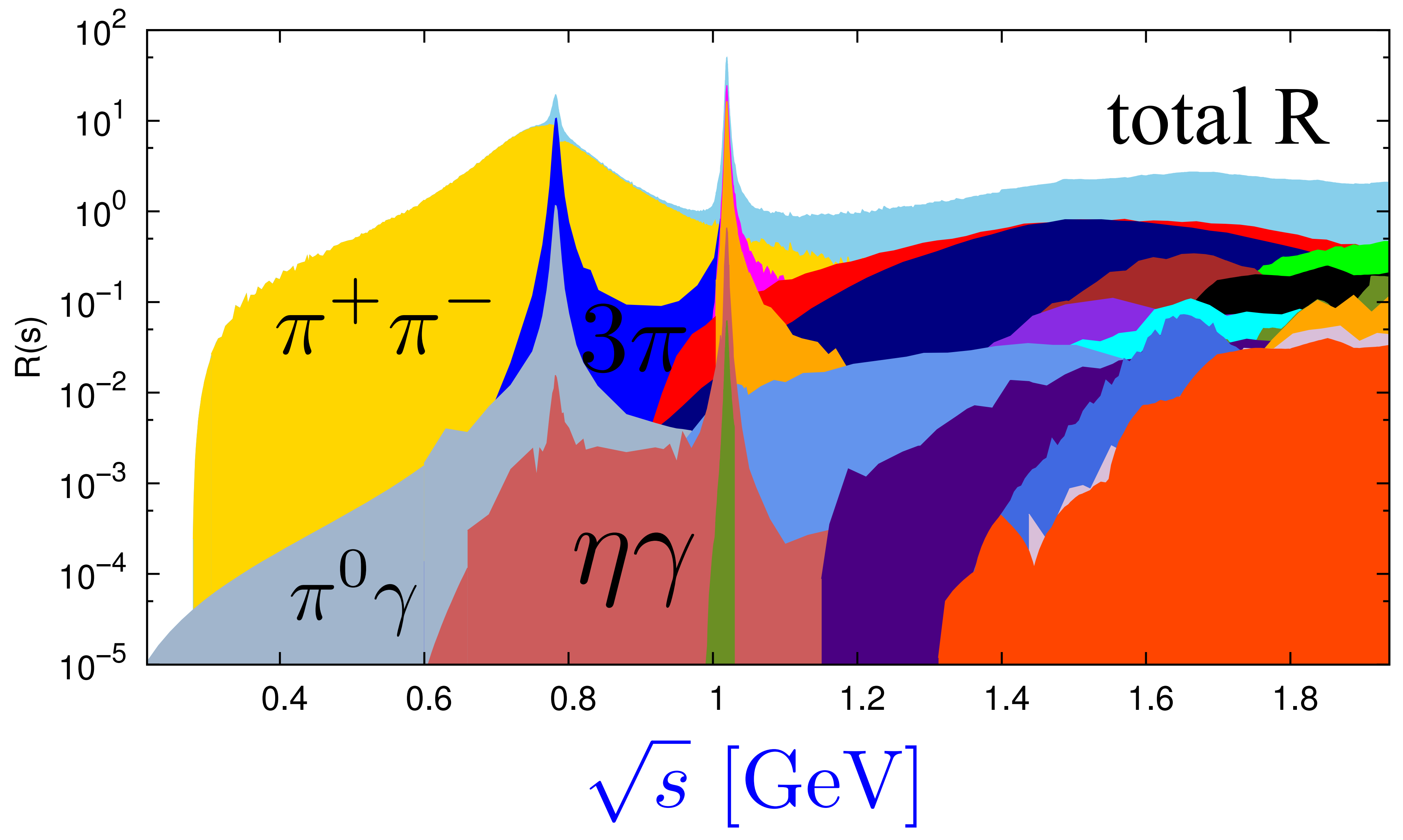
has given smallest errors so far



2) Direct computation of the vector-vector correlation function for u, d, s and c quarks in Lattice QCD

1) $\sigma(e^+e^- \to \text{hadrons})$

$R = \frac{\sigma}{\sigma_{pt}}$

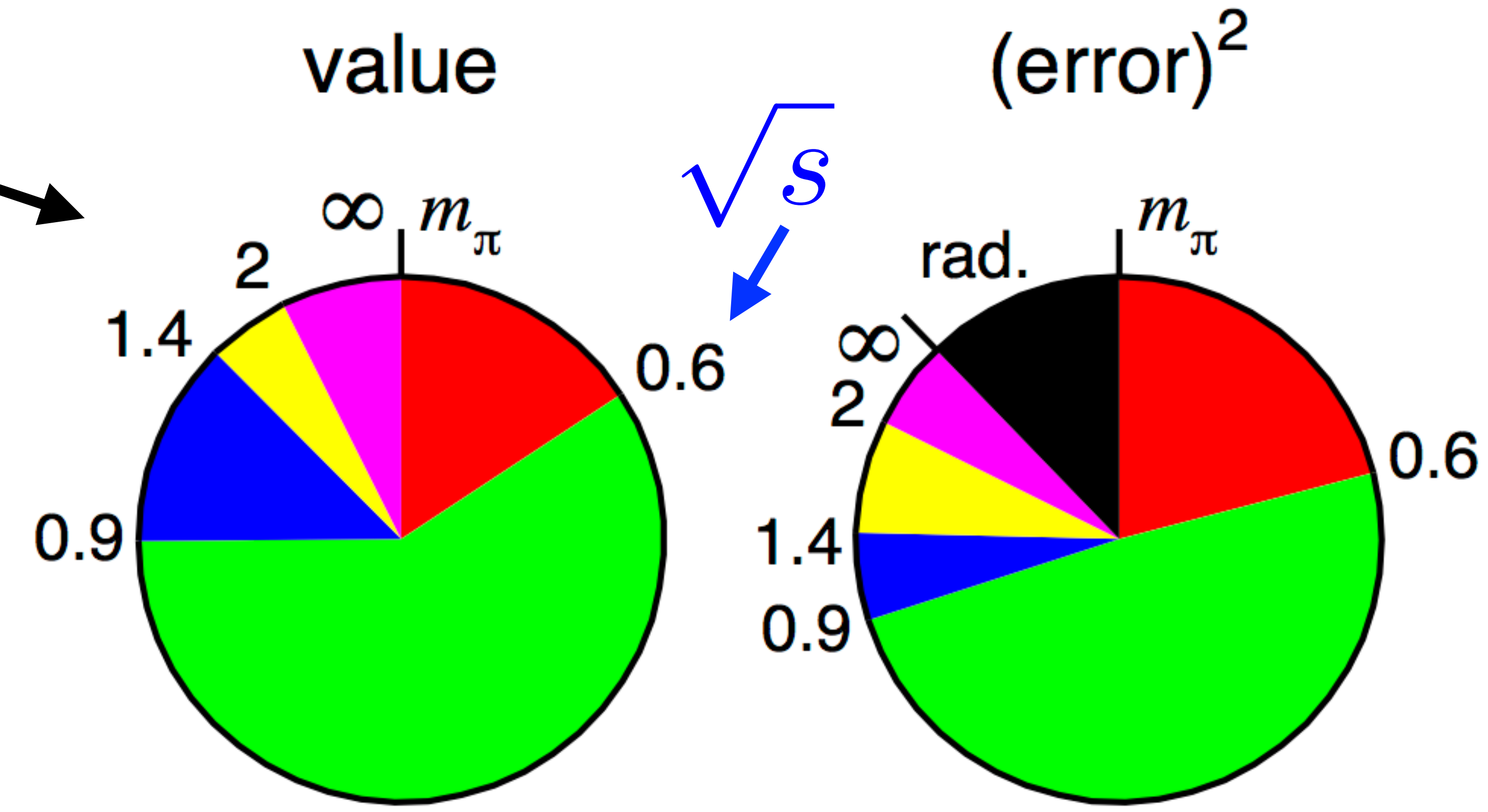


$$a_\mu^{\rm HVP} = \frac{m_\mu^2}{12\pi^3}\int_{m_\pi^2}^{\infty} ds\, \frac{\hat{K}(s)}{s}\sigma^0_{\rm had}(s)$$

s = (Centre of mass energy)^2 $\qquad e^+e^- \to \gamma^* \to hadrons$

Because of kernel function, integral is dominated by a few channels at low s.

Keshavarzi et al, 1911.00367; Davier et al, 1908.00921



Theory WP 'data-driven' average $\quad a_\mu^{\rm HVP} = 6931(40) \times 10^{-11}$

BMW lattice QCD, 2002.12347 $\quad a_\mu^{\rm HVP} = 7075(55) \times 10^{-11}$

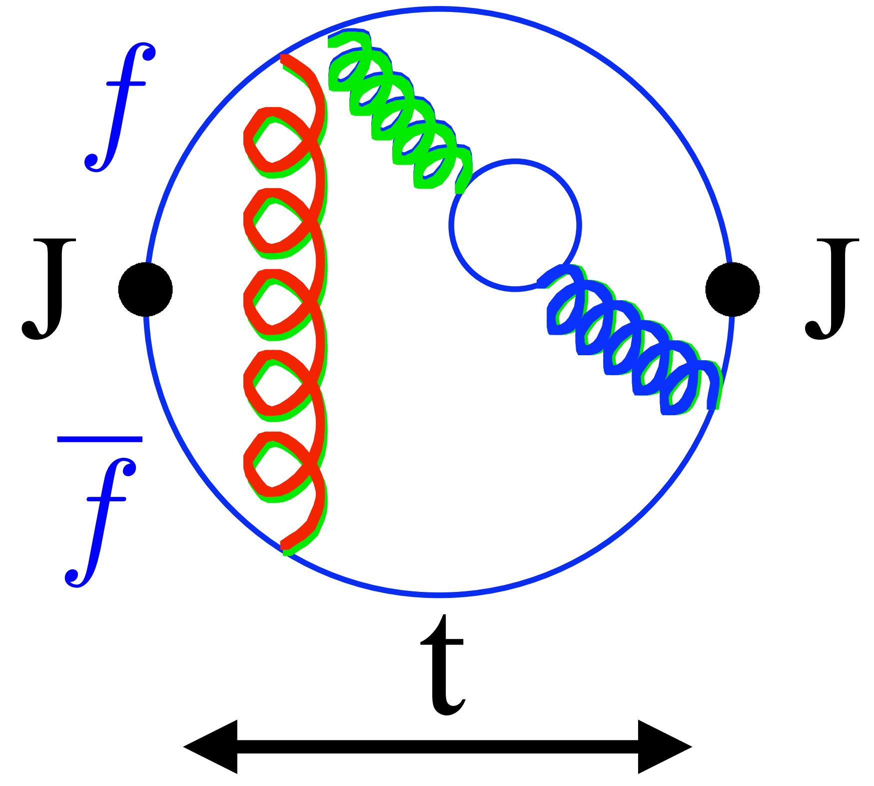
difference $= 144(68) \times 10^{-11}$

pushing SM result upwards towards expt.

But lattice QCD less accurate so far. How to do a more accurate test of data-driven HVP?

2) Lattice QCD

Calculate ‘two-point’ vector-vector correlation function C(t)

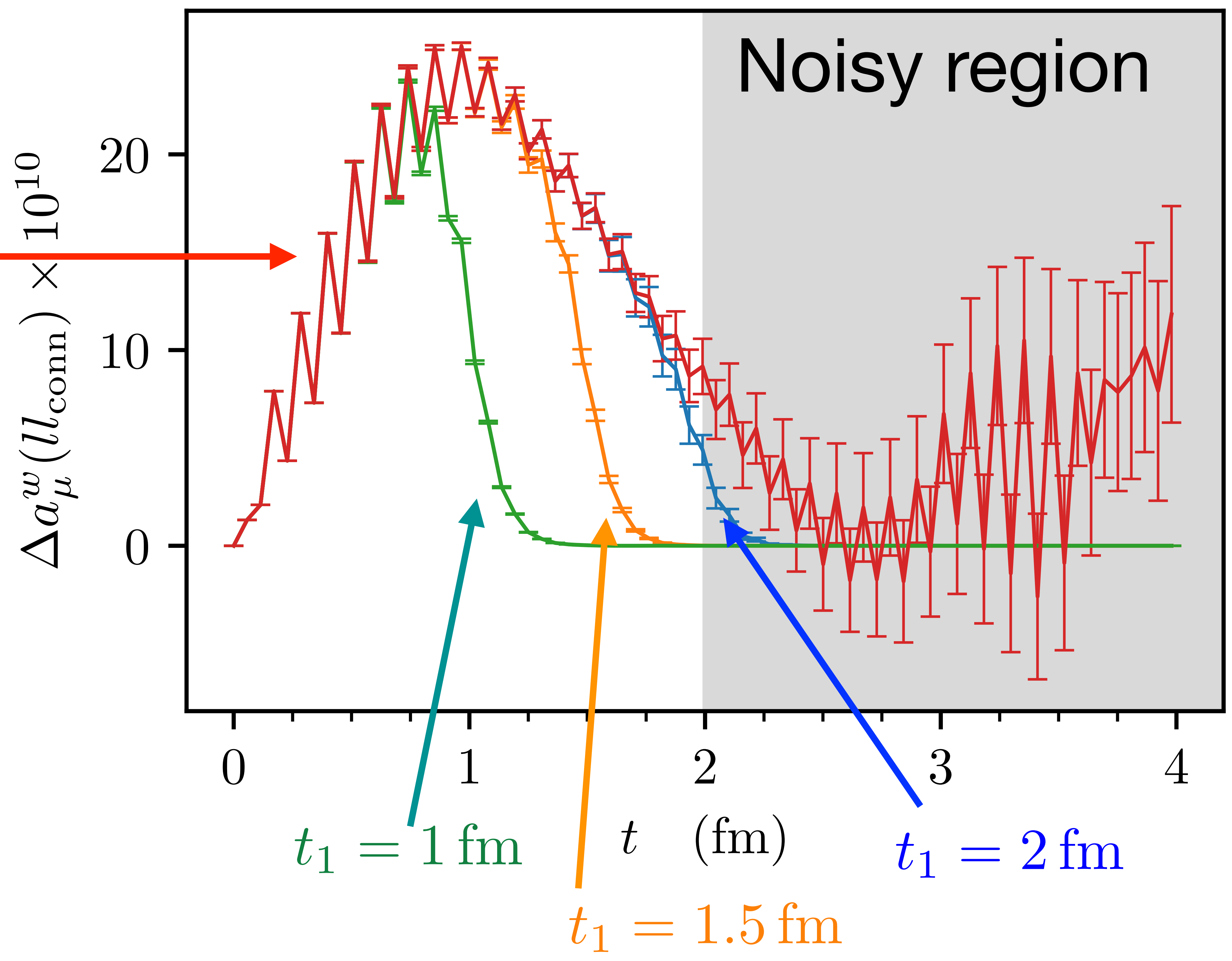


$$C(t) = \frac{1}{3}\sum_{i,x}\langle j_i(x,t)j_i(0,0)\rangle$$ falls exponentially with t

rises from 0 at t=0

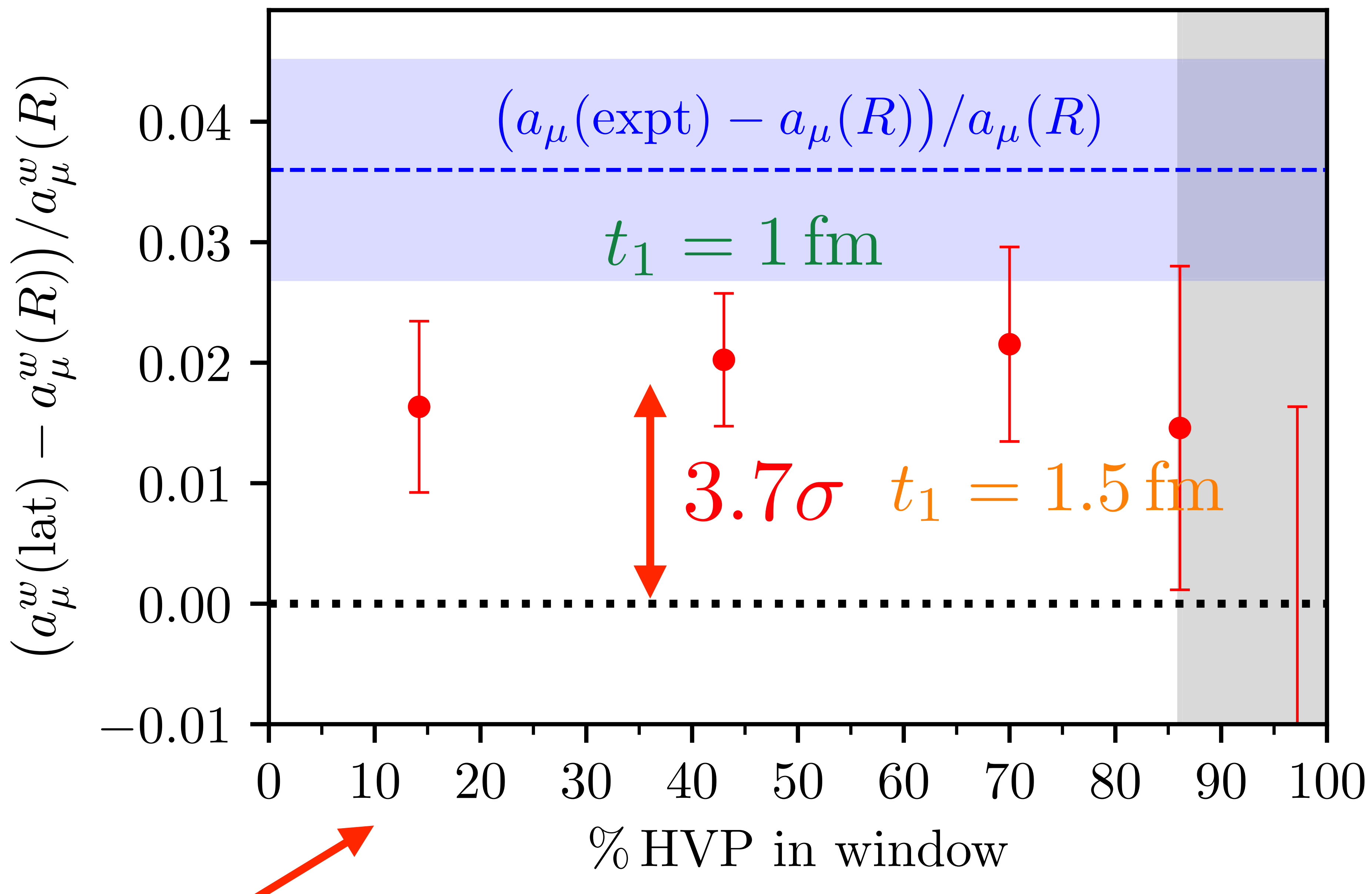
$$a_\mu^{\mathrm{HVP},f} = e_f^2\left(\frac{\alpha}{\pi}\right)^2\int_0^\infty dt\,\tilde{K}(t)C(t)$$

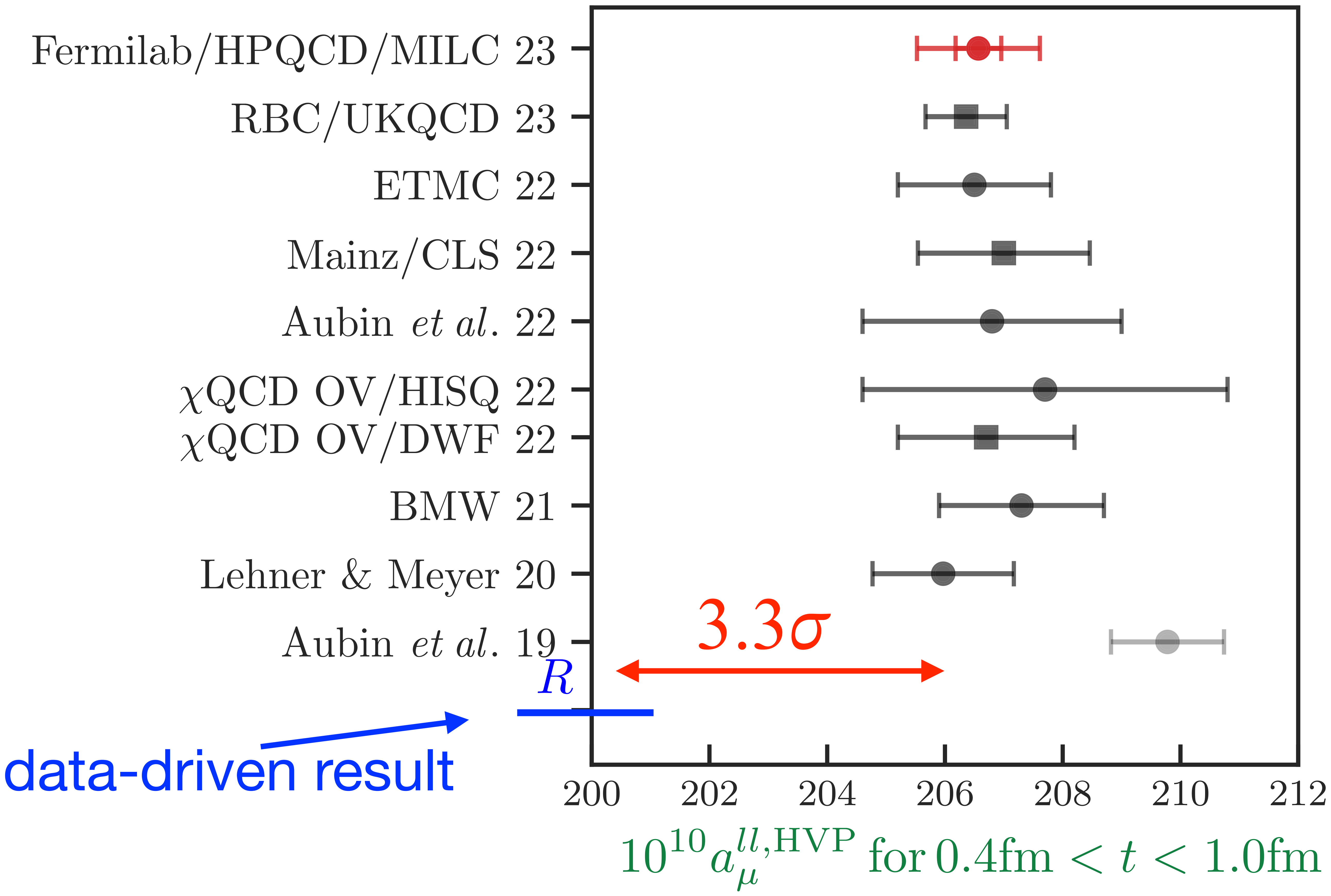
Largest (90%) and most problematic contribution is from u/d quarks - C(t) noisy at large time



Apply smooth ‘window-in-time’ from t=0 to t=t_1 to cut out noisy region. Then

- Lattice QCD results have smaller uncertainty
- Can apply SAME window to data-driven results and compare





For total HVP in window see significant tension with data-driven (R) result - 3.7σ at t_1=1fm

Fermilab/HPQCD/MILC, 2207.04765

Inferred data-driven result

Multiple lattice QCD calculations agree on 'intermediate-window' u/d result - in significant tension with data-driven value.

Conclusion: current data-driven HVP value is probably too low. i.e. there is probably less 'new physics' than we thought.

Needs more theory work and more experimental results on low-energy e+e-→hadrons to sort out. (See CMD-3 2302.08834)

WATCH THIS SPACE!

Lattice QCD has come a long way in 50 years!

We now have multiple precision tests of QCD (uncertainties below 1%)

Future

- Improve precision on quantities needed for new physics searches e.g. HVP for g-2, form factors for flavour physics … Include QED and m_d-m_u effects.

- Extend wider calculations of spectrum, including exotica, mixing with multi-hadron states to quantitative results. More baryon physics.

- Longer term - exploit quantum computing!

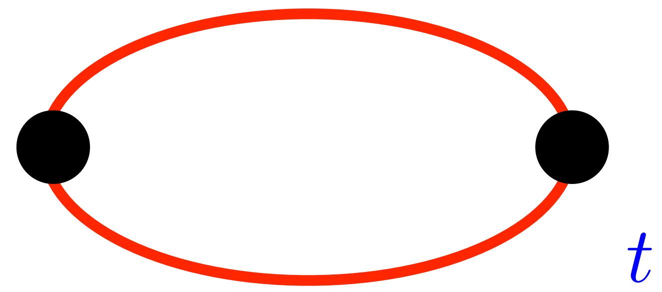
Backup slides

Lattice QCD = three-step procedure

1) Generate sets of gluon fields (inc. effect of sea quarks) for MC integrn

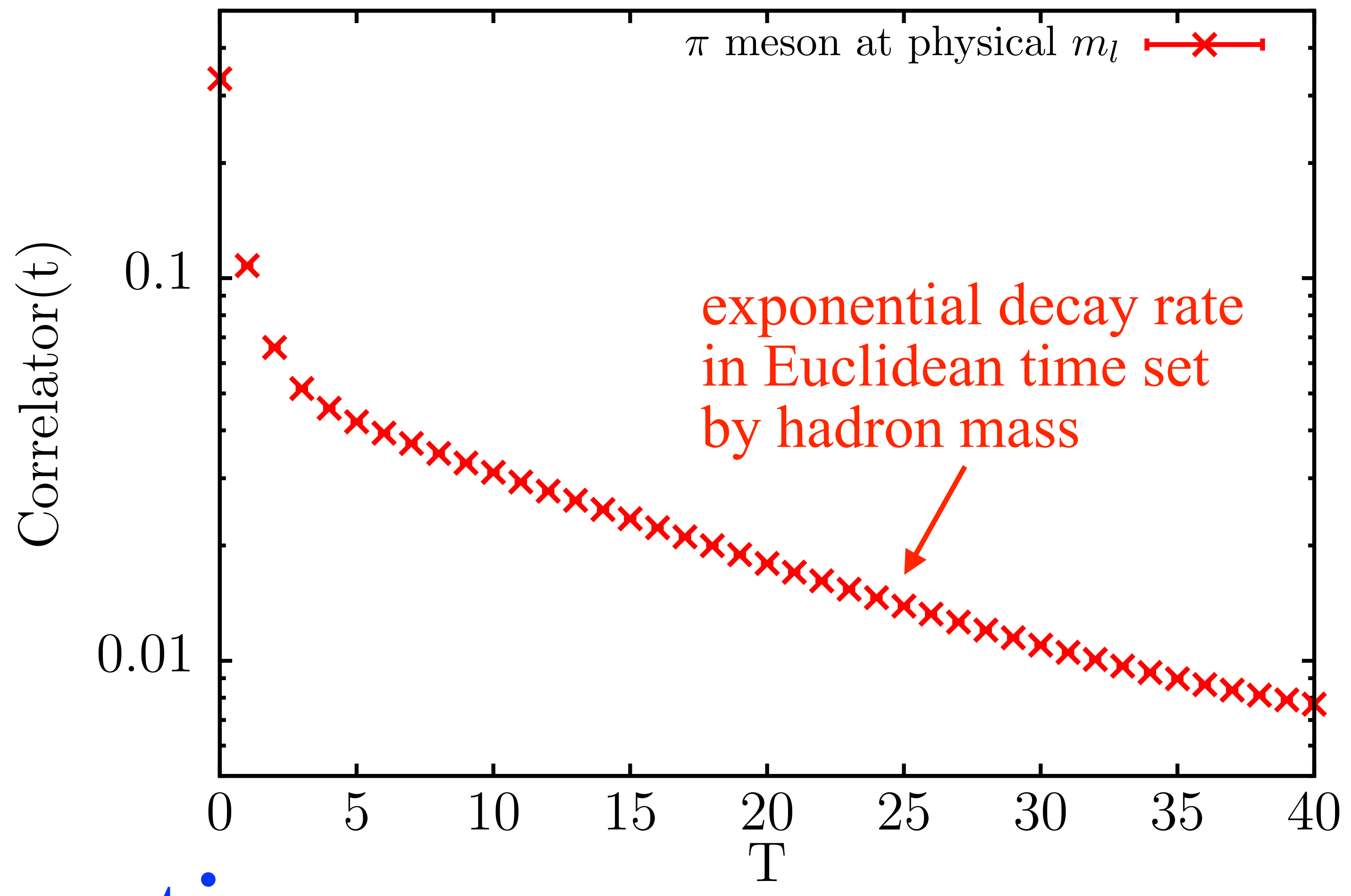
numerically extremely challenging

2) Calculate valence quark propagators and combine to make "hadron correlation functions" - average these results over the set of gluon fields for $\langle \mathcal{C} \rangle$ =



numerically costly, data intensive

3) Fit $\langle \mathcal{C} \rangle$ to obtain hadron masses and decay amplitudes in units of the lattice spacing, a. Fix a and each m_q using calibration hadron masses.



Repeat 1-3 at different a for extrapolation to a =0.

Final accuracy depends on :

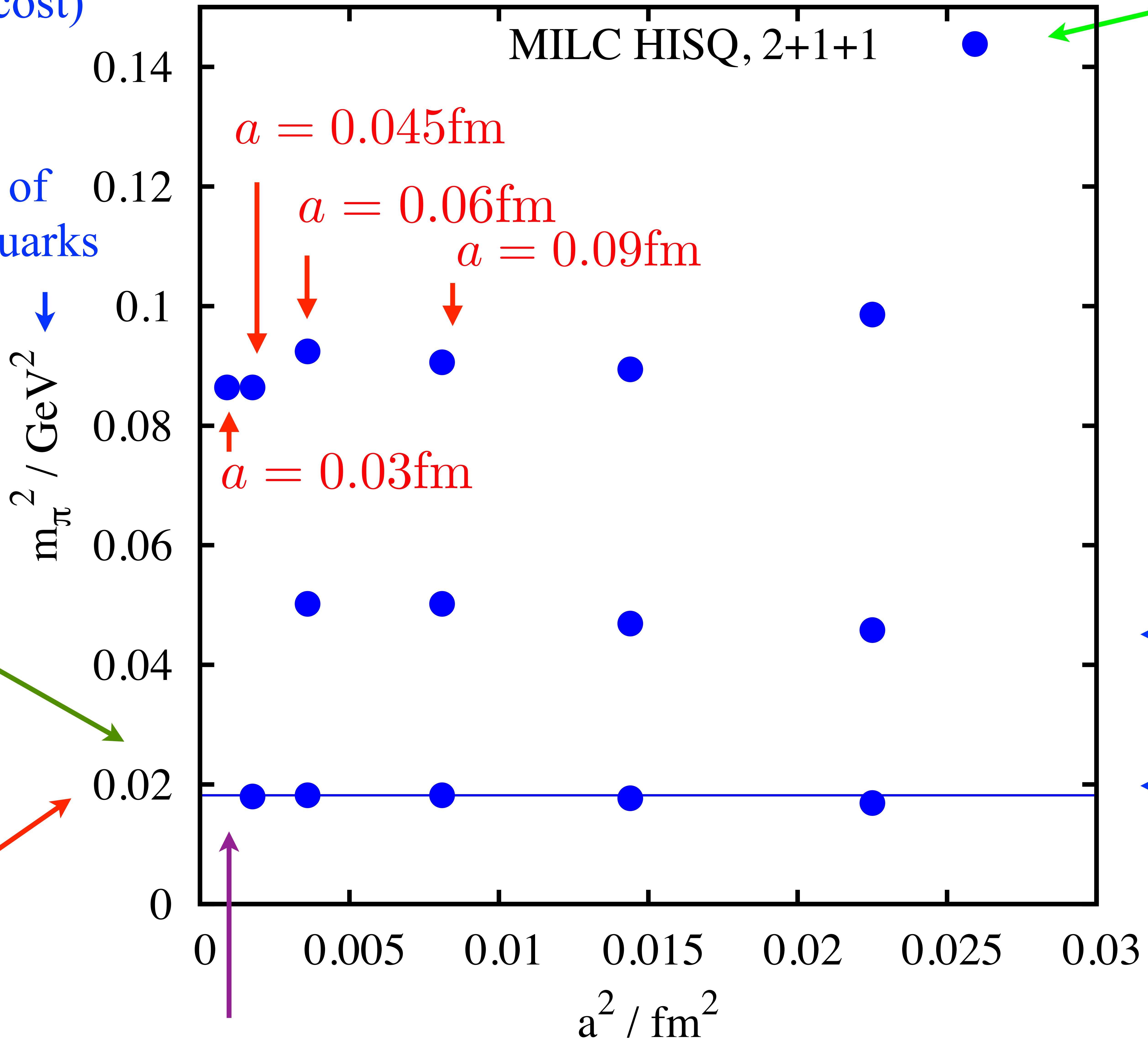
- statistical accuracy i.e. number of gluon field configurations
- control of lattice spacing dependence/ how well quark masses are tuned
- normalisation of operators (for decay amplitudes)

Example state-of-the-art: Parameters for gluon field configurations with HISQ sea quarks

$m_u = m_d$
$= m_l$ (halves cost)

Configs with $m_u \neq m_d$ also being generated now

mass of u,d quarks



"2nd generation" lattices include u/d, s and c quarks in sea

HISQ = Highly improved staggered quarks -very accurate discretisation of Dirac equation

E.Follana, et al, HPQCD, hep-lat/0610092.

Want u/d quarks with physical (light) masses for their physics - expensive!

$m_{u,d} \approx m_s/10$

$m_{u,d} \approx m_s/27$

*physical $m_{u/d}$ *

$m_{\pi^0} = 135$ MeV

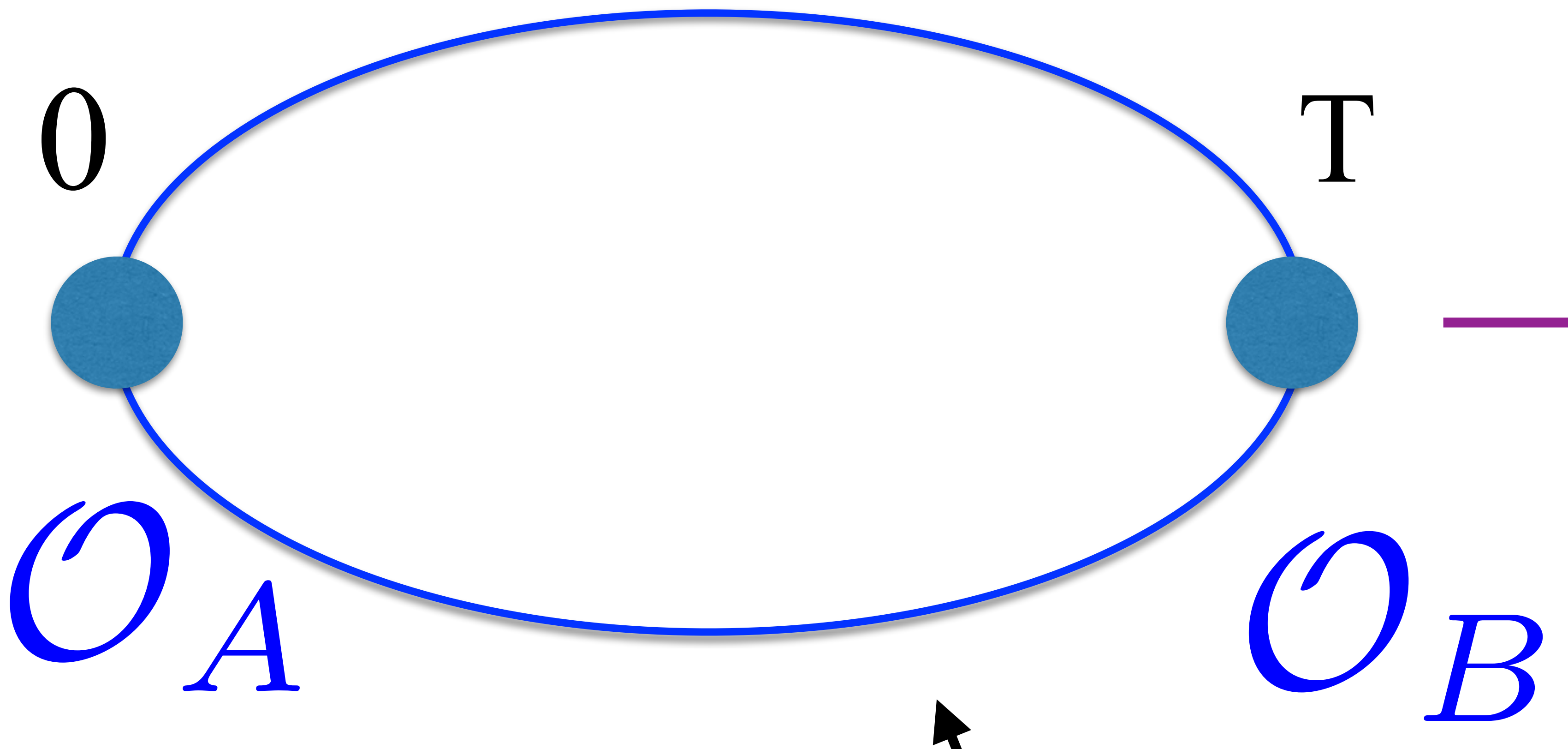
Spatial size:

$m_\pi L > 3$

~6 fm for physical m_l

Very fine lattices important for b quark physics

Meson Correlation functions are constructed from valence quark propagators



2-point function

av. over gluon fields and fit

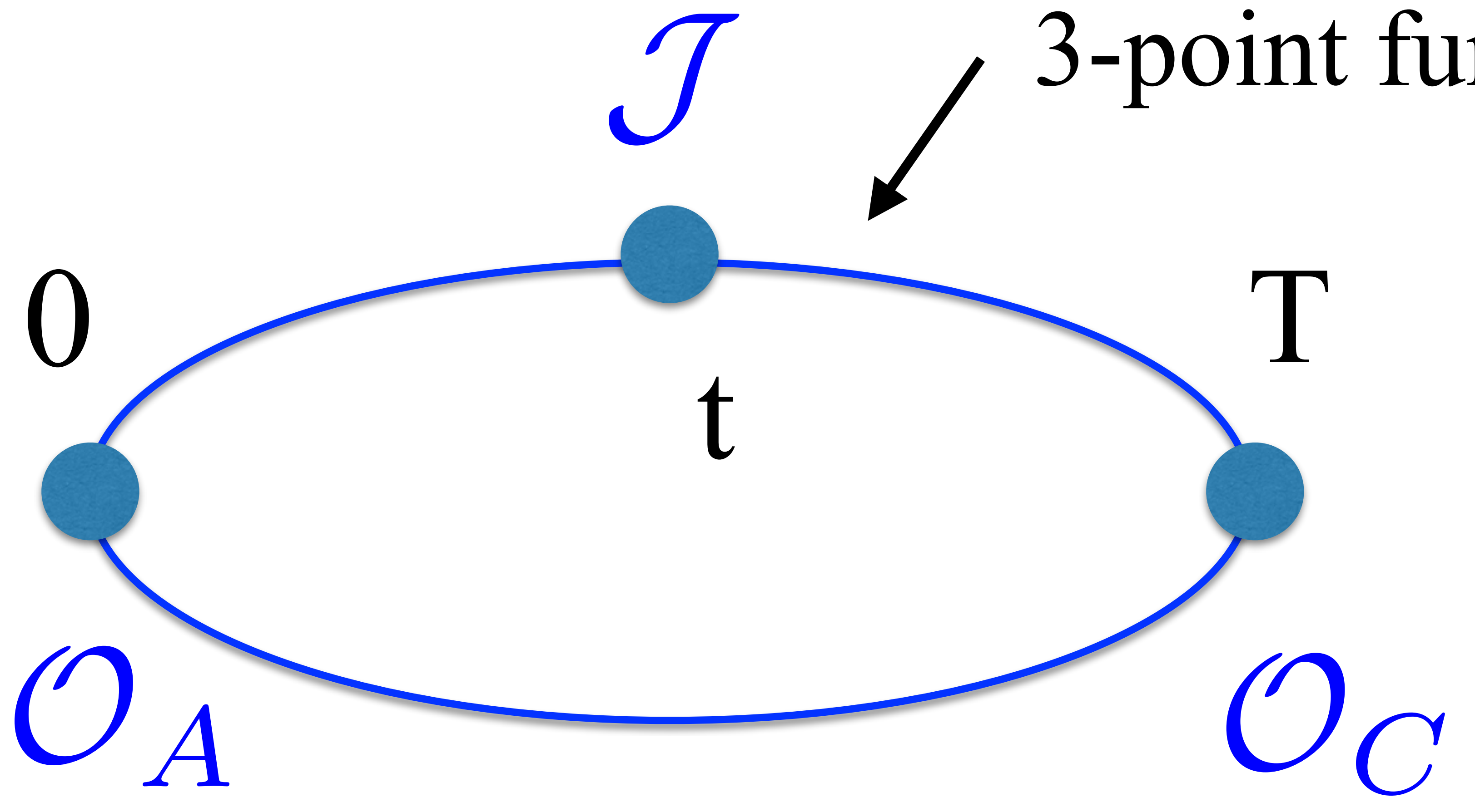
Multiple states need to be included in fit

$$C_2 = \sum_n A_n B_n e^{-M_n T}$$

A_n: $\langle 0|\mathcal{O}_A|n\rangle$ — decay constant, if O normalised

M_n: Meson mass - Ground-state mass can be very accurate. Use to tune lattice quark mass

3-point function



$$C_3 = \sum_{m,n} A_n J_{nm} C_m \, e^{-M_n t} e^{-M_m (T-t)}$$

J_{nm}: $\langle n|\mathcal{J}|m\rangle$ → form factor, if J normalised

Connected correlators shown here, some processes also have quark-line disconnected diagrams

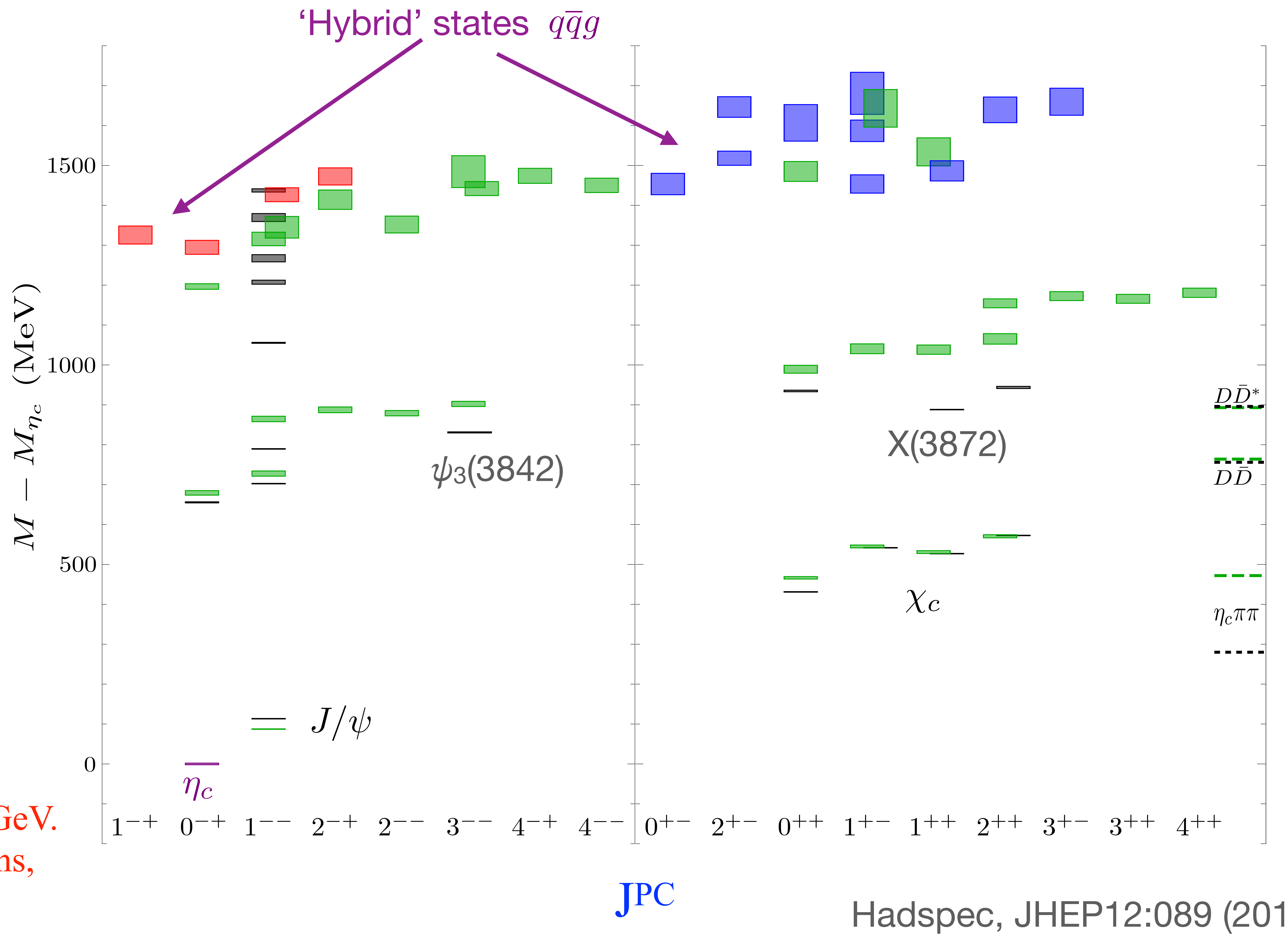
A more complete spectrum of charmonium mesons

Calculate the masses of many excited states (but with much lower accuracy)

Many operators used;
So far, calculations at only one value of the lattice spacing

black=experiment
green,red,blue=lattice

Lowest 'Hybrid' states arise from coupling to 1^{+-} gluonic excitation which adds ~1.3 GeV. Same picture seen for baryons, light mesons etc.



Hadspec, JHEP12:089 (2016)

Lattice QCD is an international endeavour

Needs huge amounts of High Performance Computing time

International collaborations of physicists - sizes: O(5) to O(50), to exploit national supercomputing facilities

Some gluon fields are made publicly available for others to calculate correlators on - improves productivity of the field.

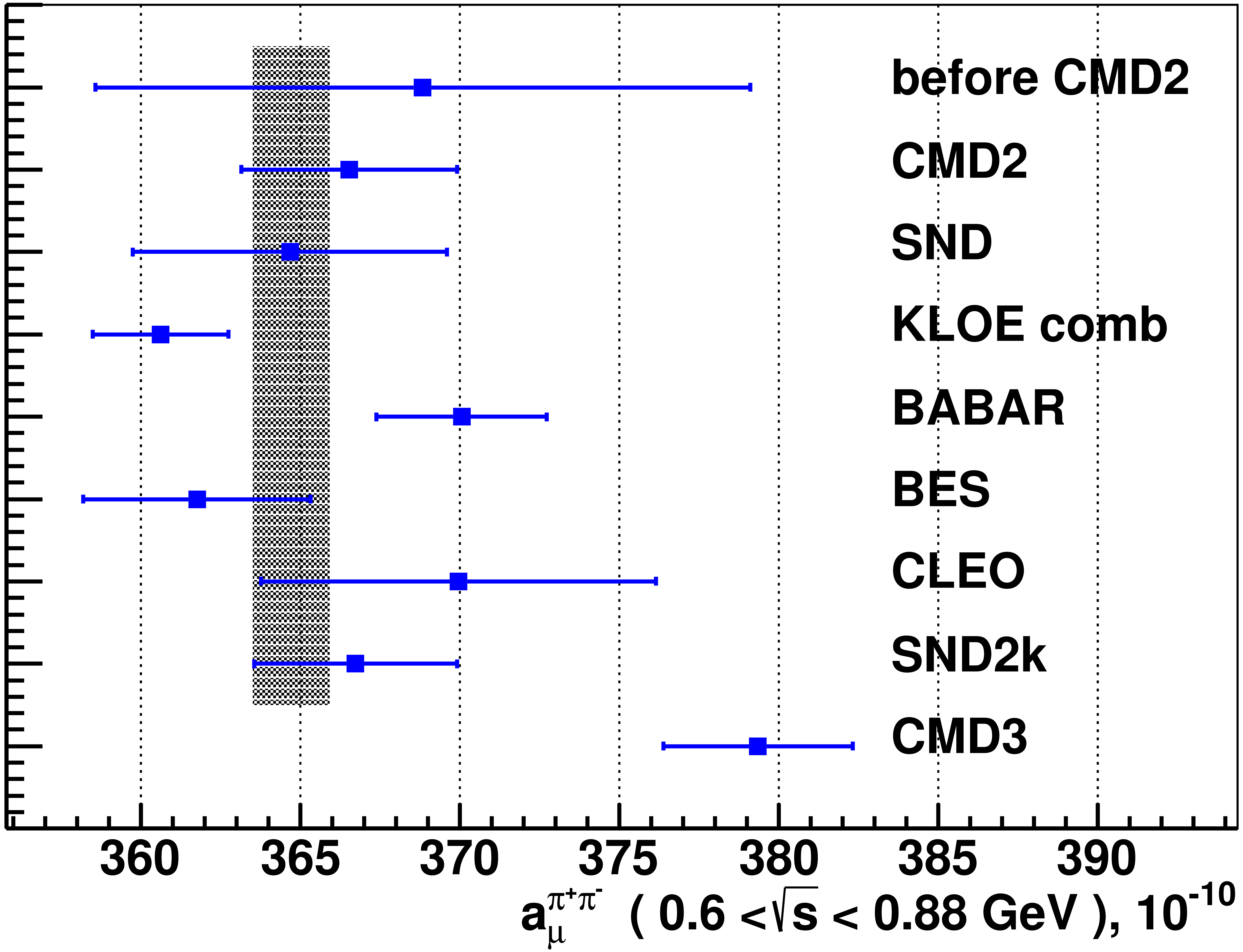
In UK : 28 DiRAC www.dirac.ac.uk

Shared by astronomy, nuclear and particle physics theorists, 3 services at 4 sites: Data Intensive (Cambridge/Leicester) ; Extreme Scaling (Edinburgh); Memory Intensive (Durham). Total Pflops computing power.

Lattice QCD calculations take weeks/millions core-hours

Tensions in experimental results for e+e- → hadrons at small s

Spread from KLOE to CMD3 = 200 x10^{-11}



CMD3 2302.08834