High Precision Physics from High Performance Computing

The 30th Anniversary Symposium of the
Center for Computational Sciences

University of Tsukuba

October 13-14, 2022

N.H. Christ

Columbia University

RBC and UKQCD Collaborations

Outline

- Lattice QCD and particle physics
- Advances in numerical methods
  - Riemannian Manifold HMC
- Application challenges
  - $K \rightarrow \pi\pi$ decay and CP violation
  - Muon g-2 and 4.2 σ SM-expt. discrepancy
- Outlook

The RBC & UKQCD collaborations

UC Berkeley/LBNL
Aaron Meyer

University of Bern & Lund
Nils Hermansson Truedsson

BNL and BNL/RBRC
Yasumichi Aoki (KEK)
Peter Boyle (Edinburgh)
Taku Izubuchi
Chulwoo Jung
Christopher Kelly
Meifeng Lin
Nobuyuki Matsumoto
Shigemi Ohta (KEK)
Amarjit Soni
Tianle Wang

CERN
Andreas Jüttner (Southampton)
Tobias Tsang

Columbia University
Norman Christ
Yikai Huo
Yong-Chull Jang
Joseph Karpie
Bob Mawhinney
Bigeng Wang (Kentucky)
Yidi Zhao

University of Connecticut
Tom Blum
Luchang Jin (RBRC)
Douglas Stewart
Joshua Swaim
Masaaki Tomii

Edinburgh University
Matteo Di Carlo
Luigi Del Debbio
Felix Erben
Vera Gülpers
Maxwell T. Hansen
Tim Harris
Ryan Hill
Raoul Hodgson
Nelson Lachini
Zi Yan Li
Michael Marshall
Fionn Ó hÓgáin
Antonin Portelli
James Richings
Azusa Yamaguchi
Andrew Z.N. Yong

Liverpool Hope/Uni. of Liverpool
Nicolas Garron

Michigan State University
Dan Hoying

University of Milano Bicocca
Mattia Bruno

Nara Women's University
Hiroshi Ohki

Peking University
Xu Feng

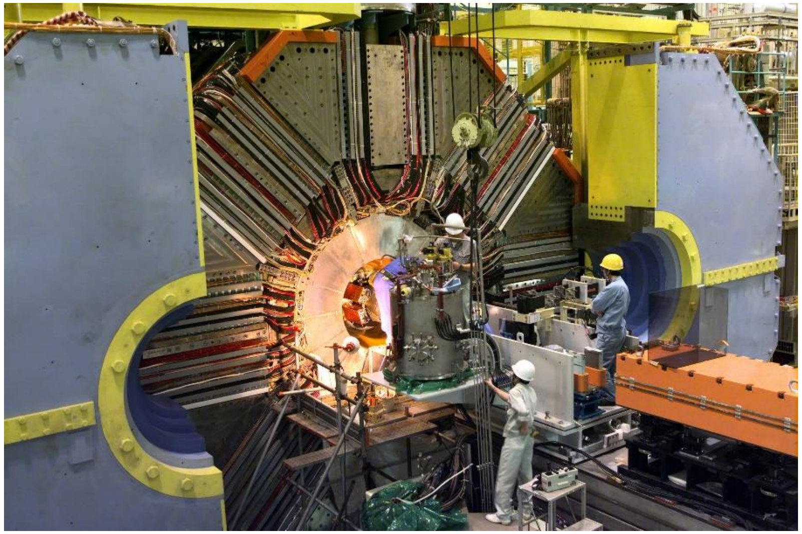
University of Regensburg
Davide Giusti
Christoph Lehner (BNL)

University of Siegen
Matthew Black
Oliver Witzel

University of Southampton
Alessandro Barone
Jonathan Flynn
Nikolai Husung
Rajnandini Mukherjee
Callum Radley-Scott
Chris Sachrajda

Stony Brook University
Jun-Sik Yoo
Sergey Syritsyn (RBRC)

Particle Physics & Lattice QCD

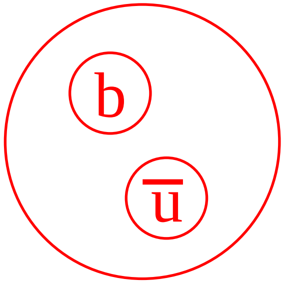


- The Standard Model does not predict everything:
  - g_μ-2 anomaly
  - Insufficiently large CP violation
  - Dark matter
  - Dark energy….
- High energy experiments at the LHC search for new particles
- High precision results at lower energies may have greater reach: Belle II at KEK.
- Most experiments involve quarks so that the strong interactions of the quarks must be untangled: Lattice QCD is required.

QCD: theory of quarks and gluons

- Do *u, d, s, c, b, t* quarks obey standard model predictions?
- Need <1% control of their binding by QCD forces.
- Much more difficult than treating atoms:
  - ***u*** and ***d*** quarks are massless and move at relativistic speeds
  - pair creation makes even a single proton a complex, many-body problem

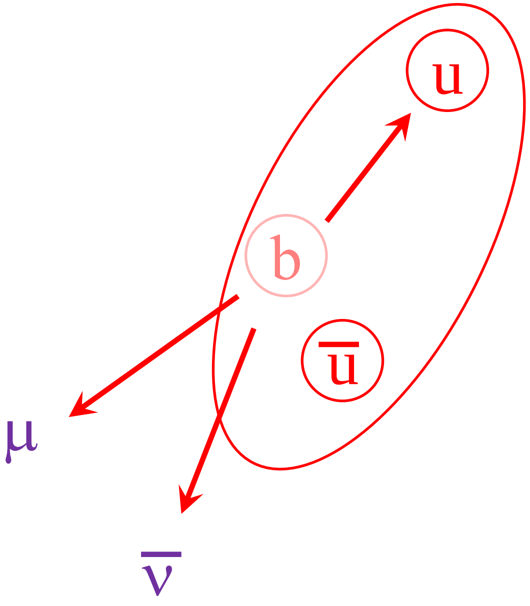
$$B \rightarrow \pi + \mu + \nu$$



QCD: theory of quarks and gluons

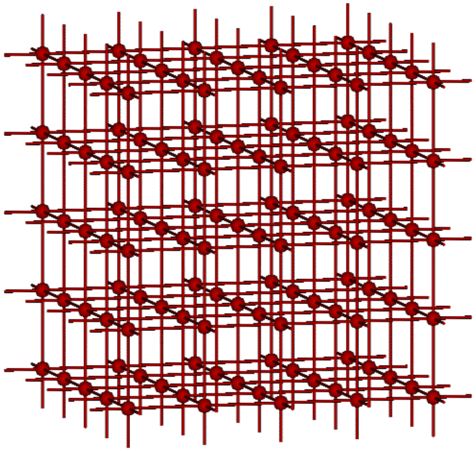
- Do *u, d, s, c, b, t* quarks obey standard model predictions?
- Need <1% control of their binding by QCD forces.
- Much more difficult than treating atoms:
  - ***u*** and ***d*** quarks are massless and move at relativistic speeds
  - pair creation makes even a single proton a complex, many-body problem

$B \rightarrow \pi + \mu + \nu$



Lattice QCD

Lattice QCD

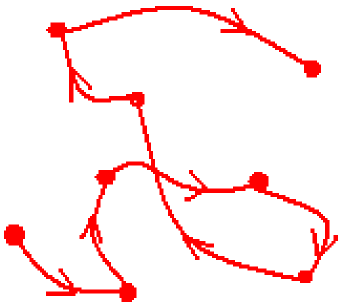


- Introduce a space-time lattice.
- Evaluate the *Euclidean* Feynman path integral.

no ***i***

  - Study $e^{-H_{QCD}\,t}$
  - 1^{st} principles non-perturbative formulation

$$\sum_n \langle n| e^{-H(T-t)} \mathcal{O} e^{-Ht} |n\rangle = \int d[U_\mu(n)] e^{-\mathcal{A}[U]} \det(D+m)\mathcal{O}[U](t)$$



- Use Monte Carlo importance sampling with a hybrid MD/Langevin evolution.
- 96^3 x 192 lattice → 5 x 10^9 dimensional integral
- ~40 samples give sub-percent errors

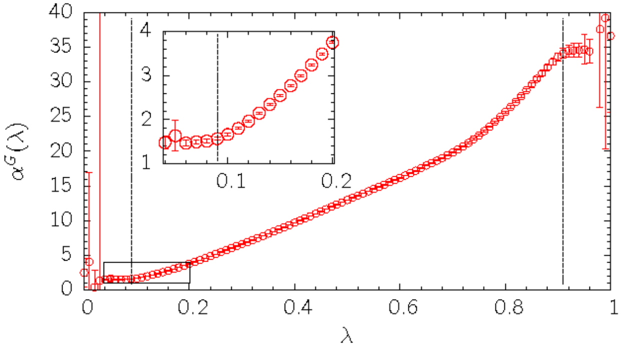
Numerical methods

- Use low eigenmodes to solve $\not{D}\, G_n = h_n$ where multiple right-hand sides allow reuse (deflation).
- Low eigenmodes also important for all-to-all propagators.
- 96^3 x 192 volume requires 5K eigenvectors (160 TB).
- Compress using local coherence: 30x (Clark, Jung & Lehner, arXiv:1710.06884)
- New directions:
  - Domain-decomposed HMC: use to reduce inter-node communication.
  - Riemannian manifold HMC.

Riemannian Manifold HMC

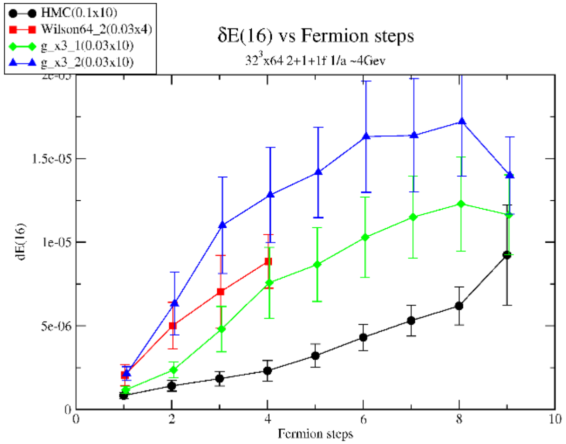
- Invented in 1986: [S. Duane, *et al.*, Phys. Lett. B 176 (1986) 143; Girolami and Calderhead, Journal of the Royal Statistical Society: Series B 73 (2011) 123]
- Modify the canonical mass term

$$\sum_{a,\mu,n} \frac{[P^a_\mu(n)]^2}{2M} \rightarrow \sum_{a,b,\mu,k,l} P^a_\mu(k)^* \left\langle k,a \left| \frac{1}{M(-\nabla^2_U)} \right| l,b \right\rangle P^b_\mu(l)$$



- Choose M(λ) to match power spectrum of the HMC force

$$M(\lambda) = \left[c + \sum_{i=0}^{4} \frac{a_0^{(i)} + a_1^{(i)}\lambda}{b_0^{(i)} + b_1^{(i)}\lambda + b_2^{(i)}\lambda^2} \right]^{-2}$$



- Suggestion of RMHMC 3x acceleration

Applications

ε'

Direct CP violation in K → $\pi\pi$ decay

$K^0 – \overline{K^0}$ mixing

- ΔS=1 weak decays allow K^0 and $\overline{K^0}$ to decay to the same $\pi\pi$ state.
- Resulting mixing described by Wigner-Weisskopf

$$i\frac{d}{dt}\begin{pmatrix} K^0 \\ \overline{K}^0 \end{pmatrix} = \left\{\begin{pmatrix} M_{00} & M_{0\bar{0}} \\ M_{\bar{0}0} & M_{\bar{0}\bar{0}} \end{pmatrix} - \frac{i}{2}\begin{pmatrix} \Gamma_{00} & \Gamma_{0\bar{0}} \\ \Gamma_{\bar{0}0} & \Gamma_{\bar{0}\bar{0}} \end{pmatrix}\right\}\begin{pmatrix} K^0 \\ \overline{K}^0 \end{pmatrix}$$

- Decaying states are mixtures of K^0 and $\overline{K^0}$

$$\begin{aligned} |K_S\rangle &= \frac{K_+ + \overline{\epsilon}K_-}{\sqrt{1+|\overline{\epsilon}|^2}} \\ |K_L\rangle &= \frac{K_- + \overline{\epsilon}K_+}{\sqrt{1+|\overline{\epsilon}|^2}} \end{aligned}$$

$$\overline{\epsilon} = \frac{i}{2}\left\{\frac{\mathrm{Im}\,M_{0\bar{0}} - \frac{i}{2}\mathrm{Im}\,\Gamma_{0\bar{0}}}{\mathrm{Re}\,M_{0\bar{0}} - \frac{i}{2}\mathrm{Re}\,\Gamma_{0\bar{0}}}\right\}$$

Indirect CP violation

CP violation

- CP violating, experimental amplitudes:

$$\eta_{+-} \equiv \frac{\langle \pi^+\pi^-|H_w|K_L\rangle}{\langle \pi^+\pi^-|H_w|K_S\rangle} = \epsilon + \epsilon'$$

$$\eta_{00} \equiv \frac{\langle \pi^0\pi^0|H_w|K_L\rangle}{\langle \pi^0\pi^0|H_w|K_S\rangle} = \epsilon - 2\epsilon'$$

- Where: $\epsilon = \overline{\epsilon} + i\frac{\mathrm{Im}\,A_0}{\mathrm{Re}A_0}$

Indirect: $|\varepsilon| = (2.228 \pm 0.011) \times 10^{-3}$

Direct: $\mathrm{Re}(\varepsilon'/\varepsilon) = (1.66 \pm 0.23) \times 10^{-3}$

$K \rightarrow \pi\,\pi$ and CP violation

- Final $\pi\pi$ states can have I = 0 or 2.

$$\langle \pi\,\pi(I=2)|H_w|K^0\rangle = A_2 e^{i\delta_2} \qquad \Delta I = 3/2$$

$$\langle \pi\,\pi(I=0)|H_w|K^0\rangle = A_0 e^{i\delta_0} \qquad \Delta I = 1/2$$

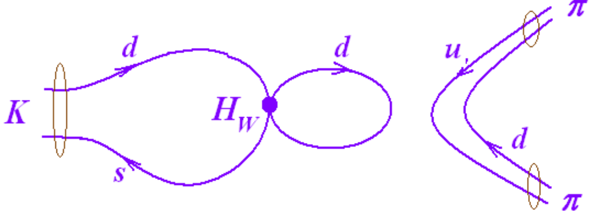
- CP symmetry requires A_0 and A_2 be real.
- Direct CP violation in this decay is characterized by:

$$\epsilon' = \frac{i e^{\delta_2-\delta_0}}{\sqrt{2}} \left|\frac{A_2}{A_0}\right| \left(\frac{\mathrm{Im} A_2}{\mathrm{Re} A_2} - \frac{\mathrm{Im} A_0}{\mathrm{Re} A_0}\right)$$

Direct CP violation

Challenging calculation

- Presence of vacuum implies exponentially falling signal/noise ratio.



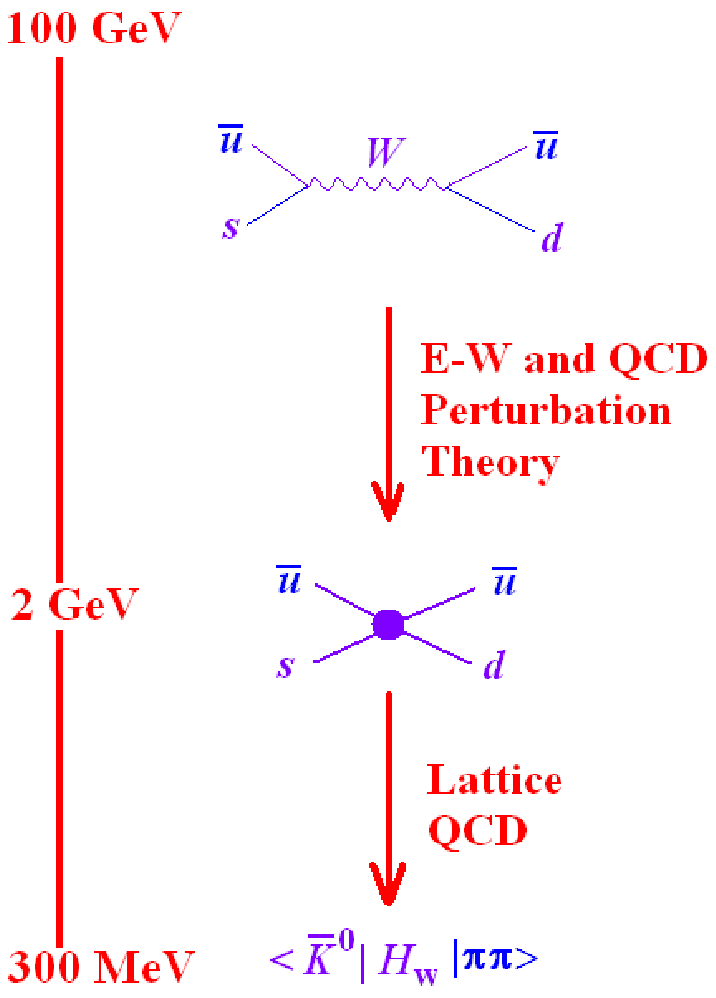
- Two-pion final state was a new challenge.
- We first attempted this calculation in 1997:
- Seven generations of graduate students:
  - Calin Christian (2002)
  - Changhoan Kim (2004)
  - Sam Li (2008)
  - Matthew Lightman (2011)
  - Qi Liu (2012)
  - Daiqian Zhang (2015)
  - Tianle Wang (2021)

Low Energy Effective Theory

- Represent weak interactions by local four-quark Lagrangian

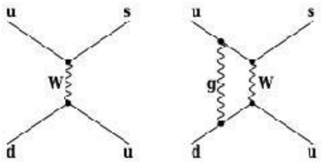
$$\mathcal{H}^{\Delta S=1} = \frac{G_F}{\sqrt{2}} V_{ud} V_{us}^* \left\{ \sum_{i=1}^{10} \Big[z_i(\mu) + \tau y_i(\mu) \Big] Q_i \right\}$$

- $\tau = -\frac{V_{td} V_{ts}^*}{V_{ud} V_{us}^*} = (1.543 + 0.635i) \times 10^{-3}$
- $V_{qq'}$ – CKM matrix elements
- z_i and y_i – Wilson Coefficients
- Q_i – four-quark operators



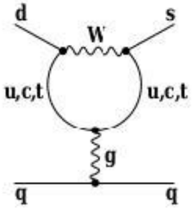
Local four quark operators

- **Current-current operators**



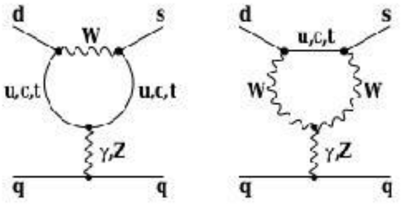
$$Q_1 \equiv (\bar{s}_\alpha d_\alpha)_{V-A}(\bar{u}_\beta u_\beta)_{V-A}$$
$$Q_2 \equiv (\bar{s}_\alpha d_\beta)_{V-A}(\bar{u}_\beta u_\alpha)_{V-A}$$

- **QCD Penguins**



$$Q_3 \equiv (\bar{s}_\alpha d_\alpha)_{V-A} \sum_{q=u,d,s} (\bar{q}_\beta q_\beta)_{V-A}$$
$$Q_4 \equiv (\bar{s}_\alpha d_\beta)_{V-A} \sum_{q=u,d,s} (\bar{q}_\beta q_\alpha)_{V-A}$$
$$Q_5 \equiv (\bar{s}_\alpha d_\alpha)_{V-A} \sum_{q=u,d,s} (\bar{q}_\beta q_\beta)_{V+A}$$
$$Q_6 \equiv (\bar{s}_\alpha d_\beta)_{V-A} \sum_{q=u,d,s} (\bar{q}_\beta q_\alpha)_{V+A}$$

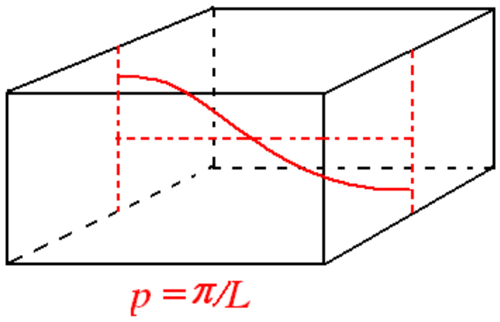
- **Electro-Weak Penguins**



$$Q_7 \equiv \frac{3}{2}(\bar{s}_\alpha d_\alpha)_{V-A} \sum_{q=u,d,s} e_q(\bar{q}_\beta q_\beta)_{V+A}$$
$$Q_8 \equiv \frac{3}{2}(\bar{s}_\alpha d_\beta)_{V-A} \sum_{q=u,d,s} e_q(\bar{q}_\beta q_\alpha)_{V+A}$$
$$Q_9 \equiv \frac{3}{2}(\bar{s}_\alpha d_\alpha)_{V-A} \sum_{q=u,d,s} e_q(\bar{q}_\beta q_\beta)_{V-A}$$
$$Q_{10} \equiv \frac{3}{2}(\bar{s}_\alpha d_\beta)_{V-A} \sum_{q=u,d,s} e_q(\bar{q}_\beta q_\alpha)_{V-A}$$

Lattice calculation of $\boxed{\langle \pi\pi | H_W | K \rangle}$

- The operator product $d(x)\overline{s}(x)$ easily creates a kaon.
- Use finite-volume energy quantization (Lellouch-Luscher) and adjust L so that *a finite-volume* state obeys: $E_{\pi\pi} = M_K$.



$$\langle \pi^+\pi^- | H_W | K^0 \rangle \quad \propto \quad \langle \overline{d}u(t_{\pi_1})\overline{u}d(t_{\pi_2})\; H_W(t_{\mathrm{op}})\; \overline{d}s(t_K) \rangle$$

- Use boundary conditions on the quarks: $E_{\pi\pi}^{(\mathrm{gnd})} = M_K$
- For $(\pi\pi)_{I=0}$ use G-parity boundary conditions
  - $G|\pi\rangle = -|\pi\rangle$
  - Complex at the quark level G: $\begin{pmatrix} u \\ d \end{pmatrix} \rightarrow \begin{pmatrix} \overline{d} \\ -\overline{u} \end{pmatrix}$

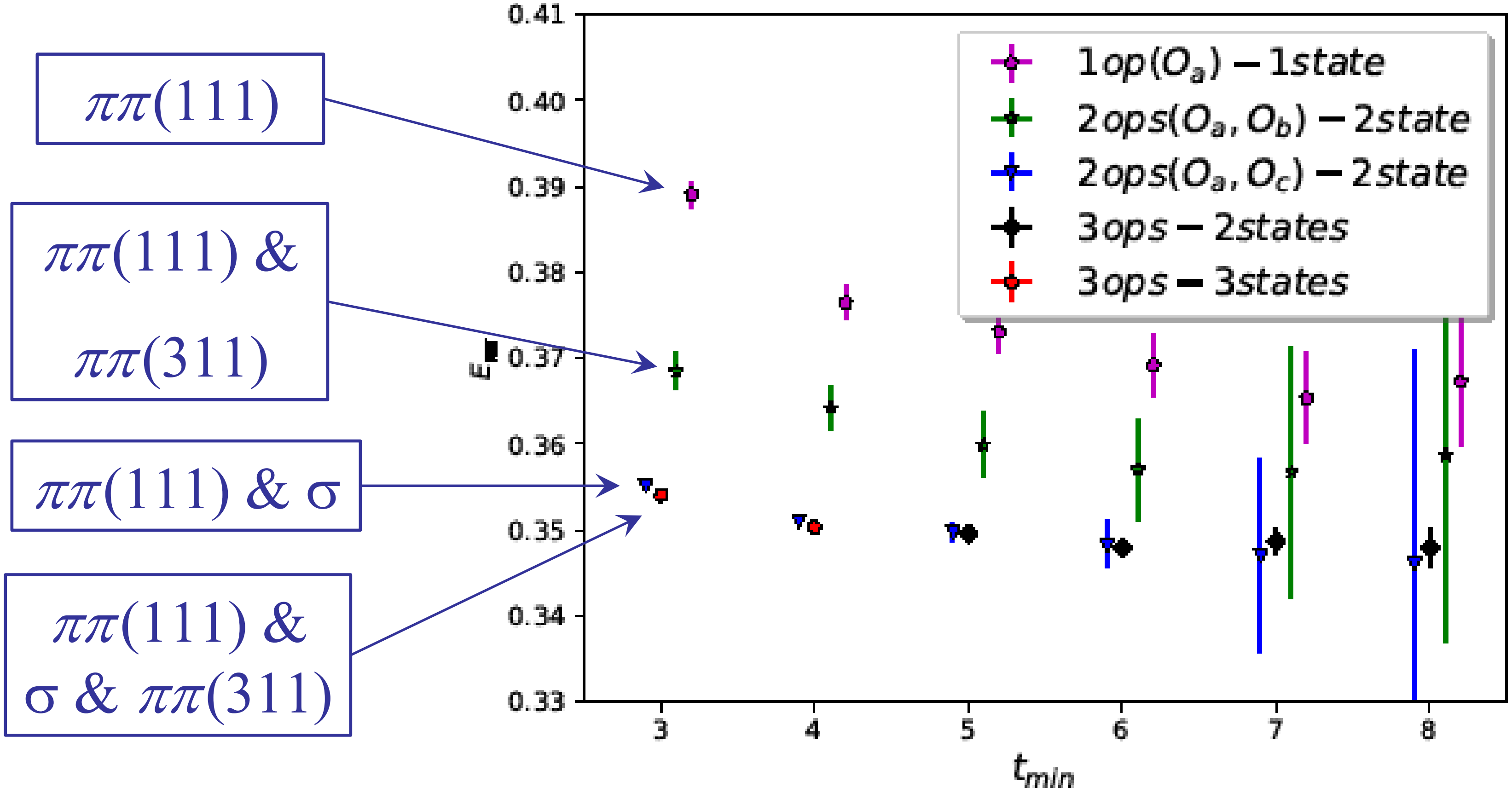
Recent results

- 2015 [Phys. Rev. Lett. 115 (2015) 212001]
  - $I = 0$ $\pi\pi$ phase shift: $\delta_0 = 23.8(5.4)^{o}$
  - Dispersion theory result: $\delta_0 = 34^{o}$
    [Colangelo, *et al.*]
  - $\mathrm{Re}(\varepsilon'/\varepsilon) = (1.38 \pm 5.15_{\mathrm{stat}} \pm 4.59_{\mathrm{sys}}) \times 10^{-4}$
  - Expt.: $(16.6 \pm 2.3) \times 10^{-4}$ (2.1 σ difference)

- Introduce more $\pi\pi$ operators to distinguish excited $\pi\pi$ states
- Increase statistics 216 → 741

- 2020 [Phys. Rev. D 102 (2020) 054509]
  - $I = 0$ $\pi\pi$ phase shift: $\delta_0 = 31.7(6)^{\circ}$
  - $\mathrm{Re}(\varepsilon'/\varepsilon) = (21.7 \pm 2.6_{\mathrm{stat}} \pm 6.2_{\mathrm{sys}} \pm 5.0_{\cancel{\mathrm{isospin}}}) \times 10^{-4}$

$I = 0$ $\pi\pi$ scattering with three operators



$\pi\pi(111)$

$\pi\pi(111)$ & $\pi\pi(311)$

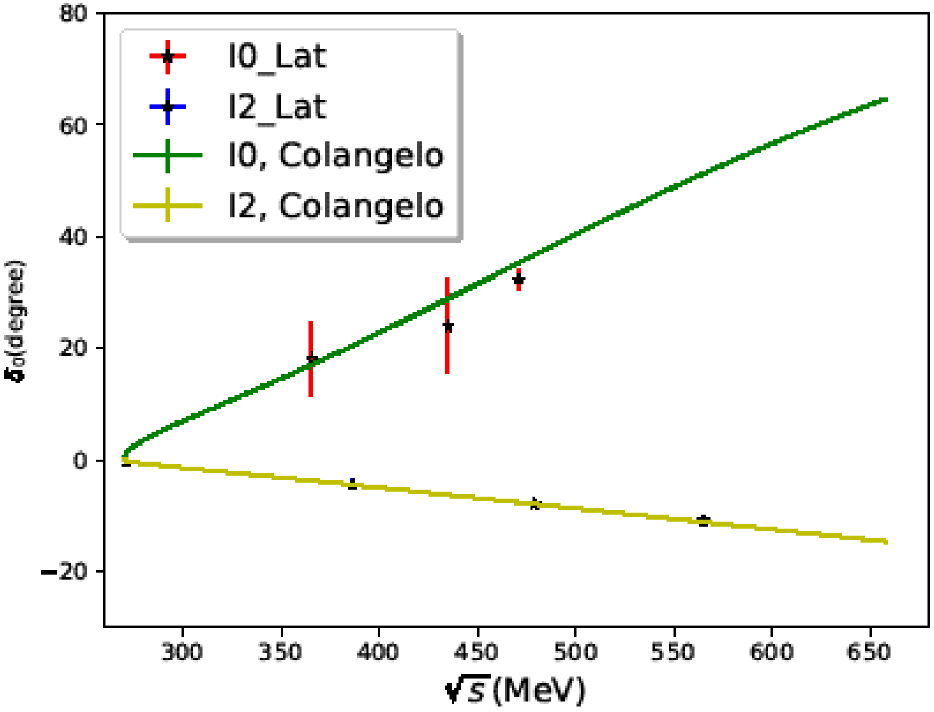
$\pi\pi(111)$ & σ

$\pi\pi(111)$ & σ & $\pi\pi(311)$

- δ_0 = 31.7(6)° vs 34° data-driven prediction (5-15 fit, statistical errors only).

Extended results for ππ phase shifts

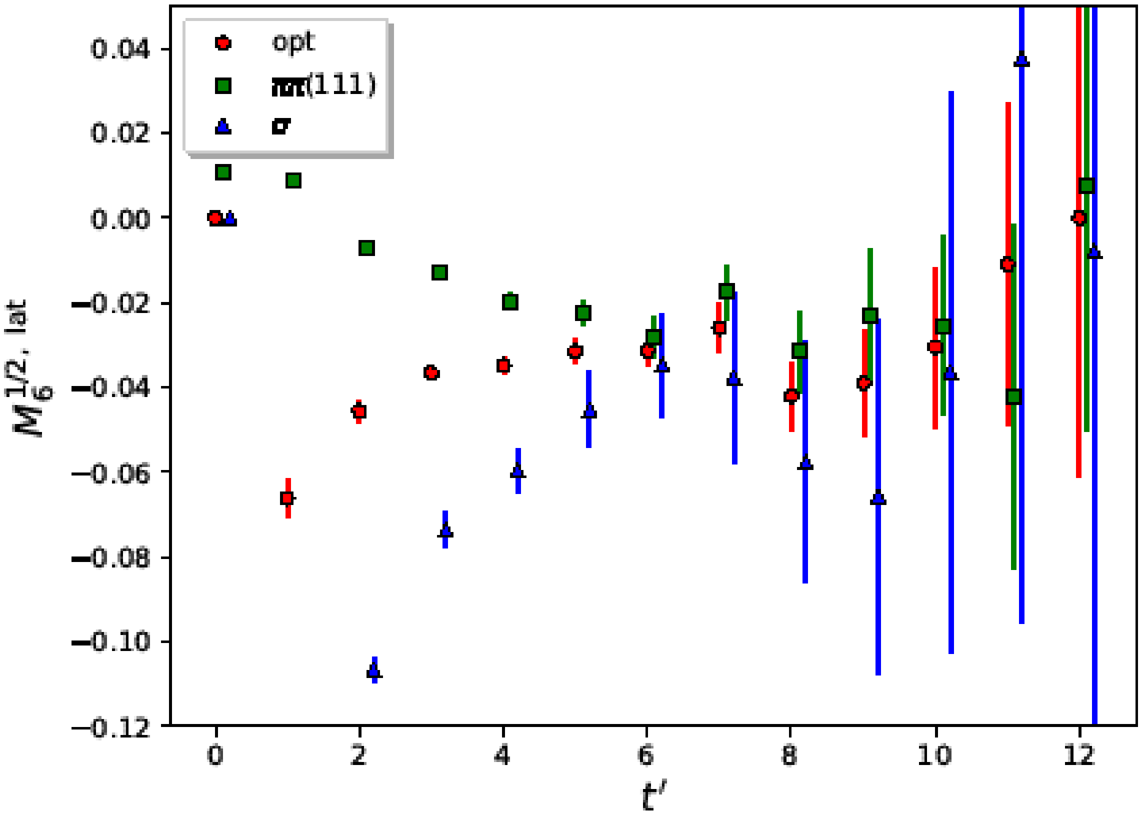
- Combine pion operators carrying various momenta to examine $P_{cm} \neq 0$ → varying *s*



- We are now in good agreement with dispersive results.

Example of $K \rightarrow \pi\pi$ data

- Examine dependence on $\pi\pi$ H_W separation plot $\langle \pi\pi(t_{\pi\pi})\ H_W\ (t_{op})\ K(t_K)\ \rangle$ versus $t' = t_{\pi\pi} - t_{op}$



$t_{op} - t_K \geq 6$

Systematic errors

Description	**Error**	
	Re(A_0)	Im(A_0)
Excited state	-	
Unphysical kinematics	5%	
Operator renormalization	4%	
Wilson coefficients	12%	
Finite lattice spacing	12%	
Lellouch-Luscher factor	1.5%	
Finite volume	7%	
Parametric errors	0.3%	6%
Missing G_1 operator	5%	
Total	19.8%	20.7%

ε' – Next steps

- Continuum limit (Chris Kelly) :
  - G-parity evolution and measurement code now optimized for GPUs
  - Now generating 40^3x96 G-parity ensemble on Perlmutter
- Isospin breaking (E&M + m_u-m_d) now an important focus (Xu Feng, Joe Karpie)
  - Work in Coulomb gauge: Coulomb + transverse photons
  - Coulomb part may be solved
- Explore periodic boundary conditions. Use GEVP to extract matrix element of excited state. (Tom Blum, Dan Hoying, Luchang Jin, Masaaki Tomii)

g_μ-2

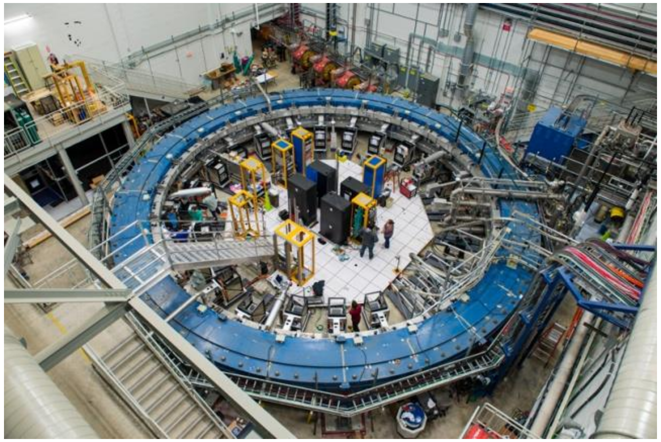
Anomalous muon magnetic moment

g - 2 for the muon

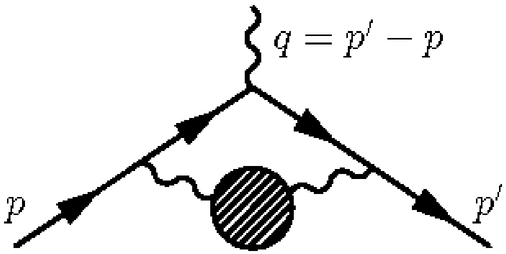
- Anomalous moment: $a_\mu = (g_\mu - 2)/2$
- FNAL expt E989 :

  $a_\mu = 11699204 \pm 5.4 \times 10^{-10}$
- 4.2σ difference between the standard model prediction and experiment:

  $a_\mu^{EXP} - a_\mu^{SM} = 25.1 \pm 5.9 \times 10^{-10}$ (0.46 ppm)
- Effects of quark and gluons enter at order α_{EM}^2:

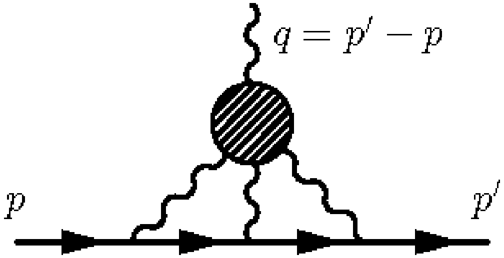


FNAL E989



HVP

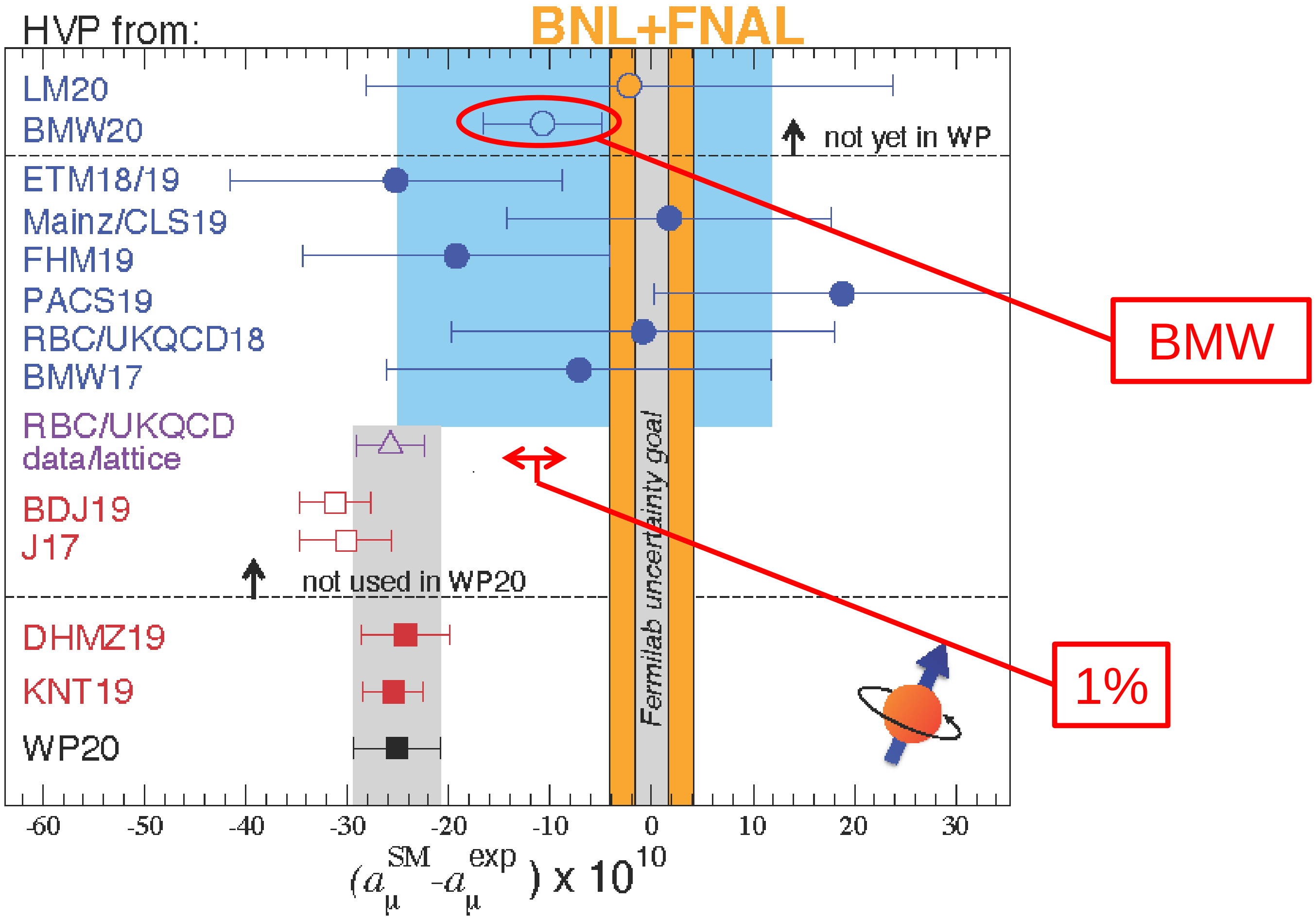
$692.5(2.7) \times 10^{-10}$



HLbL

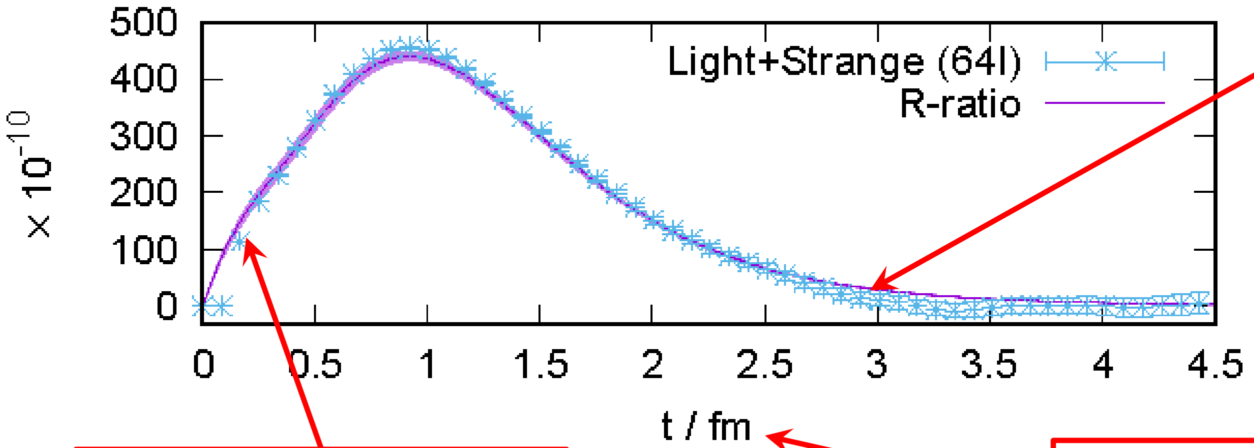
$10.5(2.6) \times 10^{-10}$

Hadronic vacuum polarization



Time-momentum analysis

(Bernecker-Meyers representation)



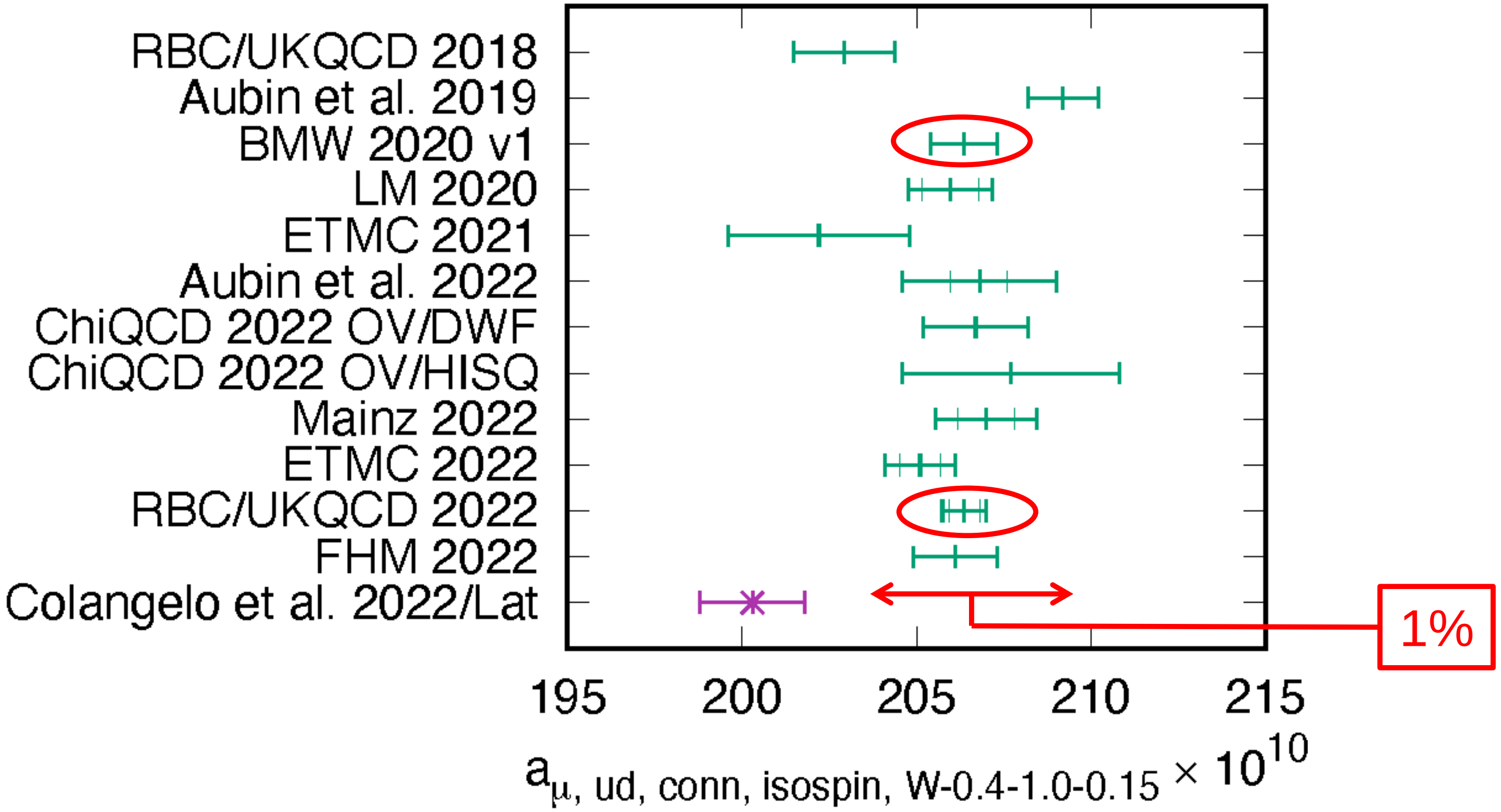
Large time
$\pi\pi$ states

Small time more
sensitive to a^2 errors

Time separation
between currents

- HVP contribution to g_μ-2 is the area under this curve.
- Compare middle region where lattice precision is greatest

``Middle Window'' comparison



Additional Calculations

- Complete calculation g_μ- 2 with reduced errors.
- K_L-K_S mass difference
- Long distance part of ε_K
- Electromagnetic corrections to $K^- \rightarrow \mu^- \nu$
- Two photon exchange contribution to $K_L \rightarrow \mu^+ \mu^-$
- Electromagnetic corrections to ε'

Outlook

- Faster machines carry us into new regimes where old and new algorithmic ideas become effective, multiplying the computers' impact.
- Exascale machines Frontier (ORNL) and Aurora (ANL) should be examples.
  - Planning new 2+1+1 flavor ensembles: 96^3x384, 1/a=3 GeV
    128^3x512, 1/a=4 GeV
    160^3x640, 1/a=5 GeV:
  - $(m_{charm}\ a)^2 = (1.2\ \text{GeV} / 5\ \text{GeV})^2 = 6\%$ -- should allow accurate calculation of charm quark loops.
  - We can move from 3-flavor calculation in the Standard Model to calculations which involve an active charm quark: $K^0 – \overline{K}^0$ mixing is the easiest example.
- By the 60th anniversary of CSS we will have learned much more about the Standard Model and what lies beyond it!