Lattice calculation of the $\Delta I=1/2$ $K\rightarrow\pi\pi$ amplitude

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Motivation for studying K→ππ Decays

- Likely explanation for matter/antimatter asymmetry in Universe, baryogenesis, requires violation of CP.

- Direct CPV first observed in late 90s at CERN and Fermilab in $K^0 \to \pi\pi$:

$$\eta_{00} = \frac{A(K_\mathrm{L} \to \pi^0\pi^0)}{A(K_\mathrm{S} \to \pi^0\pi^0)}, \qquad \eta_{+-} = \frac{A(K_\mathrm{L} \to \pi^+\pi^-)}{A(K_\mathrm{S} \to \pi^+\pi^-)}.$$

$$\mathrm{Re}(\epsilon'/\epsilon) \approx \frac{1}{6}\left(1 - \left|\frac{\eta_{00}}{\eta_{\pm}}\right|^2\right) = 16.6(2.3) \times 10^{-4} \qquad \text{(experiment)}$$

measure of direct CPV

measure of indirect CPV

- In terms of isospin states: $\Delta I=3/2$ decay to I=2 final state, amplitude A_2
  $\Delta I=1/2$ decay to I=0 final state, amplitude A_0

$$\omega = \mathrm{Re}A_2/\mathrm{Re}A_0$$

$$A(K^0 \to \pi^+\pi^-) = \sqrt{\frac{2}{3}}A_0 e^{i\delta_0} + \sqrt{\frac{1}{3}}A_2 e^{i\delta_2},$$
$$A(K^0 \to \pi^0\pi^0) = \sqrt{\frac{2}{3}}A_0 e^{i\delta_0} - 2\sqrt{\frac{1}{3}}A_2 e^{i\delta_2}.$$

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

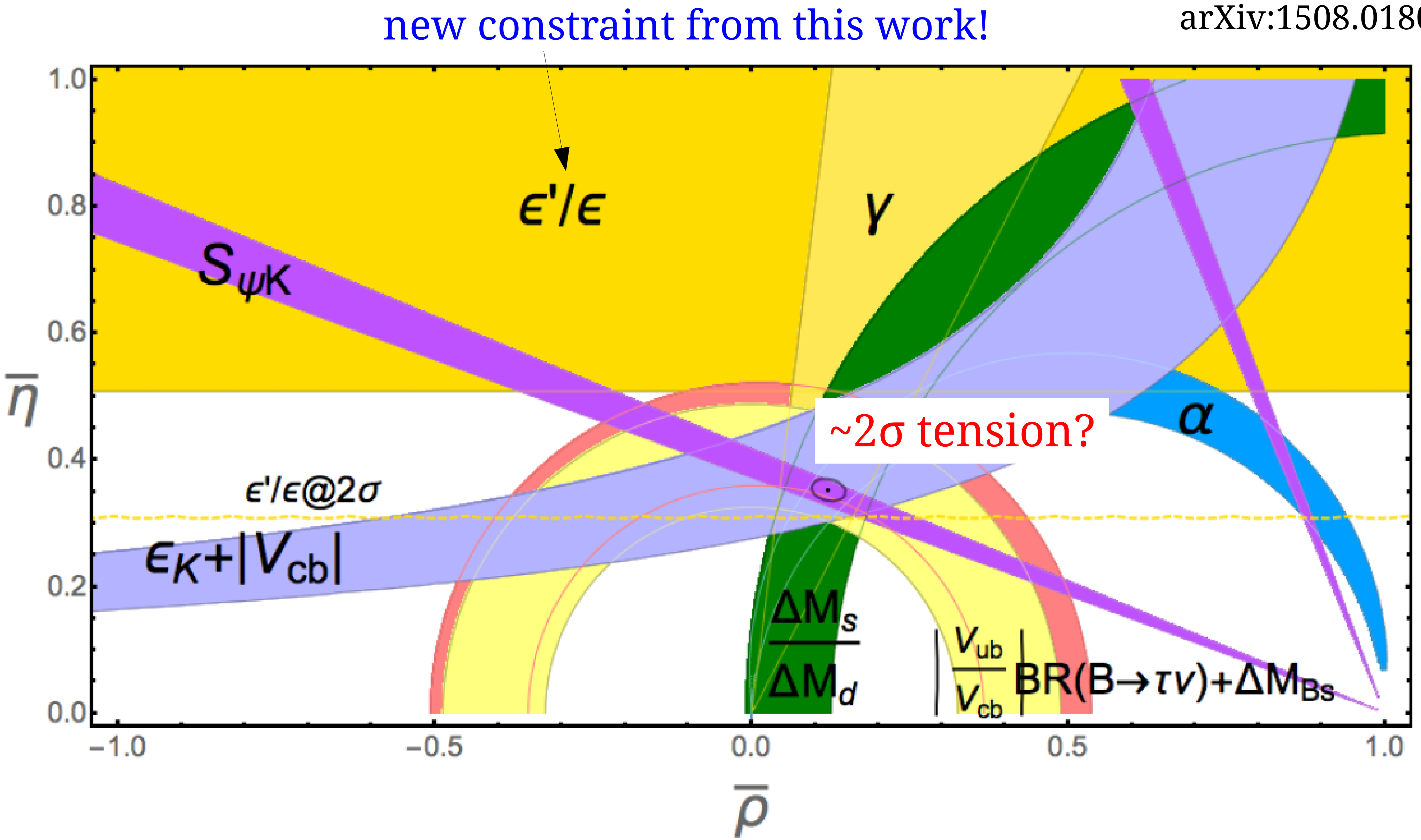
(δ_I are strong scattering phase shifts.)

- Amount of direct CPV in Standard Model appears too low to describe measured M/AM asymmetry: tantalizing hint of new physics.

- Small size of ε' makes it particularly sensitive to new direct-CPV introduced by most BSM models.

- ε' also provides a new horizontal band constraint on CKM matrix:

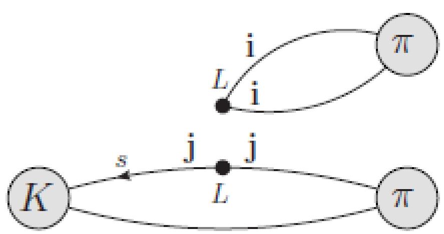
[Lehner et al arXiv:1508.01801]



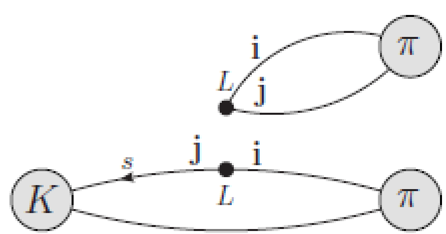
The role of the lattice

- In experiment kaons approx 450x (!) more likely to decay into I=0 pi-pi states than I=2. $$\frac{\mathrm{Re}A_0}{\mathrm{Re}A_2} \simeq 22.5$$ (the ΔI=1/2 rule)
- Perturbative running to charm scale accounts for about a factor of 2. Is the remaining 10x non-perturbative or New Physics?
- The answer is **low-energy *QCD!*** RBC/UKQCD [arXiv:1212.1474, arXiv:1502.00263]

  Strong cancellation between the two dominant contractions



Contraction ①.



Contraction ②.

$$\mathrm{Re}(A_2) \sim ① + ②$$

$$② \approx -0.7①$$

heavily suppressing $\mathrm{Re}(A_2)$.

- Lattice QCD only *ab initio*, systematically improvable technique for studying QCD at hadronic scale.

Lattice Determination of K→ππ

- At energy scales μ«$M_{W,}$ K→ππ decays accurately described by weak effective theory.

$$H_W^{\Delta S=1} = \frac{G_F}{\sqrt{2}} V_{ud}^* V_{us} \sum_{j=1}^{10} [z_j(\mu) + \tau y_j(\mu)] Q_j$$

10 effective 4-quark operators

perturbative Wilson coeffs.

- On the lattice compute $M_j^{I,\,\mathrm{lat}} = \langle (\pi\pi)_I | Q_j | K \rangle$
- Operators must be renormalized into same scheme as Wilson coeffs: Use RI-(S)MOM NPR and perturbatively match to MSbar at high scale.
- Mixing under renormalization, hence Z is a matrix.

$$A^I = F \frac{G_F}{\sqrt{2}} V_{ud} V_{us} \sum_{i=1}^{10} \sum_{j=1}^{7} \left[(z_i(\mu) + \tau y_i(\mu)) Z_{ij}^{\mathrm{lat}\to\overline{\mathrm{MS}}} M_j^{I,\,\mathrm{lat}} \right]$$

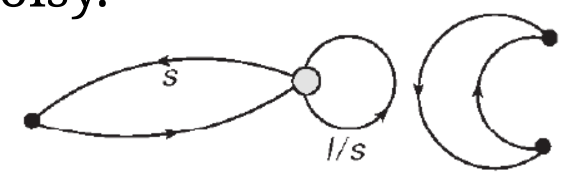
- F is finite-volume correction calculated using LL method.

[Phys.Rev. D91 (2015) 7, 074502]

- A_2 computable using standard lattice techniques. Most recent determination ~12% total error (3% stat) dominated by PT truncation in NPR.
- A_0 considerably more difficult for 2 reasons:

Disconnected Diagrams

- "Type-4" disconnected diagrams (coupling between subdiagrams only via sea gluons) are *very* noisy.



- Use computationally expensive (and non-trivial to implement) Trinity-style all-to-all (A2A) propagators:
    - 900 exact low-eigenmodes computed using Lanczos algorithm
    - Stochastic high-modes with full dilution of indices
- Allows us to tune ππ source shape to minimize vacuum overlap.
- Also to perform all spatial and temporal translations to boost statistics.

Physical Kinematics

- Important to calculate with physical (energy-conserving) kinematics.
- With physical masses: $2 \times m_\pi \sim 270 \text{ MeV} \ll m_K \sim 500 \text{ MeV}$
- Requires moving pions!
- This is excited state of the ππ-system. Possibilities:
    - try to perform multi-state fits to very noisy data (esp. A_0 where there are disconn. diagrams)
    - modify boundary conditions to remove the ππ ground-state
- Second approach optimal. Straightforward for A_2 (APBC on d-quark) but additional requirements for A_0 not satisfied by APBC: must conserve isospin and apply momentum to both charged and neutral pions.
- Solution: Use G-parity BCs:

$$\hat{G} = \hat{C} e^{i\pi \hat{I}_y} \quad : \quad \hat{G}|\pi^\pm\rangle = -|\pi^\pm\rangle \qquad \hat{G}|\pi^0\rangle = -|\pi^0\rangle$$

- As a boundary condition: (i=+, -, 0)

$$\pi^i(x+L) = \hat{G}\pi^i(x) = -\pi^i(x) \longrightarrow |p| \in (\pi/L,\, 3\pi/L,\, 5\pi/L \ldots)$$

(moving ground state)

- Technically very challenging to implement.

Calculation details

- 32^3x64 Mobius DWF ensemble with IDSDR gauge action at β=1.75. Coarse lattice spacing (a^{-1}=1.378(7) GeV) but large, (4.6 fm)^3 box.
- Using Mobius params (b+c)=32/12 and L_s=12 obtain same action as the L_s=32 Shamir DWF + IDSDR ens. used for ΔI=3/2 but at reduced cost.
- G-parity BCs in 3 spatial directions results in close matching of kaon and $\pi\pi$ energies:

$$m_K=490.6(2.4)\ \mathrm{MeV}$$

$$E_{\pi\pi}(I=0) = 498(11)\ \mathrm{MeV}$$

$$E_\pi=274.6(1.4)\ \mathrm{MeV} \quad (m_\pi = 143.1(2.0)\ \mathrm{MeV})$$

- First calculation (Phys.Rev.Lett. 115 (2015) 21, 212001) utilized 216 independent measurements (4 MDTU sep.).
- Resources primarily from previous USQCD grants: 44.6M BG/Q core hours (2013-2014) and 42M BG/Q core hours + 29% ALCF 0-priority time (2014-2015).
- Highly optimized BG/Q CPS/Bagel/BFM code. Optimal performance for both ensemble generation and measurements on 512-1024 nodes BG/Q.
- Cost is 0.9 BG/Q rack-day per complete measurement (4 configs generated + 1 set of contractions).

Issue with ensemble generation

- Recently discovered mistake with RNG seeding used in ensemble generation:
  - With GPBC we have independent u and d quarks fields.
  - Dirac matrix is 2x2 in flavor space with components spanning boundary.
  - Pseudofermion field

$$\phi = (M^\dagger[U])^{1/2} \begin{pmatrix} \eta_d \\ \eta_u \end{pmatrix} \quad \text{where} \quad P[\eta_i] \sim e^{-\eta_i^\dagger \eta_i}$$

independent for each flavor

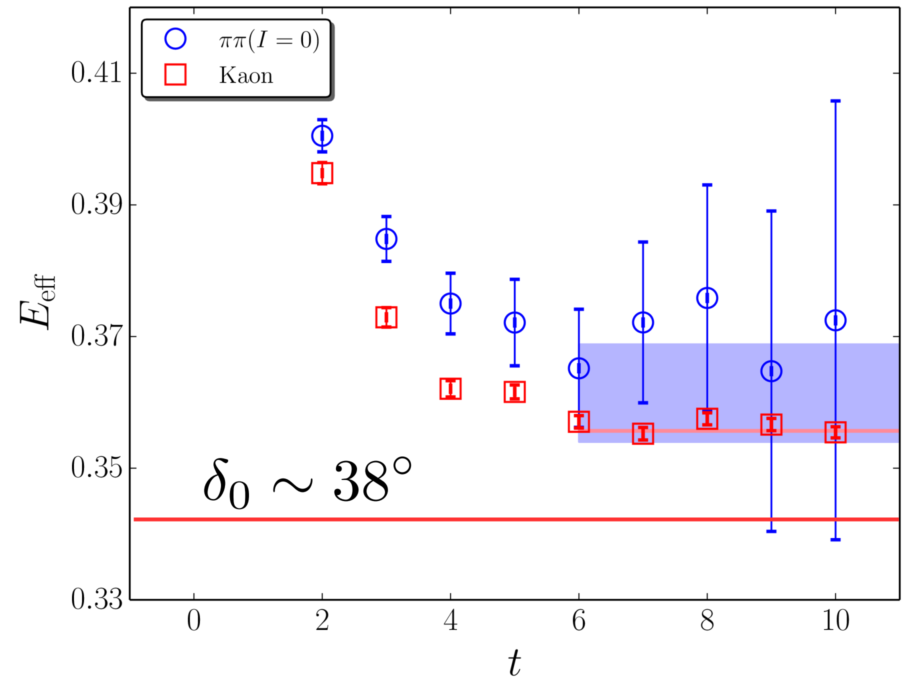
  - Due to coding error, identical random numbers were used for η_u and η_d up to a relative shift of 12 sites in the y-direction:

$$\eta_u(x) = \eta_d(x + 12\hat{y})$$

  - Persists through entire ensemble.
- At present have not found theoretical interpretation that would allow effect to be estimated.
- However, strong empirical evidence that effect is negligible for present calculation.
- E.g. statistically resolvable correlation observed in plaquettes separated by 12 in y-dir but only at ~5×10^{-5}, unlikely to have strong effect on paper results where errors are 100x – 1000x larger.

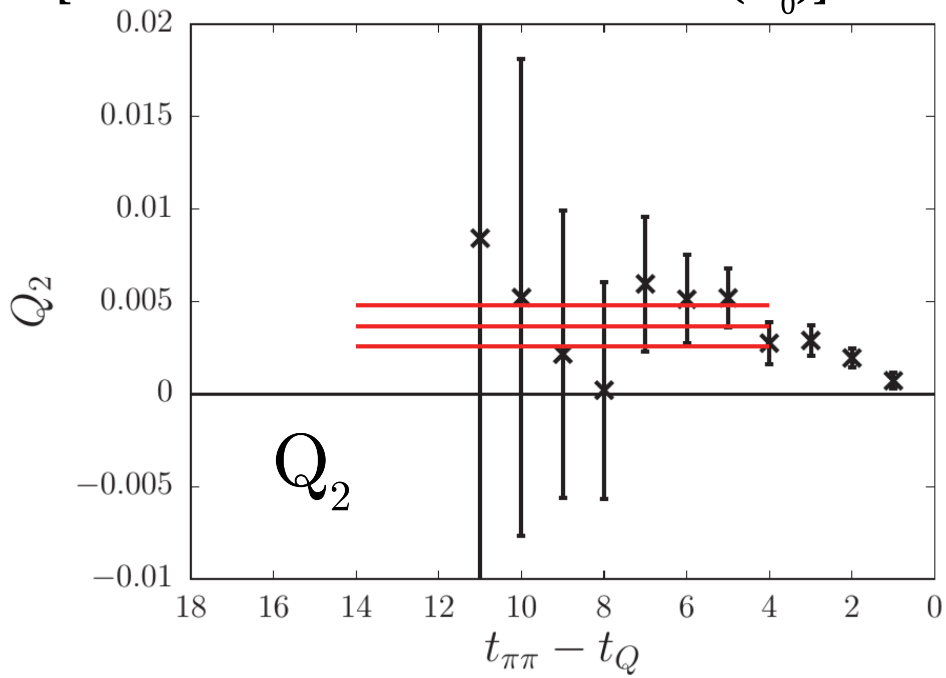
Results of first calculation

- Our phase shift $\delta_0 = 23.8(4.9)(1.2)^\circ$ ~2.7σ below conventional Roy equation determination of $\delta_0 = 38.0(1.3)^\circ$
  [G.Colangelo, private communication]
- Possibly low statistics concealing delayed plateau start?
- Incorrect estimate of Roy equation errors or use of wrong high-energy 'experimental' ππ scattering data?

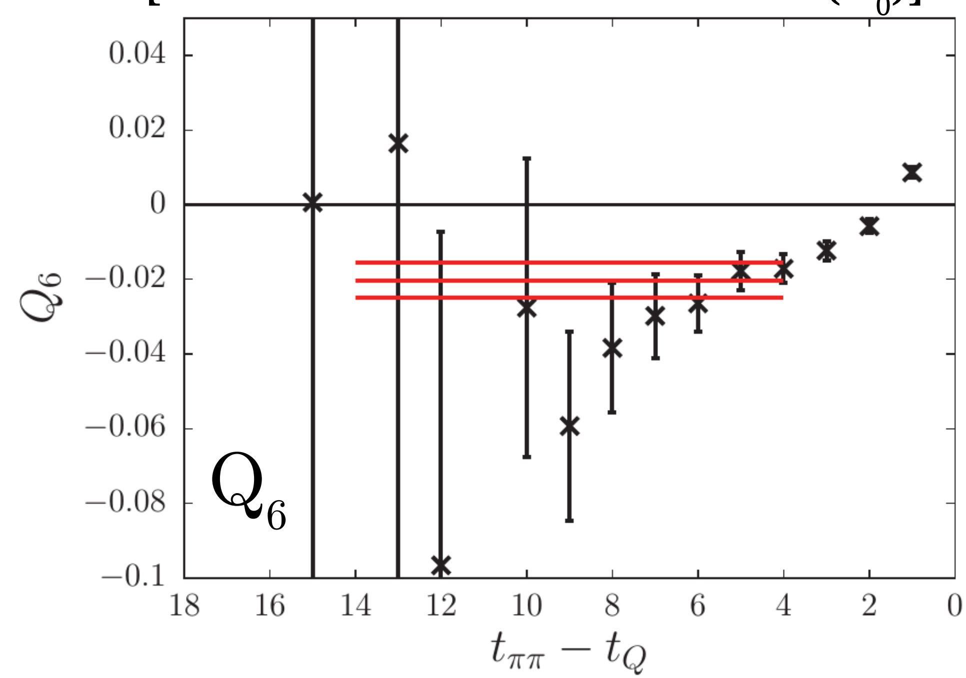


- Matrix elements:

[Dominant contribution to Re(A_0)]



[Dominant contribution to Im(A_0)]



$$\mathrm{Re}(A_0) = 4.66(1.00)_{\mathrm{stat}}(1.21)_{\mathrm{sys}} \times 10^{-7}\ \mathrm{GeV}$$ (This work)

$$\mathrm{Re}(A_0) = 3.3201(18) \times 10^{-7}\ \mathrm{GeV}$$ (Experiment)

- Good agreement for Re(A_0) serves as test for method.

$$\mathrm{Im}(A_0) = -1.90(1.23)_{\mathrm{stat}}(1.04)_{\mathrm{sys}} \times 10^{-11}\mathrm{GeV}$$ (This work)

- First ab initio prediction of Im(A_0).
- ~85% total error on the predicted Im(A_0) due to strong cancellation between dominant Q_4 and Q_6 contributions:

$$\begin{aligned}\Delta[\mathrm{Im}(A_0), Q_4] &= \quad 1.82(0.62)(0.32) \times 10^{-11} \\ \Delta[\mathrm{Im}(A_0), Q_6] &= -3.57(0.91)(0.24) \times 10^{-11}\end{aligned}$$

despite only 40% and 25% respective errors for the matrix elements.

- Dominant systematic (15%) is due to PT truncation errors in the NPR exacerbated by low renormalization scale 1.53 GeV.
- Since publication we have applied step-scaling procedure to raise this to 2.29 GeV, utilizing our 24^3 a^{-1}=1.78 GeV ensemble.

- Re(A_0) and Re(A_2) from expt.
- Lattice values for Im(A_0), Im(A_2) and the phase shifts,

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

$$\boxed{\begin{array}{ll} = \quad 1.38(5.15)(4.43)\times 10^{-4}, & \text{(this work)} \\ \quad 16.6(2.3)\times 10^{-4} & \text{(experiment)} \end{array}}$$

- Present error ~3x experimental error.
- Find possible discrepancy between lattice and experiment at 2.1σ level.

  - strong motivation for continued study!

- Calculation error is dominated by statistics: clear mandate for extending present calculation.

Proposal

- Primary goal is to generate more statistics. Presently enacting programme to increase the number of measurements by at least 4x (including replacing existing, flawed measurements).
- For optimal throughput, generating multiple evolution streams originating from widely separated points on the original ensemble, leaving O(100) MDTU for thermalization to eradicate any effect of the RNG error.
- Already running streams on KEKSC (24.6M BG/Q core hours grant) and on DiRAC BG/Q installation at Edinburgh University.
- Intend to make use of Blue Waters allocation (separate USQCD BW proposal), and Cori phase-II early access for evolution/measurement.
- We request 71M BG/Q core hours on the BNL 512-node machine and 50M in zero-priority time at Mira (ALCF).
- This will enable us to perform an additional 200+141 complete measurements; a factor of 1.6 over our current stats by itself.
- Alternative: generate 535 independent gauge configurations and exploit Cori phase-II for the measurements.

SPC Questions (paraphrased)

Can these ensembles be used to compute other "simple" quantities, e.g. decay constants and form factors?

Yes, quantities like f_pi, f_K and B_K can be computed but extra cost and theoretical considerations make this unattractive unless property of having no stationary pions in the spectrum can be utilized.

What allocations have you received on Cori Phase II and Blue Waters

Blue Waters - somewhat unclear. The RBC/MILC proposal received 17.4M core hours, which prorates to 5.9M for K->pipi. Believe sufficient to generate 475 new independent configs.

Cori Phase II – unclear. If we get 5% of the machine over 2 months we might expect to measure on ~800 configs. Evolution is not optimal on this machine due to network.

What progress has been made investigation TWQCD's "exact one-flavor action" and what improvement do you anticipate?

Currently in preliminary stages but looks promising; if successful we will be able to reduce our reliance on multishift, which is hampered by large linear algebra overheads and reduced scope for mixed-precision and evolution tuning. Factor of 2 in evolution speed may be possible.

Are you in a position to make use of KNL / cluster / GPU resources?

G-parity evo and K->pipi fully implemented in CPS/Grid optimized for KNL/KNH. Straightforward to include new architecture using intrinsics. DWF code heavily constrained by network bandwidth, limiting performance on clusters. New comms-efficient CG-variant (P.Boyle) might help alleviate. Investigating into utilizing OPENACC directives in Grid to offload computation in colab. with BNL CSI.

Thank you!

Evidence from 32^3x64 calculation

- Measured plaquette vs. value obtained from non-GPBC ensemble (with extrap to same quark mass):

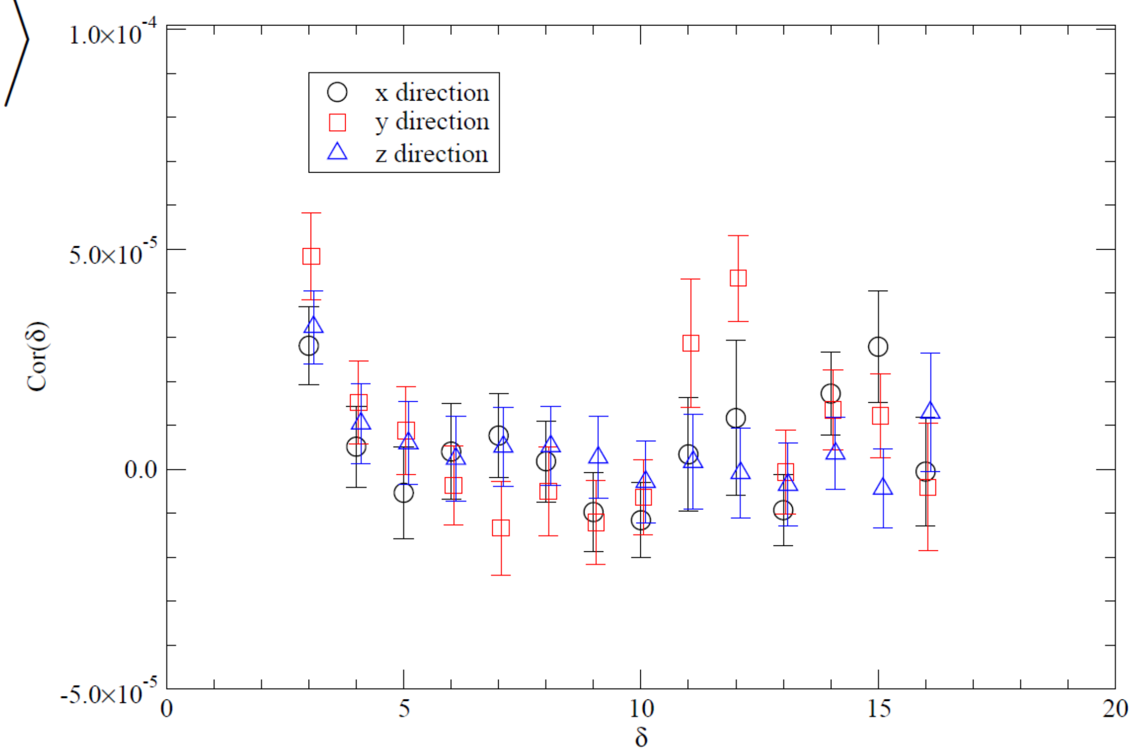
GPBC, incorrect ensemble	Standard
0.512239(6)	0.512239(3)(7)

- More sensitive test: as u, d fields couple to same gauge field we should observe correlations between observables separated by 12 in y-direction.

$$\mathrm{Cov}(\delta) = \left\langle \frac{1}{6V} \sum_{x,\mu<\nu} \left[P_{\mu\nu}(x) P_{\mu\nu}(x+\delta) - \mathcal{P}^2 \right] \right\rangle$$

$$\mathrm{Cor}(\delta) = \frac{\mathrm{Cov}(\delta)}{\mathrm{Cov}(0)}$$

- Statistically significant (3 sigma) correlation between plaquettes seen at sep 12.
- However effect is tiny, ~5x10^{-5}, unlikely to have strong effect on paper results where errors are 100x – 1000x larger.

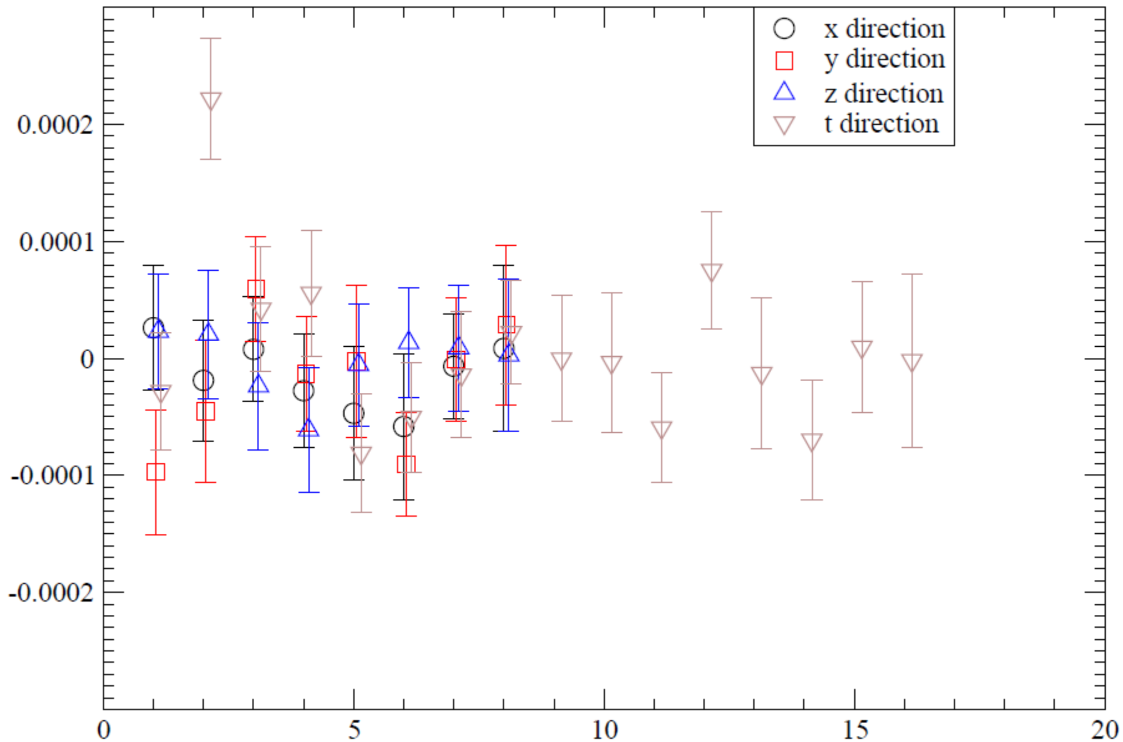


Evidence from 16^3x32 calculation

- 16^3x32 DWF+Iwasaki (β=2.13) test ensembles.

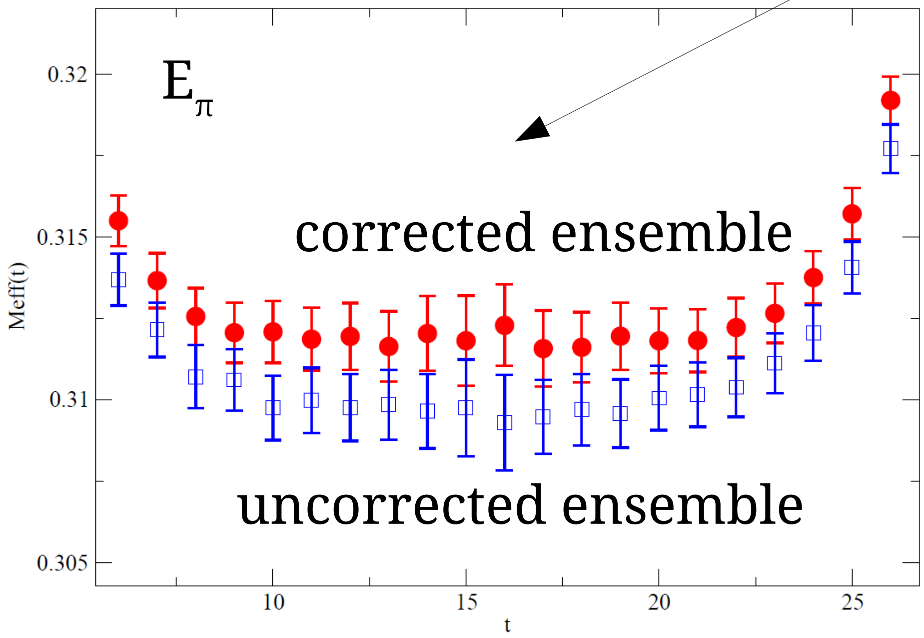
$$\eta_u(x) = \eta_d(x + 2\hat{t})$$

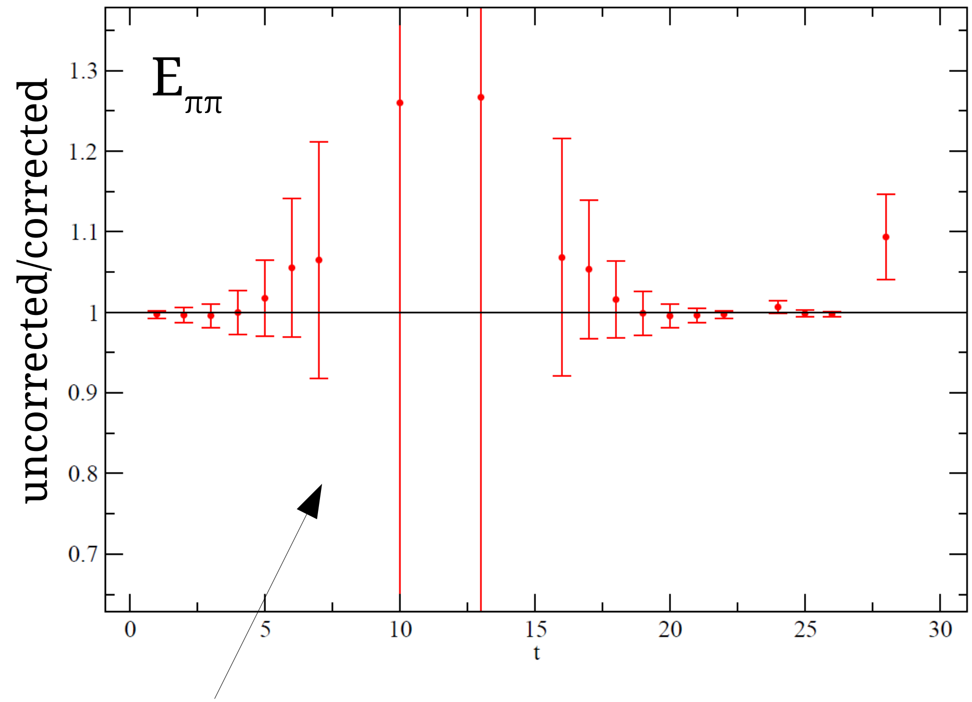
- Smaller lattice separation between correlated sites likely enhances effect.
- Generated an ensemble without error for comparison.
- Presently ~860 meas on corrected ensemble and 670 on uncorrected.
- Cannot see correlation in plaquette due to natural correlation between neaby sites. However evidence in link trace:



- Here at 2x10^{-4} level.

- Inconclusive, ~1.5 sigma, ~0.8% discrepancy in pion energy





- No presently measurable difference between $\pi\pi$(I=0) effective energies (important for validity of $K \to \pi\pi$ calculation)
- While apparently negligible, this error is uncontrolled theoretically and detracts from our claim of a first-principles calculation.
- Error will be corrected as part of our plans to extend the present calculation in near future.

An old homework problem

- 1964: CP-violation (indirect) first observed at BNL (Cronin, Fitch et al → 1980 Nobel prize)
- 1973: Framework for Standard Model CPV established (Kobayashi, Maskawa)
- 1993: Publication of first evidence of direct CPV from NA31 expt at CERN.
- 1999: KTeV at FermiLab and NA48 at CERN confirm direct CPV.
- 2001: First quenched calculations of ε' performed by CP-PACS and RBC using single particle amplitudes and LO ChPT to correct for missing pion.
- 2001: Technique established for lattice measurement of decays (Lellouch, Luscher)
- 2011: First full threshold (stationary, unphysically-heavy pions) calc. of A_0 and A_2 using dynamical domain wall fermions performed by RBC/UKQCD.
- 2012: First calculation of A_2 performed by RBC/UKQCD using DWF with physical kinematics, pion masses and large physical volume but single lattice spacing.
- 2015: Continuum calculation of A_2 performed by RBC/UKQCD
- 2015: Full threshold calculation of A_0 and A_2 using Wilson fermions by Ishizuka *et al* [arXiv:1505.05289]
- 2015: (This work) First complete, *ab initio* determination of ε' with physical kinematics and pion masses.

$\Delta I=3/2$ Calculation

Phys.Rev. D 91 (2015) 7, 074502 [arXiv:1502.00263 [hep-lat]].

Calculation Strategy

- A_2 can be computed directly from charged kaon decay:

$$\langle(\pi\pi)^{I=2}_{I_3=1}|H_W|K^+\rangle = \sqrt{2}A_2 e^{i\delta_2}$$

- Remove stationary (charged) pion state using antiperiodic BCs on d-quark propagator: $d(x+L) = -d(x) \longrightarrow |p| \in (\pi/L,\, 3\pi/L,\, 5\pi/L\ldots)$

$$\pi^+(x+L) = [\bar{u}d](x+L) = -\pi^+(x)$$ Moving ground state!

$$\pi^0(x+L) = [\bar{u}u - \bar{d}d](x+L) = +\pi^0(x)$$ Stationary ground state....

- Use Wigner-Eckart theorem to remove neutral pion from problem

$$\langle(\pi^+\pi^0)_{I=2}|Q^{\Delta I_z=1/2}|K^+\rangle = \frac{\sqrt{3}}{2}\langle(\pi^+\pi^+)_{I=2}|Q^{\Delta I_z=3/2}|K^+\rangle$$

- APBCs on d-quark break isospin symmetry allowing mixing between isospin states: however $\pi^+\pi^+$ is the only charge-2 state with these Q-numbers hence it cannot mix.

- Calculation performed on RBC & UKQCD 48^3x96 and 64^3x128 Mobius DWF ensembles with (5 fm)^3 volumes and a=0.114 fm, a=0.084 fm. Continuum limit computed.
- Make full use of eigCG and AMA to translate over all timeslices. Obtain 0.7-0.9% stat errors on all bare matrix elements!
- Results:

$$\mathrm{Re}(A_2) = 1.50(4)_{\mathrm{stat}}(14)_{\mathrm{sys}} \times 10^{-8}\ \mathrm{GeV}$$
$$\mathrm{Im}(A_2) = -6.99(20)_{\mathrm{stat}}(84)_{\mathrm{sys}} \times 10^{-13}\ \mathrm{GeV}$$

10%, 12% total errors on Re, Im!

- Systematic error completely dominated by perturbative error on NPR and Wilson coefficients.