

BSM Physics from Kaon Decays

Lattice QCD at Fermilab:
Celebrating the Career of
Paul Mackenzie

November 7-8, 2019

N.H. Christ

RBC/UKQCD Collaboration

Outline

- Thoughts about Paul
- Physics
 - $K_L \rightarrow \mu^+ \mu^-$
 - $K \rightarrow \pi\pi$ decay and ε'
- Conclusions

Thoughts about Paul

- Many places where Paul's work has had a large impact on me:
 - Tadpole improvement of lattice perturbation theory.
 - QCD machines: ACPMAPS
 - Fermilab heavy quark action
- Founding member and then spokesperson for USQCD.
- Common physics goal of searching for phenomena not predicted by the standard model.



The RBC & UKQCD collaborations

BNL and BNL/RBRC

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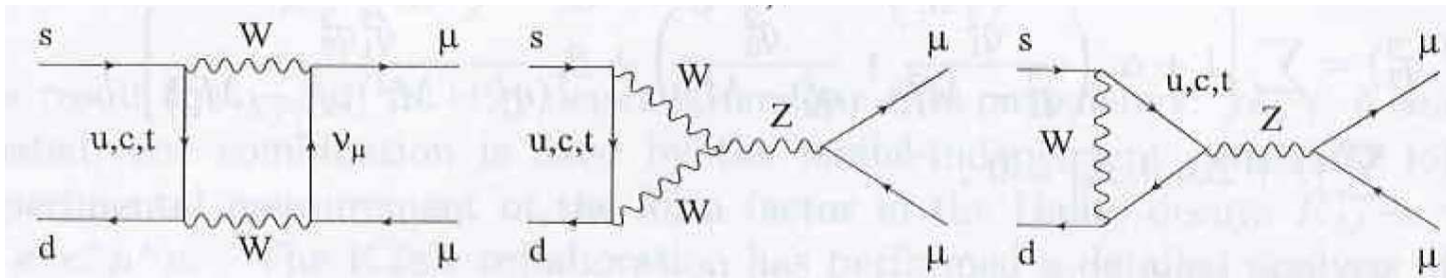
Jun-Sik Yoo

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$$K \rightarrow \mu^+ \mu^-$$

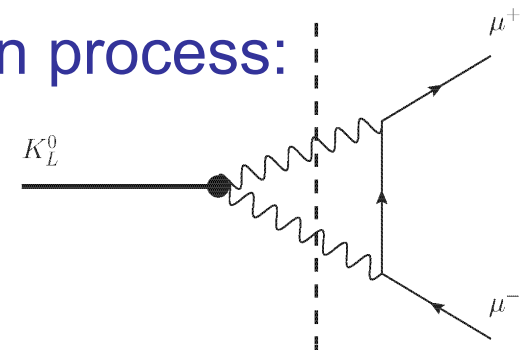
Physics of $K_L \rightarrow \mu^+ \mu^-$

- A second order weak, “strangeness changing neutral current”



(Cirigliano, *et al.*, Rev. Mod. Phys., **84**, 2012)

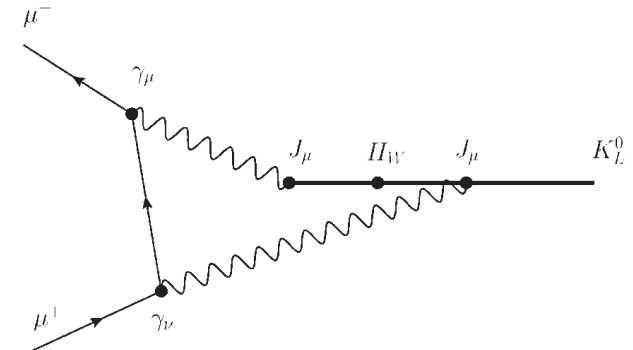
- $K_L \rightarrow \mu^+ \mu^-$ decay rate is known:
 - $\text{BR}(K_L \rightarrow \mu^+ \mu^-) = (6.84 \pm 0.11) \times 10^{-9}$
- Large “background” from two-photon process:
 - Third-order electroweak amplitude
 - Optical theorem gives imaginary part.
 - $K_L \rightarrow \gamma\gamma$ decay rate is known



Physics of $K_L \rightarrow \mu^+ \mu^-$ (con't)

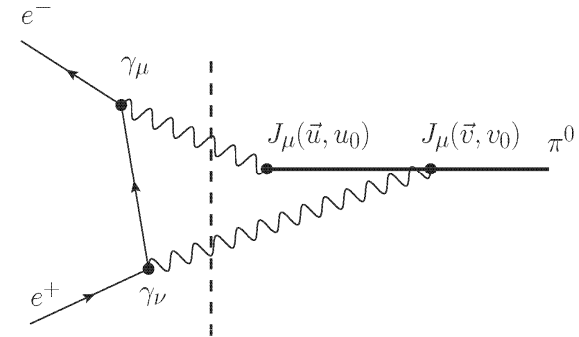
- Define: $\frac{\Gamma(K_L \rightarrow \mu^+ \mu^-)}{\Gamma(K_L \rightarrow \gamma\gamma)} = 2\beta_\mu \left(\frac{\alpha m_\mu}{\pi M_K}\right)^2 (|F_{\text{imag}}|^2 + |F_{\text{real}}|^2)$
- Optical theorem + experiment determine:

$$|F_{\text{real}}| = |(F_{\text{real}})_{\text{E\&M}} + (F_{\text{real}})_{\text{Weak}}| = 1.167 \pm 0.094$$
- Standard model: $(F_{\text{real}})_{\text{Weak}} = -1.82 \pm 0.04$
- A 10% lattice calculation of $(F_{\text{real}})_{\text{E\&M}}$ would allow a test of $(F_{\text{real}})_{\text{Weak}}$ with 6 – 17% accuracy
- Lattice calculation more difficult than ΔM_K
 - 5 vertices, 60 time orders
 - many states $|n\rangle$ with $E_n < M_K$
- First try simpler $\pi^0 \rightarrow e^+ e^-$

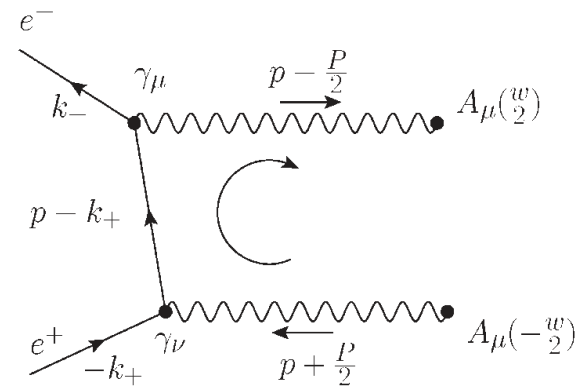
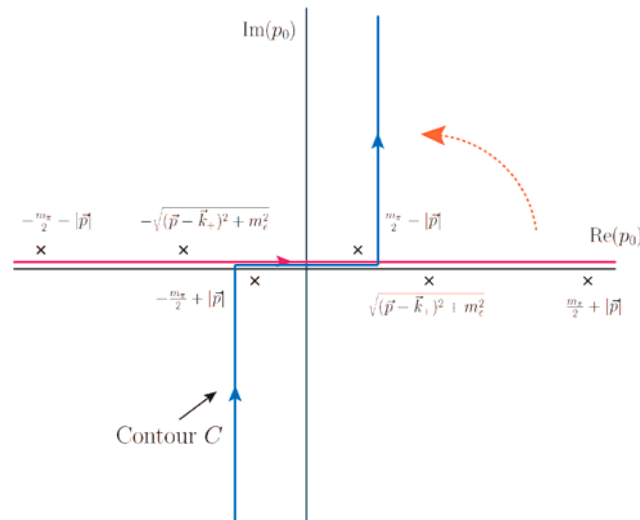


Consider simpler $\pi^0 \rightarrow e^+ e^-$

- Euclidean non-covariant P.T. difficult:
 - 12 time orders,
 - $E_{\gamma\gamma} < M_{\pi^0}$
- Try something different:
 - Evaluate in Minkowski space
 - Wick rotate internal time integral:



$$\mathcal{A}_{\pi^0 \rightarrow e^+ e^-} \rightarrow \int d^4 w \tilde{L}(k_-, k_+, w)_{\mu\nu} \langle 0 | T \left\{ J_\mu\left(\frac{W}{2}\right) J_\nu\left(-\frac{W}{2}\right) \right\} | \pi^0(\vec{P} = 0) \rangle$$

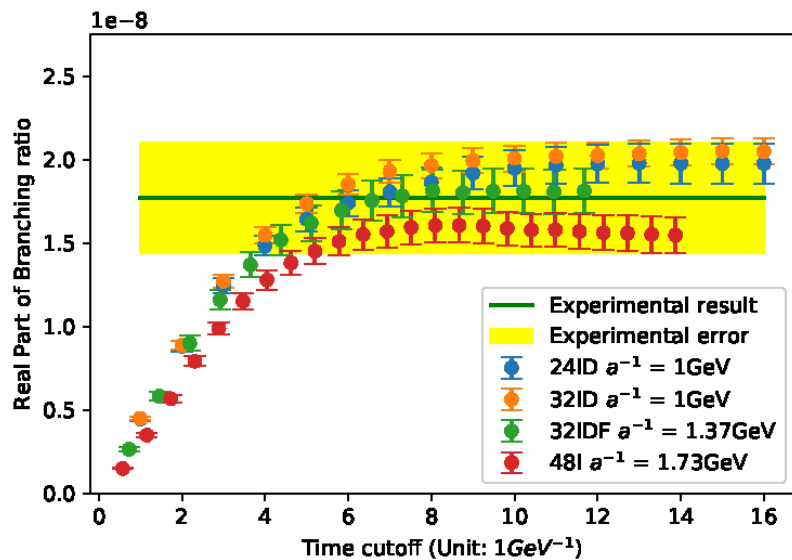
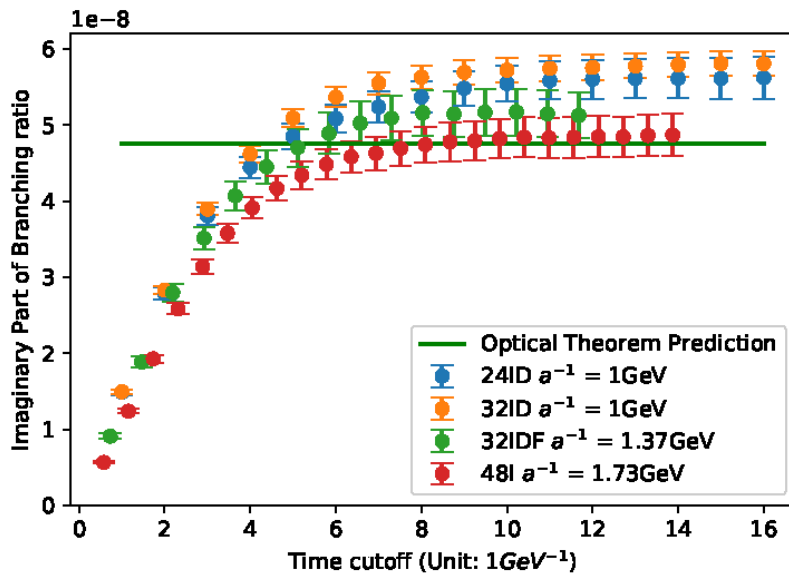


Lattice Results

(Yidi Zhao)

$$\mathcal{A}_{\pi^0 \rightarrow e^+e^-} \rightarrow \int d^4w \tilde{L}(k_-, k_+, w)_{\mu\nu} \langle 0 | T \left\{ J_\mu\left(\frac{w}{2}\right) J_\nu\left(-\frac{w}{2}\right) \right\} | \pi^0(\vec{P} = 0) \rangle$$

- Lattice result is literally complex:
 - Exponentially small FV corrections
 - Physical kinematics, $1/a \leq 1.73 \text{ GeV}$:
 - $\text{Im}(A) = 35.94(1.01)(1.09)$ [Expt: 35.07(37)]
 - $\text{Re}(A) = 20.39(72)(70)$. [Expt: 21.51(2.02)]



$K \rightarrow \pi\pi$ decay and ε'

Cabibbo-Kobayashi-Maskawa mixing

- W^\pm emission scrambles the quark flavors

$$\begin{pmatrix} u \\ c \\ t \end{pmatrix} \xleftrightarrow{W^\pm} \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} d \\ s \\ b \end{pmatrix}$$

CP
violation!

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} = \begin{pmatrix} 1 - \frac{\lambda^2}{2} & \lambda & A\lambda^3(\bar{\rho} - i\bar{\eta}) \\ -\lambda & 1 - \frac{\lambda^2}{2} & A\lambda^2 \\ A\lambda^3(1 - \bar{\rho} - i\bar{\eta}) & -A\lambda^2 & 1 \end{pmatrix} + \mathcal{O}(\lambda^4)$$

$$\lambda = 0.22535 \pm 0.00065, \quad A = 0.811^{+0.022}_{-0.012},$$

$$\bar{\rho} = 0.131^{+0.026}_{-0.013}, \quad \bar{\eta} = 0.345^{+0.013}_{-0.014}.$$

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:

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

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

Direct CP violation in $K \rightarrow \pi \pi$

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

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

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

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

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

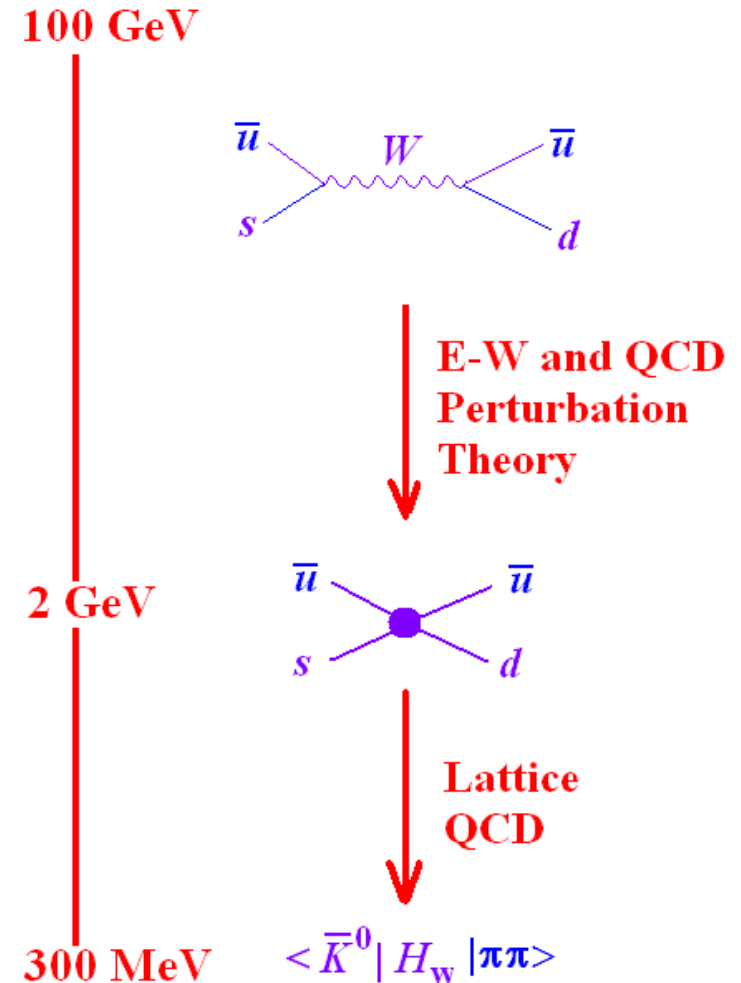
Direct CP
violation

Low Energy Effective Theory

- Represent weak interactions by local four-quark Lagrangian

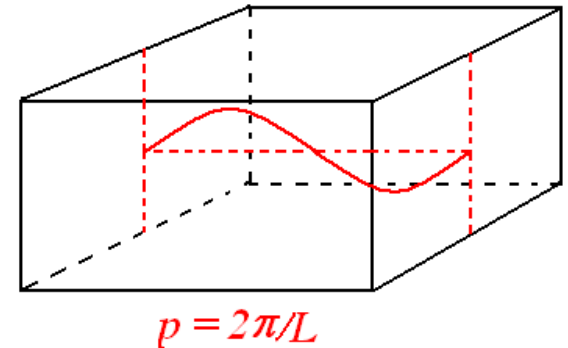
$$\mathcal{H}^{\Delta S=1} = \frac{G_F}{\sqrt{2}} V_{ud} V_{us}^* \left\{ \sum_{i=1}^{10} [z_i(\mu) + \tau y_i(\mu)] Q_i \right\}$$

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



Lattice calculation of $\langle \pi\pi | H_W | K \rangle$

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



$$\langle \pi^+ \pi^- | H_W | K^0 \rangle \propto \langle \bar{d}u(t_{\pi_1}) \bar{u}d(t_{\pi_2}) H_W(t_{\text{op}}) \bar{d}u(t_K) \rangle$$

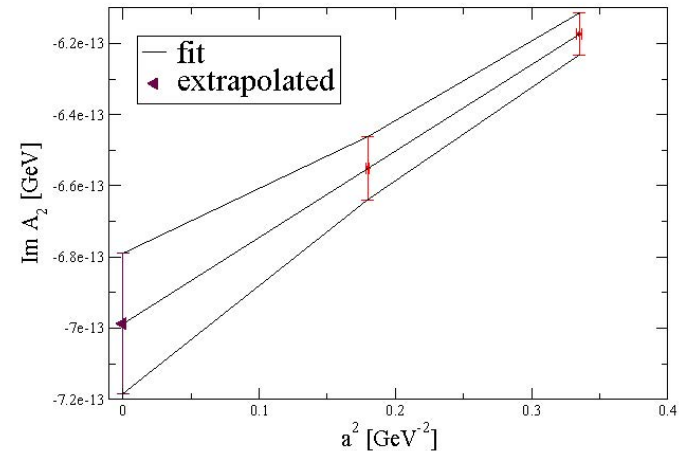
- Use boundary conditions on the quarks: $E_{\pi\pi}^{(\text{gnd})} = M_K$
- For $(\pi\pi)_{I=2}$ make d anti-periodic
- For $(\pi\pi)_{I=0}$ use G-parity boundary conditions: [arXiv:1908.08](https://arxiv.org/abs/1908.08)

Calculation of A_2

$\Delta I = 3/2$ – Continuum Results

(M. Lightman, E. Goode, T. Janowski)

- Use two large ensembles to remove a^2 error ($m_p = 135$ MeV, $L = 5.4$ fm)
 - $48^3 \times 96$, $1/a = 1.73$ GeV
 - $64^3 \times 128$, $1/a = 2.28$ GeV
- Continuum results:
 - $\text{Re}(A_2) = 1.50(0.04_{\text{stat}}) (0.14)_{\text{syst}} \times 10^{-8}$ GeV
 - $\text{Im}(A_2) = -6.99(0.20)_{\text{stat}} (0.84)_{\text{syst}} \times 10^{-13}$ GeV
- Experiment: $\text{Re}(A_2) = 1.479(4) 10^{-8}$ GeV
- $E_{\pi\pi} \rightarrow \delta_2 = -11.6(2.5)(1.2)^\circ$
- [Phys. Rev. **D91**, 074502 (2015)]



Calculation of A_0 and ε'

Overview of 2015 calculation

(Chris Kelly and Daiqian Zhang)

- Use $32^3 \times 64$ ensemble
 - $1/a = 1.3784(68)$ GeV, $L = 4.53$ fm.
 - G-parity boundary condition in 3 directions
 - 216 configurations separated by 4 time units
- Essentially physical kinematics:
 - $M_\pi = 143.1(2.0)$
 - $M_K = 490.6(2.2)$ MeV
 - $E_{\pi\pi} = 498(11)$ MeV

2015 Results

[Phys. Rev. Lett. 115 (2015) 212001]

- $E_{\pi\pi}(499 \text{ MeV})$ determines δ_0 :
 - $l = 0$ $\pi\pi$ phase shift: $\delta_0 = 23.8(4.9)(2.2)^\circ$
 - Dispersion theory result: $\delta_0 = 34^\circ$ [G. Colangelo, *et al.*]
- $\text{Re}(\varepsilon'/\varepsilon) = (1.38 \pm 5.15_{\text{stat}} \pm 4.59_{\text{sys}}) \times 10^{-4}$
 - Expt.: $(16.6 \pm 2.3) \times 10^{-4}$
 - 2.1 σ difference
- **Unanswered questions:**
 - Is this 2.1 σ difference real? \rightarrow **Reduce errors**
 - Why is δ_0 so different from the dispersive result? \rightarrow **Introduce more $\pi\pi$ operators to distinguish excited states**

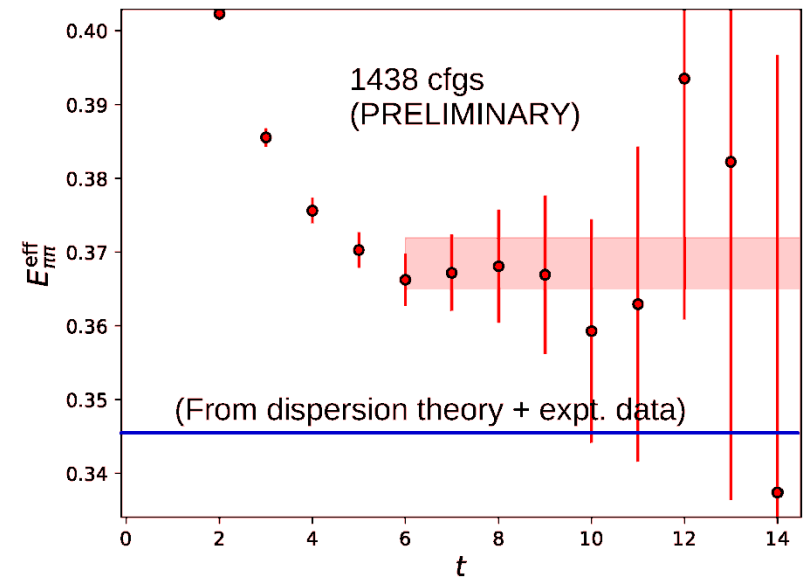
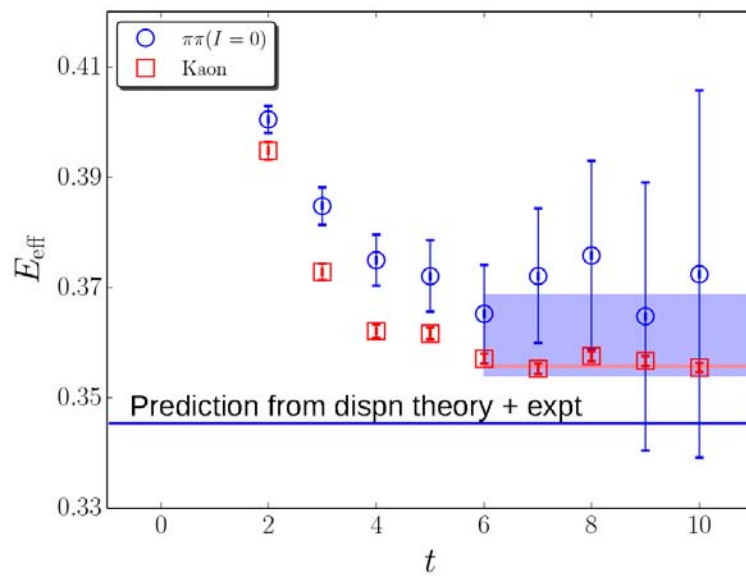
Extend and improve calculation

(Chris Kelly and Tianle Wang)

- ✓- Increase statistics: 216 → 1438 configs.
 - Reduce statistical errors
 - Allow deeper study of systematic errors
- ✓- Study operators neglected in our NPR implementation
- ✓- Use step-scaling to allow perturbative matching at a higher energy
- ✓- Use an expanded set of $\pi\pi$ operators
 - Use X-space NPR to cross charm threshold (Masaaki Tomii).

Adding more statistics

- Increasing statistics: 216 \rightarrow 1438 configs.
 - $\pi\pi - \pi\pi$ correlator well-described by a single $\pi\pi$ state
 - $\delta_0 = 23.8(4.9)(2.2)^\circ \rightarrow 19.1(2.5)(1.2)^\circ$
 $\chi^2 / \text{DoF} = 1.6$



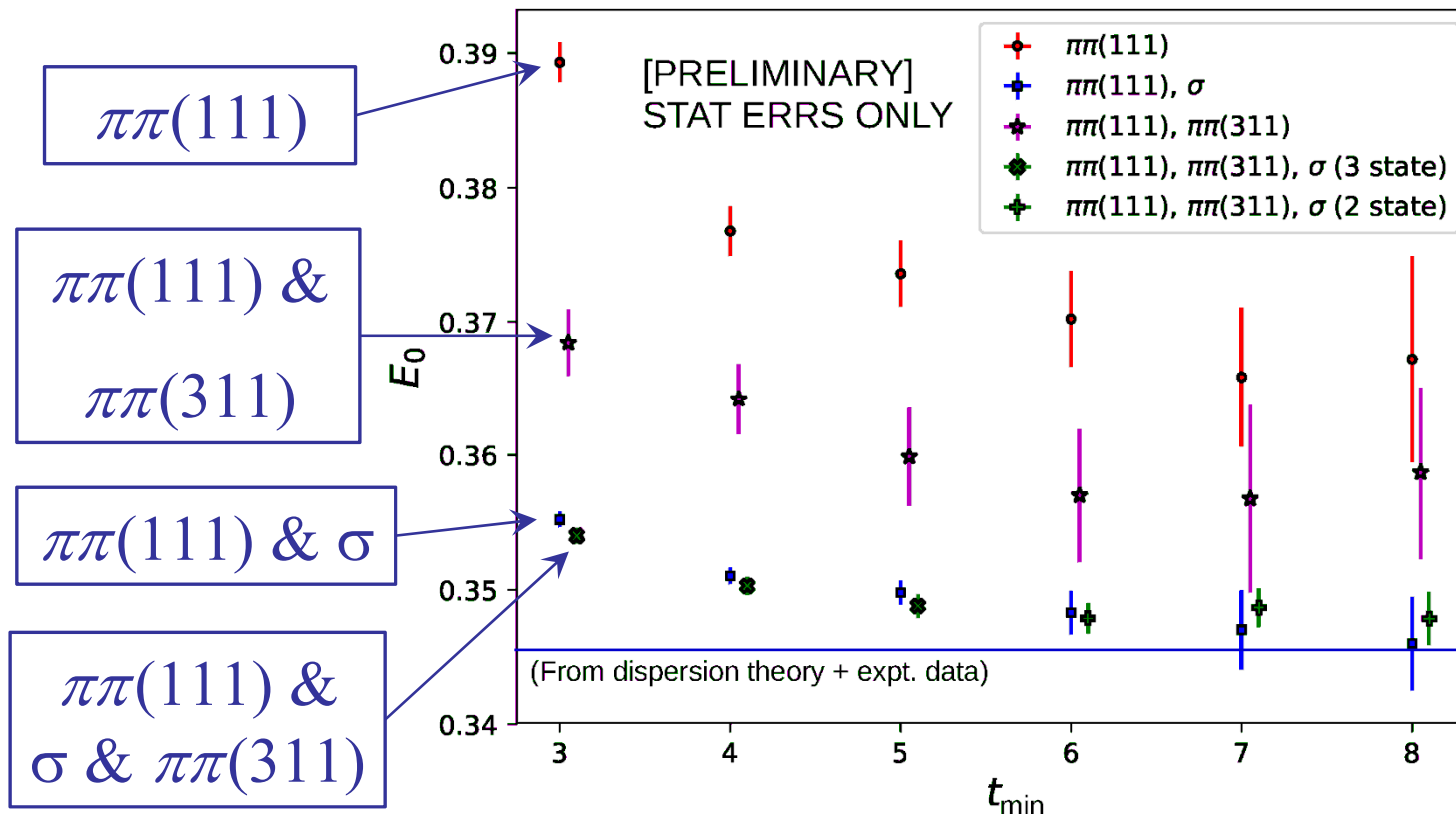
Adding more $\pi\pi$ operators

- Adding a second σ -like ($\bar{u}u + \bar{d}d$) operator reveals a second state!
- If only one state, 2 x 2 correlator matrix will have determinant = 0. For $t_f - t_i = 5$:

$$\det \begin{pmatrix} \langle \pi\pi(t_f)\pi\pi(t_i) \rangle & \langle \pi\pi(t_f)\sigma(t_i) \rangle \\ \langle \sigma(t_f)\pi\pi(t_i) \rangle & \langle \sigma(t_f)\sigma(t_i) \rangle \end{pmatrix} = 0.439(50)$$

- Add a third operator giving each pion a larger momentum: $p = \pm (3, 1, 1) \pi / L$
- Label operators as $\pi\pi(111)$, σ , $\pi\pi(311)$
- Only 741 configurations with new operators

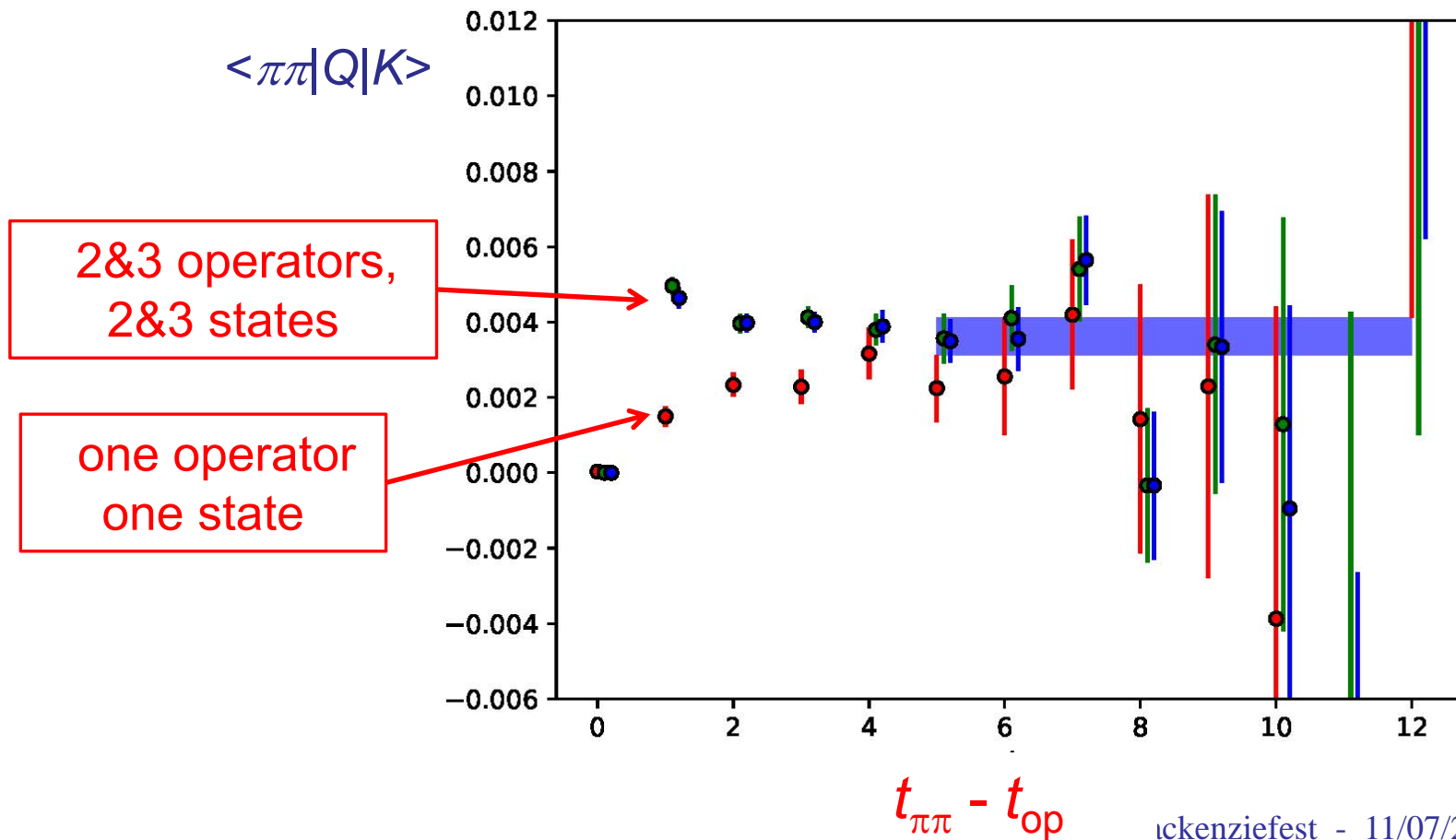
$l = 0$ $\pi\pi$ scattering with three operators



- Third $\pi\pi(311)$ operator not important.
- $\delta_0 = 31.7(6)^\circ$ vs 34° prediction (5-15 fit, statistical errors only).

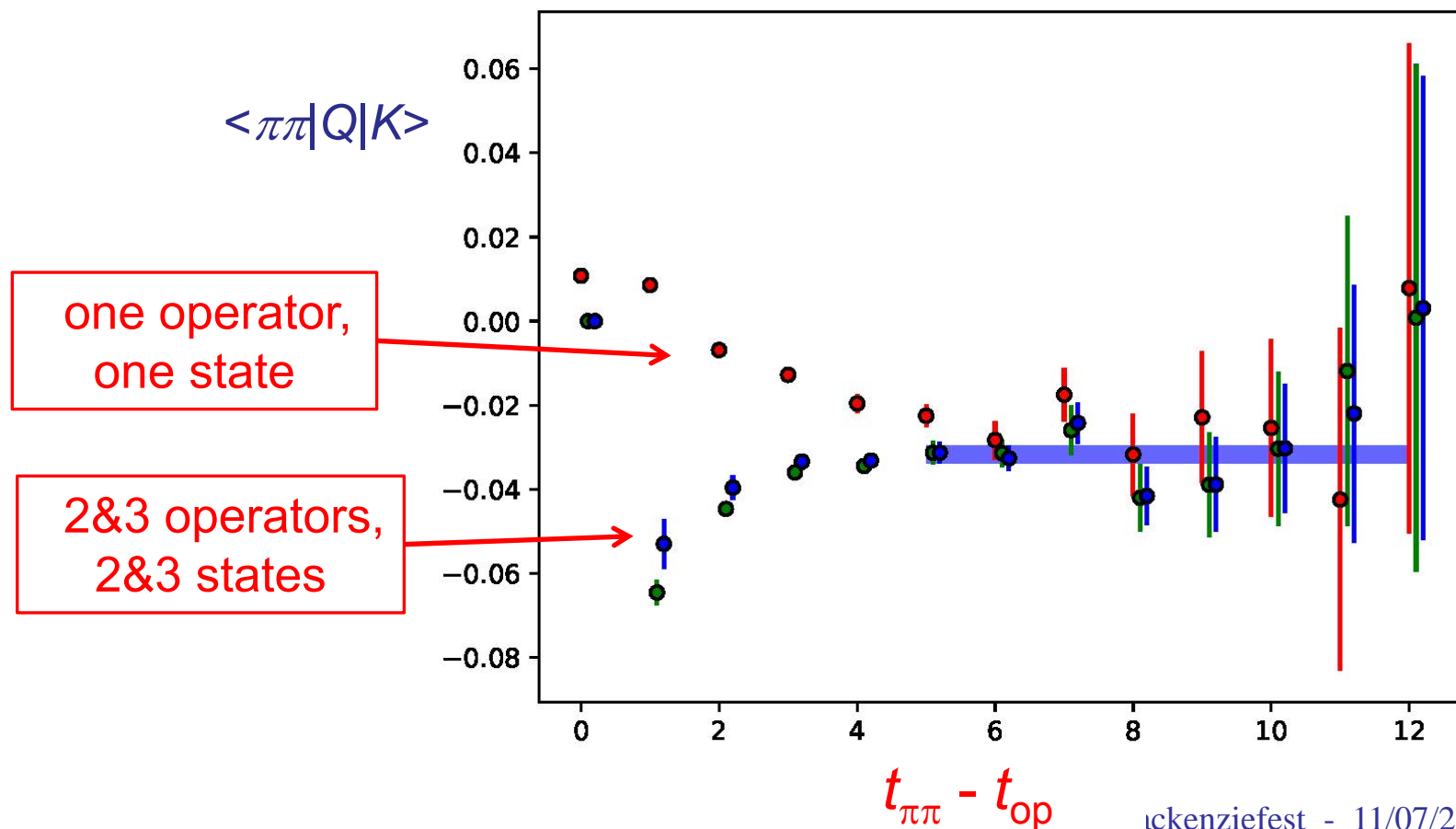
$K \rightarrow \pi\pi$ from 3-operator fits (case I)

- Fit using up to 3 operators and 3 states with energies and amplitudes from $\pi\pi$ scattering:



$K \rightarrow \pi\pi$ from 3-operator fits (case II)

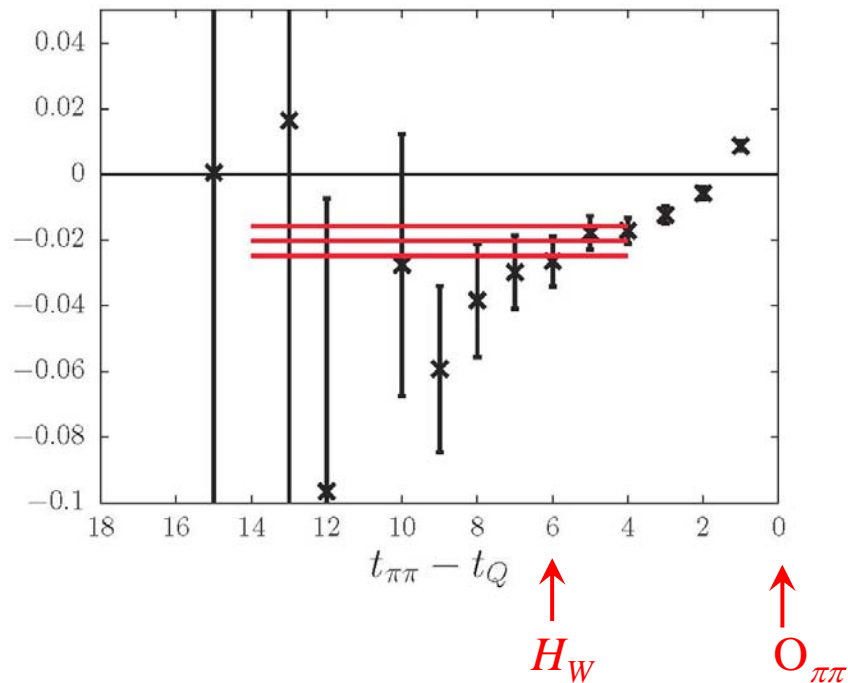
- Fit using up to 3 operators and 3 states with energies and amplitudes from $\pi\pi$ scattering:



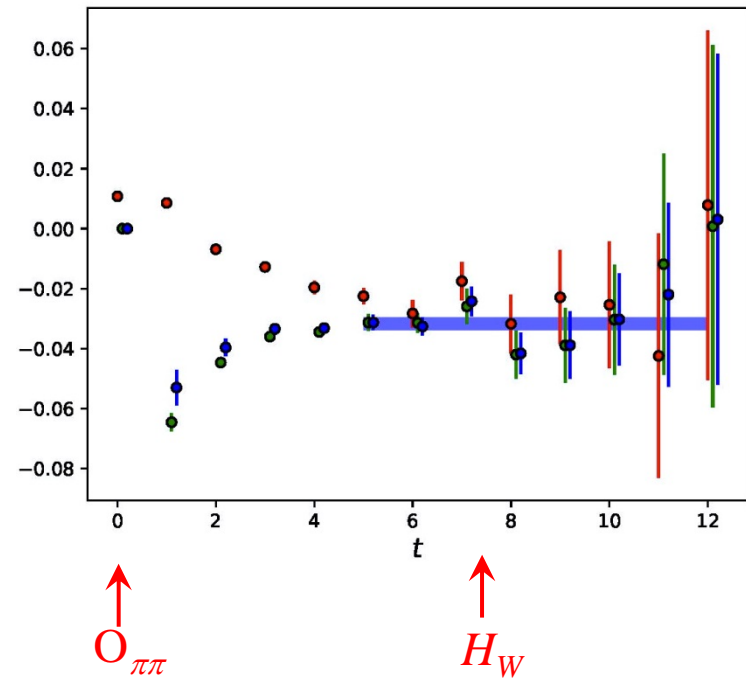
$K \rightarrow \pi \pi$ matrix elements

- Compare old and new results (case I)

215 samples [2015]



741 samples [2019]



Two data analysis challenges

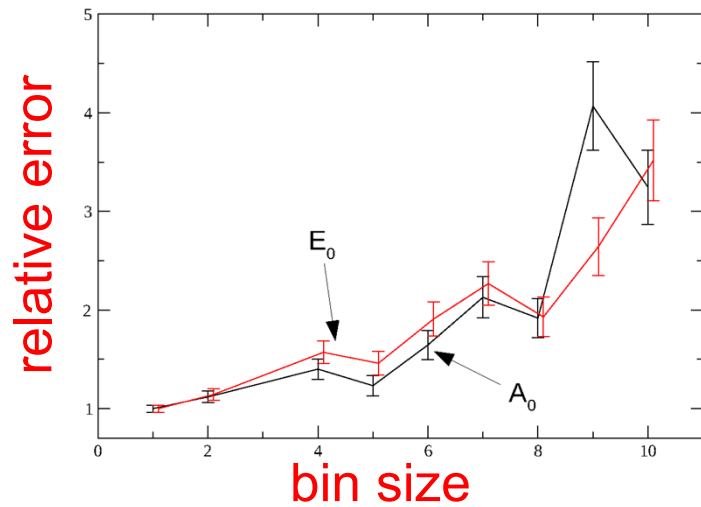
- Auto-correlations – we must be careful that our errors are accurate
- We need estimates of goodness of fit (p -values)
 - Demonstrate that our fits describe the data.
 - Decide if alternative fits used to estimate systematic errors are plausible.
 - However, our lattice QCD p -values are traditionally unreasonably small!

Auto-correlations

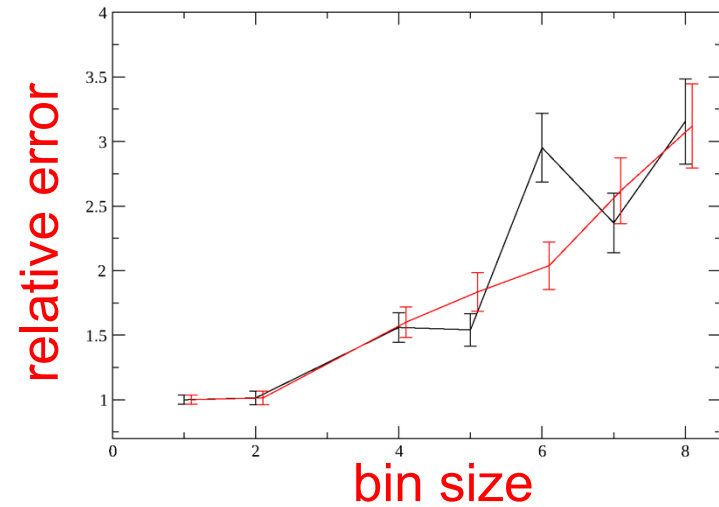
- Our measurements are made every 4 MD time units and are mildly correlated.
- While we have $N=741$ configurations, the covariance matrix for three operators and $t = 5-15$ time slices is 66×66 !
- Noise grows as we bin the data and have fewer samples to measure the fluctuations.
- Solved by the *blocked jackknife* method:
 - Identify N/B blocks of size B .
 - Sequentially remove each block and analyze the remaining $N-B$ (not $N/B-1$) samples

$l=0$ $\pi\pi$ two-point function fit errors

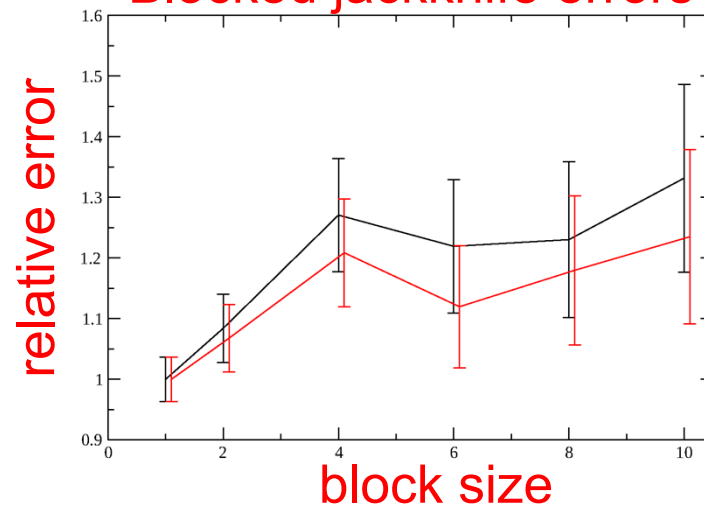
Binned data errors



Binned scrambled data errors



Blocked jackknife errors



Poor p -values

- We obtain p -values of 0.1– 0.2 for most “best fits”!
- This is often caused by ignoring fluctuations in the covariance matrix (Tanmoy Bhattacharya).
- Including covariance matrix fluctuations broadens the χ^2 distribution into the Hotelling T^2 distribution (related to F distrib.).

Hotelling T^2 is *insufficient*

- Hotelling assumes that the data (not their averages) are Gaussian and uncorrelated.
- Both are not true for our case.
- Use a bootstrap analysis to determine the correct generalized χ^2 distribution from the data. (C. Kelly)

q^2 distribution

- Define
$$q^2 = \sum_{t,t'=t_{\min}}^{t_{\max}} [\bar{v}_t - f(t, \vec{p})] [C^{-1}]_{tt'} [\bar{v}_{t'} - f(t', \vec{p})]$$

where
$$C_{tt'} = \frac{1}{N(N-1)} \sum_{i=1}^N [v_{i,t} - \bar{v}_t] [v_{i,t'} - \bar{v}_{t'}]$$

- Find $P(q^2)$ where

$$\int_0^{\infty} P(q^2) dq^2 = 1 \quad \text{and} \quad p_{\text{int}}(q^2) = \int_{q^2}^{\infty} P(q^2) dq^2$$

- Here $p_{\text{int}}(q^2)$ gives the “p-value”

Find q^2 distribution from the data (Chris Kelly)

- Start with the original ensemble $\{v_{it}\}_{1 \leq i \leq N}$
- Draw N values from this set (allowing the same value to be drawn multiple times).
- Create N_{boot} such ensembles of N values: $\{b_{it}^\alpha\}_{1 \leq i \leq N}$ where $1 \leq \alpha \leq N_{\text{boot}}$
- *Recenter* these ensembles so $f(t, \vec{p})$ will fit the average over boot strap ensembles perfectly:

$$b_{i,t}^\alpha \rightarrow \tilde{b}_{i,t}^\alpha = b_{i,t}^\alpha - \bar{v}_t + f(t, \vec{p})$$

- Here the parameters \vec{p} fit the average data \bar{v}_t

q^2 distribution

- $\tilde{b}_{i,t}^\alpha$ has the fluctuation in the population but is fit perfectly by $f(t, \vec{p})$

$$b_{i,t}^\alpha \rightarrow \tilde{b}_{i,t}^\alpha = b_{i,t}^\alpha - \bar{v}_t + f(t, \vec{p})$$

Fit to ensemble α

- Thus

$$(q^2)^\alpha = \sum_{t, t'=t_{\min}}^{t_{\max}} \left[\tilde{b}_t^\alpha - f(t, \vec{p}^\alpha) \right] \left[(C^\alpha)^{-1} \right]_{tt'} \left[\tilde{b}_{t'}^\alpha - f(t', \vec{p}^\alpha) \right]$$

will obey (and give) the correct q^2 distribution.

- $p(q^2) = N(q^2)/N_{\text{boot}}$ where $N(q^2)$ is the number of bootstrap ensembles with $(q^2)^\alpha > q^2$.
- Now p -values can be computed for any definition of q^2 including for uncorrelated fits!

$K \rightarrow \pi\pi$ calculation (2019)

- Calculation of $K \rightarrow \pi\pi$ decay substantially improved over 2015 result.
- 216 \rightarrow 741 configurations.
- Three $\pi\pi$ interpolating operators: discriminate between ground and excited states $\rightarrow \delta_0(E=M_K) = 31.7(6)^\circ$
- Errors reduced by using correlated fits.
- Bootstrap-determined q^2 distribution gives correct p -values. [$p=0.261$ (BS) vs $0.037(\chi^2)$]
- **Results available soon.**

Thanks !

- Precision measurement + lattice QCD is a long-term direction of great promise.
 - Paul is a leading contributor
 - Important new results lie ahead.
- Importance of Paul's national leadership is hard to overstate:
 - USQCD hardware has enabled frontier calculations
 - Many careers advanced by USQCD projects.
 - Collaborative good will and combined strengths of USQCD attract new talent and enhanced funding!

