$K \rightarrow \pi\pi$ decay and ε'

Lattice QCD

Santa Fe, New Mexico

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RBC/UKQCD Collaboration

Outline

- Quick review of standard model ~~CP~~
- Overview of 2015 calculation
- Overview of 2019 calculation
- Multi-operator results for $\pi\pi$ scattering
- $K \rightarrow \pi\pi$ decay amplitudes (no new result yet for ε')
- Improved statistical methods:
  - Control auto-correlations
  - Determine goodness of fit
- Conclusion

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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!

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

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

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

$K^0 - \overline{K^0}$ 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 $\overline{K^0}$

$$|K_S\rangle = \frac{K_+ + \bar{\epsilon} K_-}{\sqrt{1+|\bar{\epsilon}|^2}}$$

$$|K_L\rangle = \frac{K_- + \bar{\epsilon} K_+}{\sqrt{1+|\bar{\epsilon}|^2}}$$

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

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

$K \to \pi\,\pi$ 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:

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

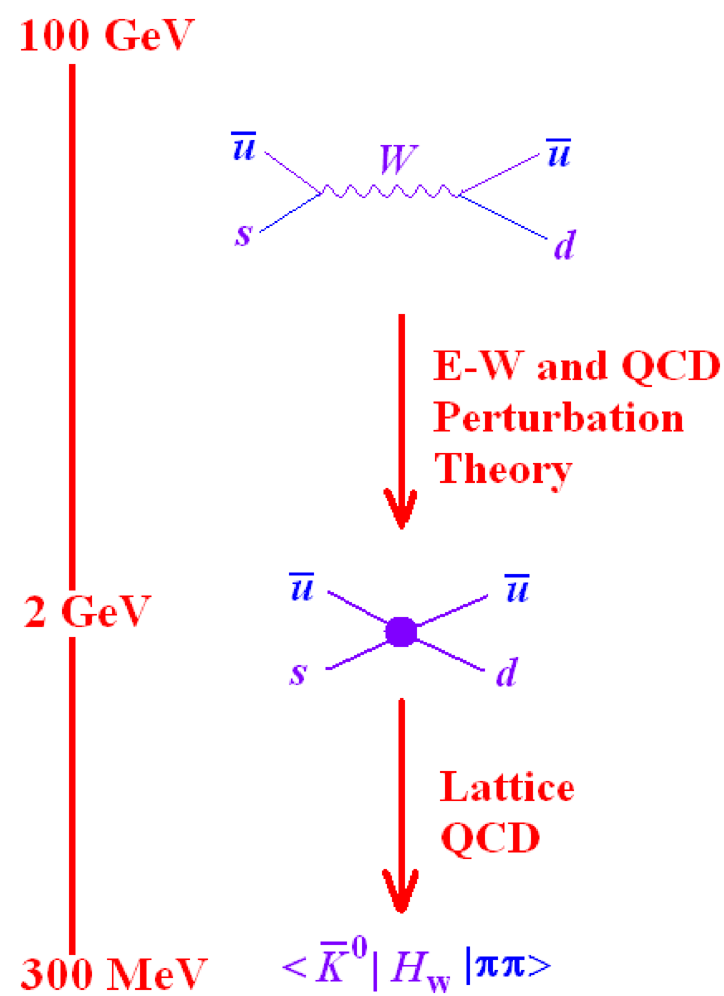
Direct CP violation

Low Energy Effective Theory

- Represent weak interactions by local four-quark Lagrangian

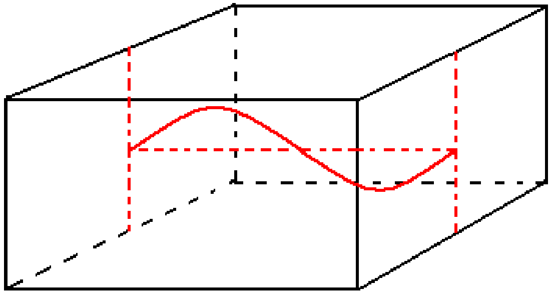
$$\mathcal{H}^{\Delta S=1} = \frac{G_F}{\sqrt{2}} V_{ud} V_{us}^* \left\{ \sum_{i=1}^{10} \left[z_i(\mu) + \tau y_i(\mu) \right] Q_i \right\}$$

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



Lattice calculation of $\boxed{<\pi\pi\,|H_W|K>}$

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



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

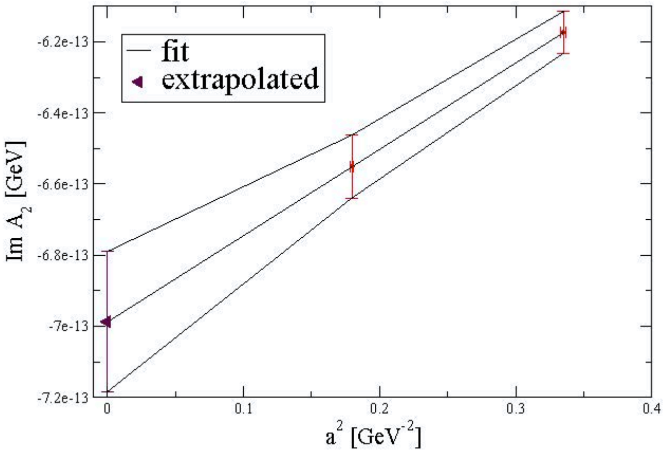
- Use boundary conditions on the quarks: $E_{\pi\pi}^{(\mathrm{gnd})} = M_K$
- For $(\pi\pi)_{I=2}$ make d anti-periodic
- For $(\pi\pi)_{I=0}$ use G-parity boundary conditions

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 x 96, 1/a=1.73 GeV
  - 64^3 x 128, 1/a=2.28 GeV



- Continuum results:
  - $\mathrm{Re}(A_2) = 1.50(0.04_{\mathrm{stat}})\,(0.14)_{\mathrm{syst}} \times 10^{-8}$ GeV
  - $\mathrm{Im}(A_2) = -6.99(0.20)_{\mathrm{stat}}\,(0.84)_{\mathrm{syst}} \times 10^{-13}$ GeV
- Experiment: $\mathrm{Re}(A_2) = 1.479(4)\ 10^{-8}$ GeV
- $E_{\pi\pi} \rightarrow \delta_2 = -11.6(2.5)(1.2)^{\circ}$
- [Phys.Rev. **D91**, 074502 (2015)]

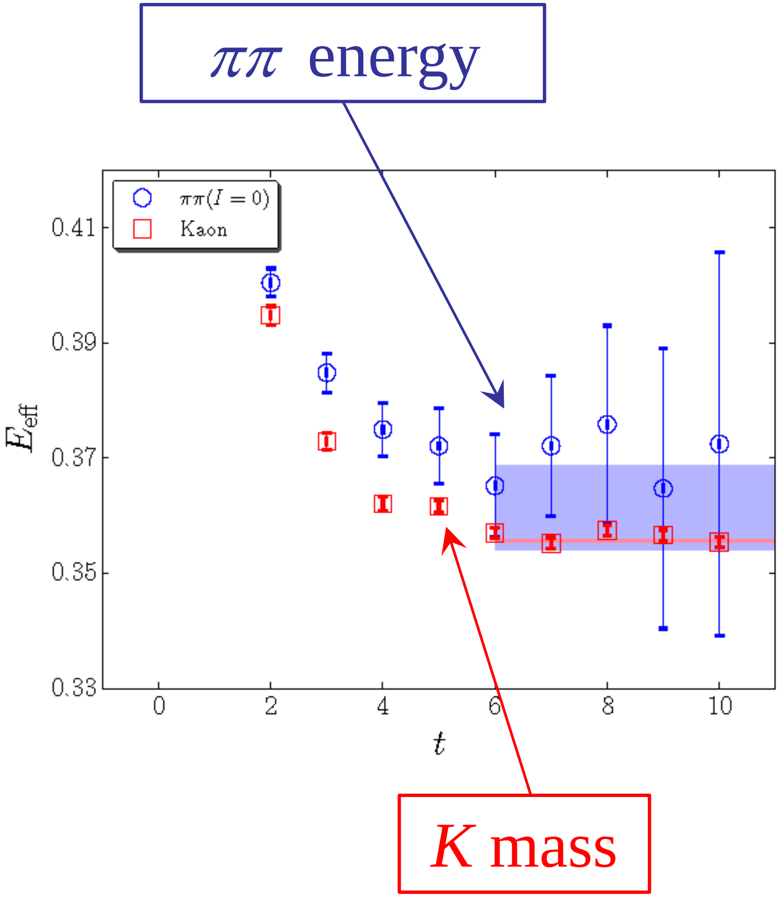
Calculation of A_0 and ε'

Overview of 2015 calculation
(Chris Kelly and Daiqian Zhang)

- Use 32^3 x 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
- Achieve essentially physical kinematics:
  - M_π = 143.1(2.0)
  - M_K = 490.6(2.2) MeV
  - $E_{\pi\pi}$ = 498(11) MeV

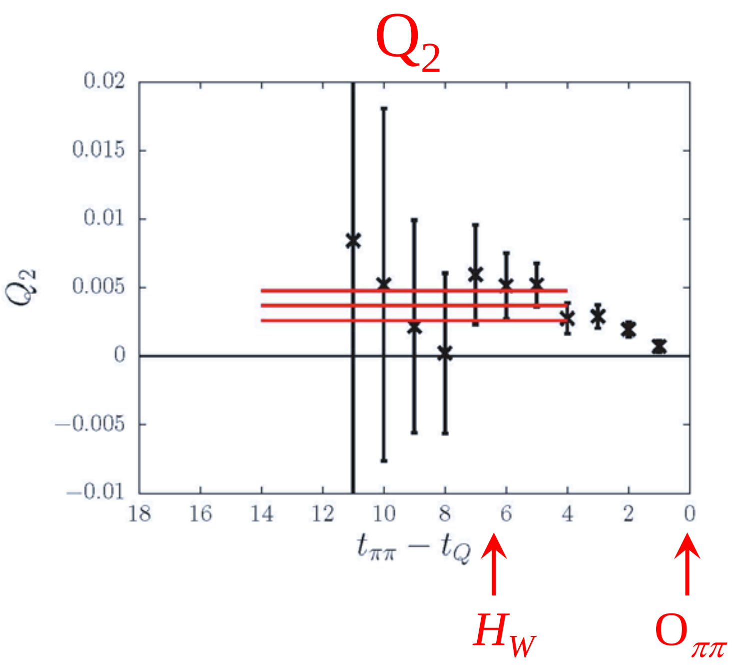
$I = 0$, $\pi\pi - \pi\pi$ correlator

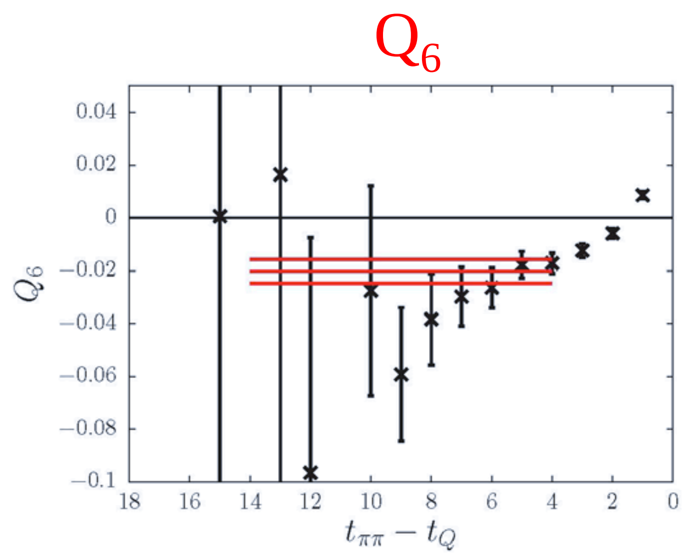
- Determine normalization of $\pi\pi$ interpolating operator
- Determine energy of finite volume, $I = 0$, $\pi\pi$ state: $E_{\pi\pi} = 498(11)$ MeV
- Obtained consistent results from a one-state fit with t_{min}=6 or a two-state fit with t_{min}=4.



$I = 0$ $K \to \pi\pi$ matrix elements

- Vary time separation between H_W and $\pi\pi$ operator.
- Show data for all $K - H_W$ separations $t_Q - t_K \geq 6$ and $t_{\pi\pi} - t_K = 10, 12, 14, 16$ and 18.
- Fit correlators with $t_{\pi\pi} - t_Q \geq 4$
- Obtain consistent results for $t_{\pi\pi} - t_Q \geq 3$ or 5





Systematic errors

Description	Error
Operator renormalization	15%
Wilson coefficients	12%
Finite lattice spacing	12%
Lellouch-Luscher factor	11%
Finite volume	7%
Parametric errors	5%
Excited states	5%
Unphysical kinematics	3%
Total	27%

2015 Results

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

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

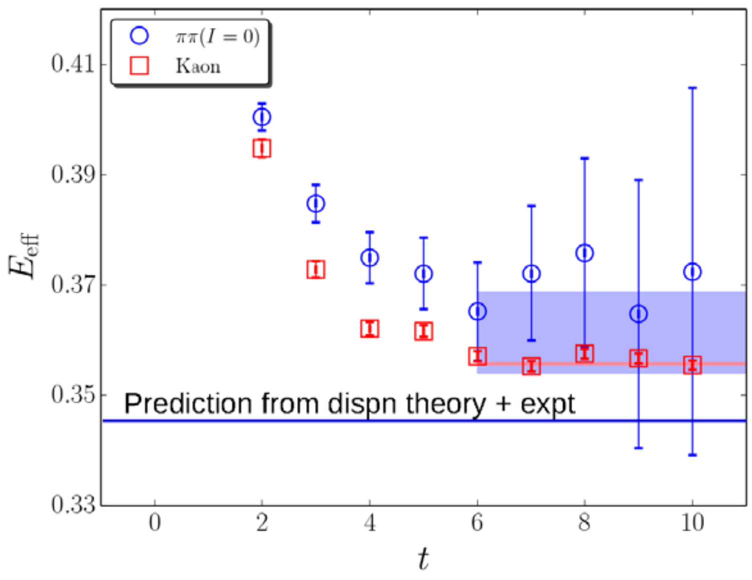
Extend and improve calculation

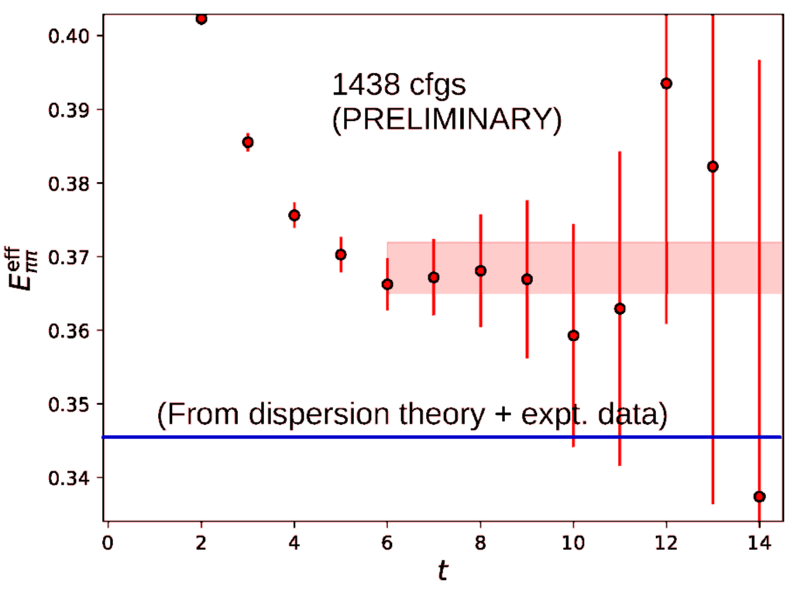
(Chris Kelly and Tianle Wang)

- ✓ Increase statistics: 216 → 1438 configs.
  - Reduce statistical errors
  - Allow in depth 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 → 1438 configs.
  - $\pi\pi - \pi\pi$ correlator well-described by a single $\pi\pi$ state
  - δ_0 = 23.8(4.9)(2.2)° → 19.1(2.5)(1.2)°
    χ^2 / 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

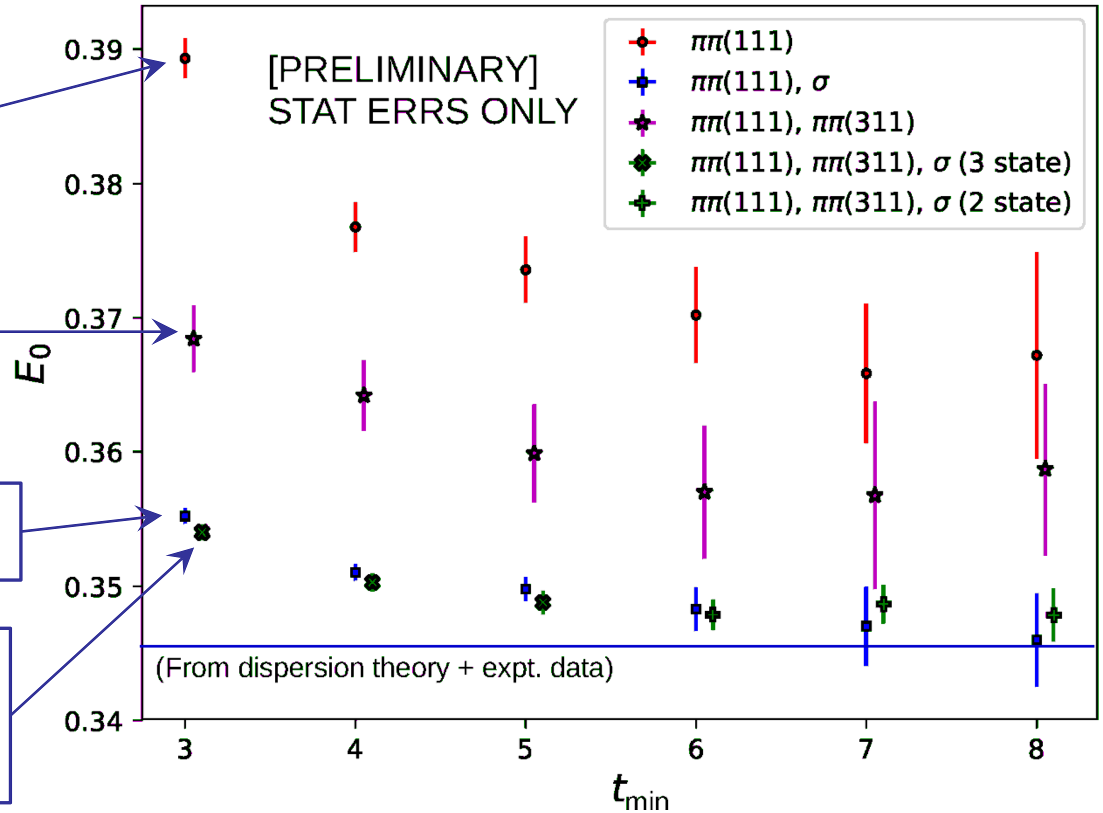
I = 0 $\pi\pi$ scattering with three operators

$\pi\pi(111)$

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

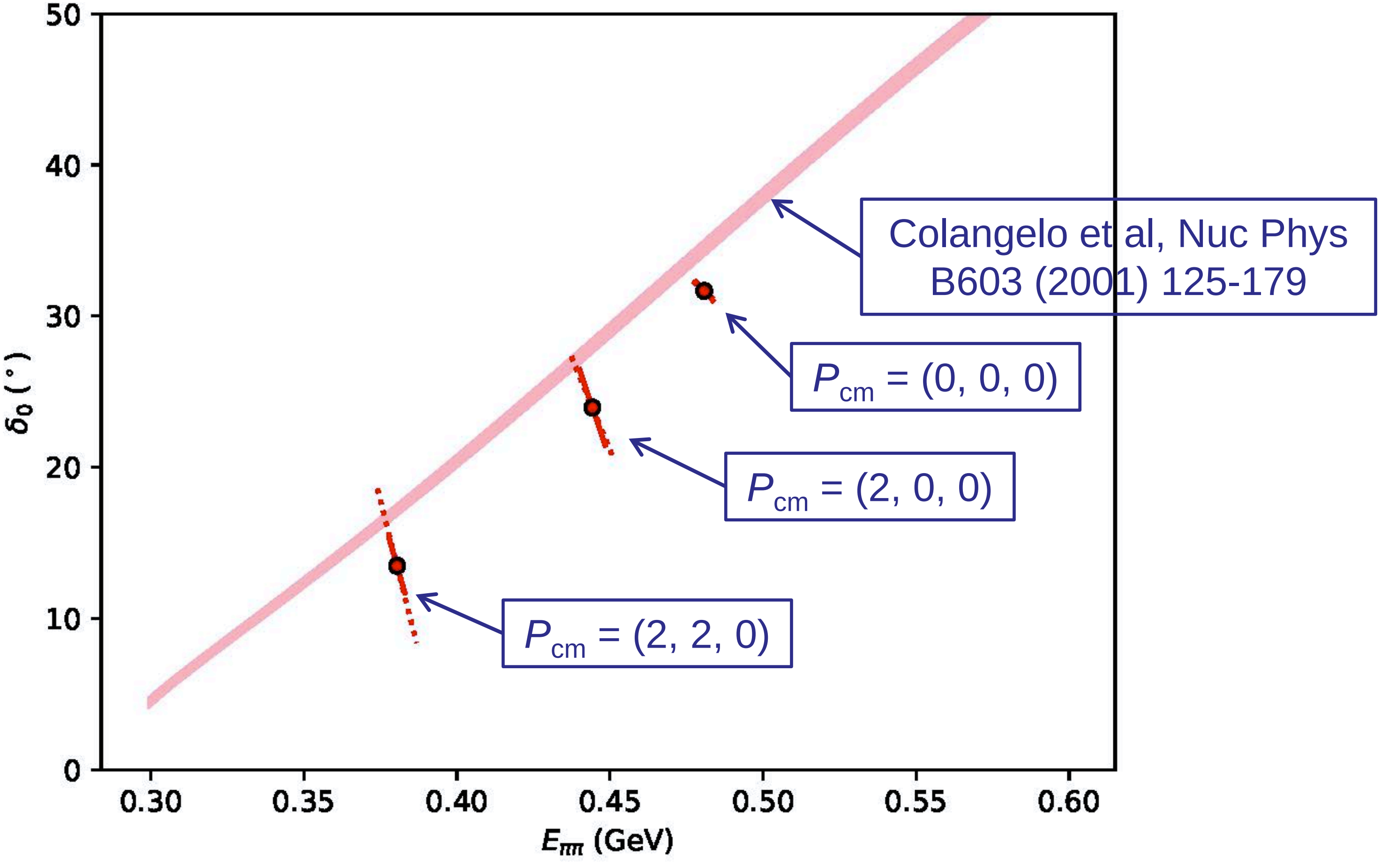
$\pi\pi(111)$ & σ

$\pi\pi(111)$ & σ & $\pi\pi(111)$



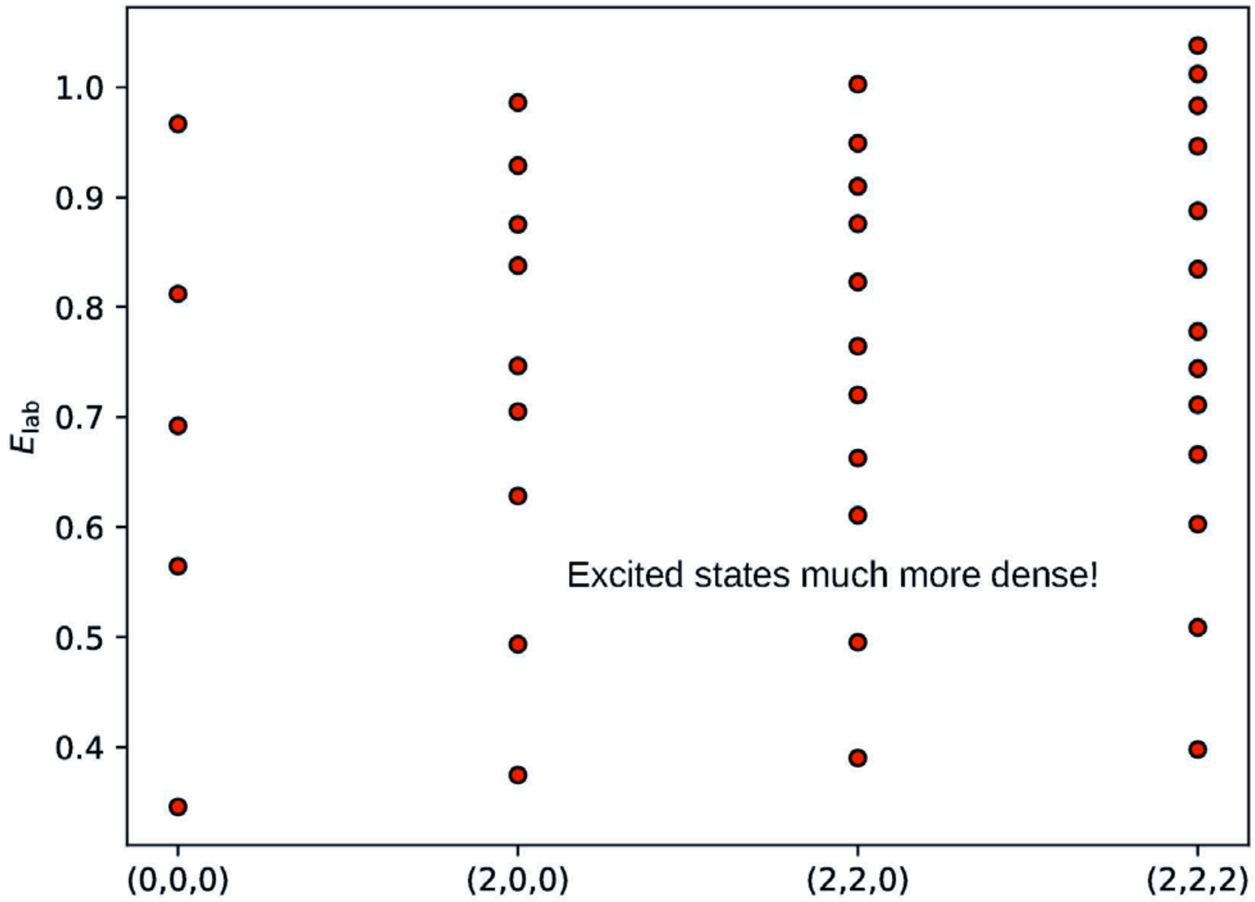
- Third $\pi\pi(311)$ operator not important.
- δ_0 = 31.7(6)° vs 34° prediction (5-15 fit, statistical errs only).

$I = 0$ $\pi\pi$ scattering with $P_{cm} \geq 0$



$I = 0$ $\pi\pi$ scattering with $P_{cm} \geq 0$

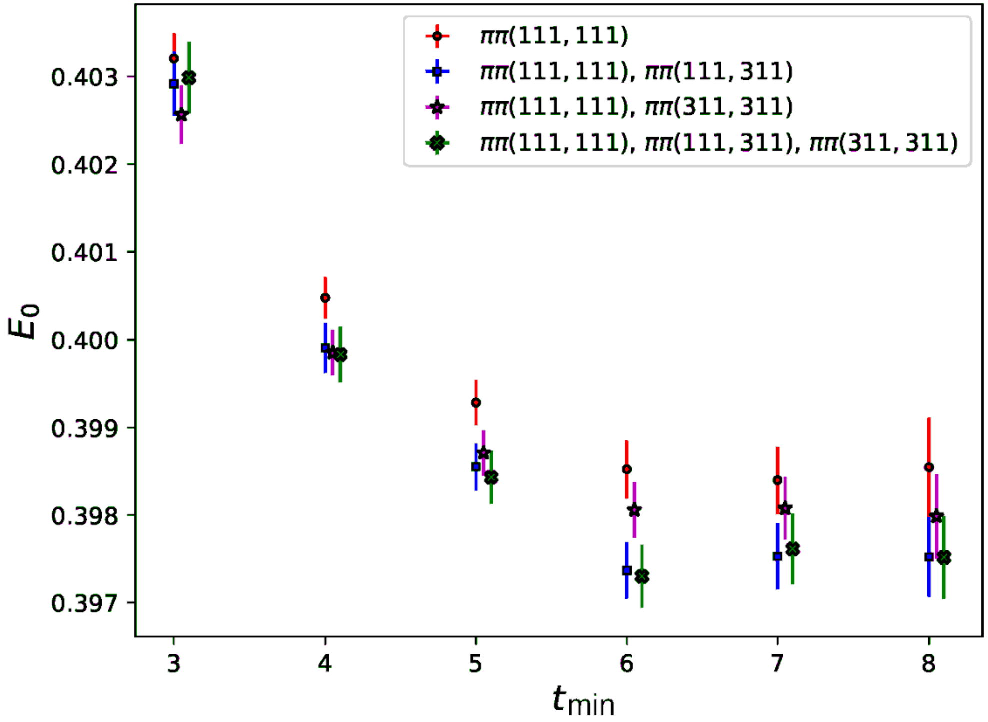
- Expect increased difficulty separating excited states for $P_{cm} \geq 0$.



$I = 0$ $\pi\pi$ scattering with $P_{cm} \geq 0$

- Failure of 3-operator fit easy to recognize:

$P_{cm} = (222)\pi/L$



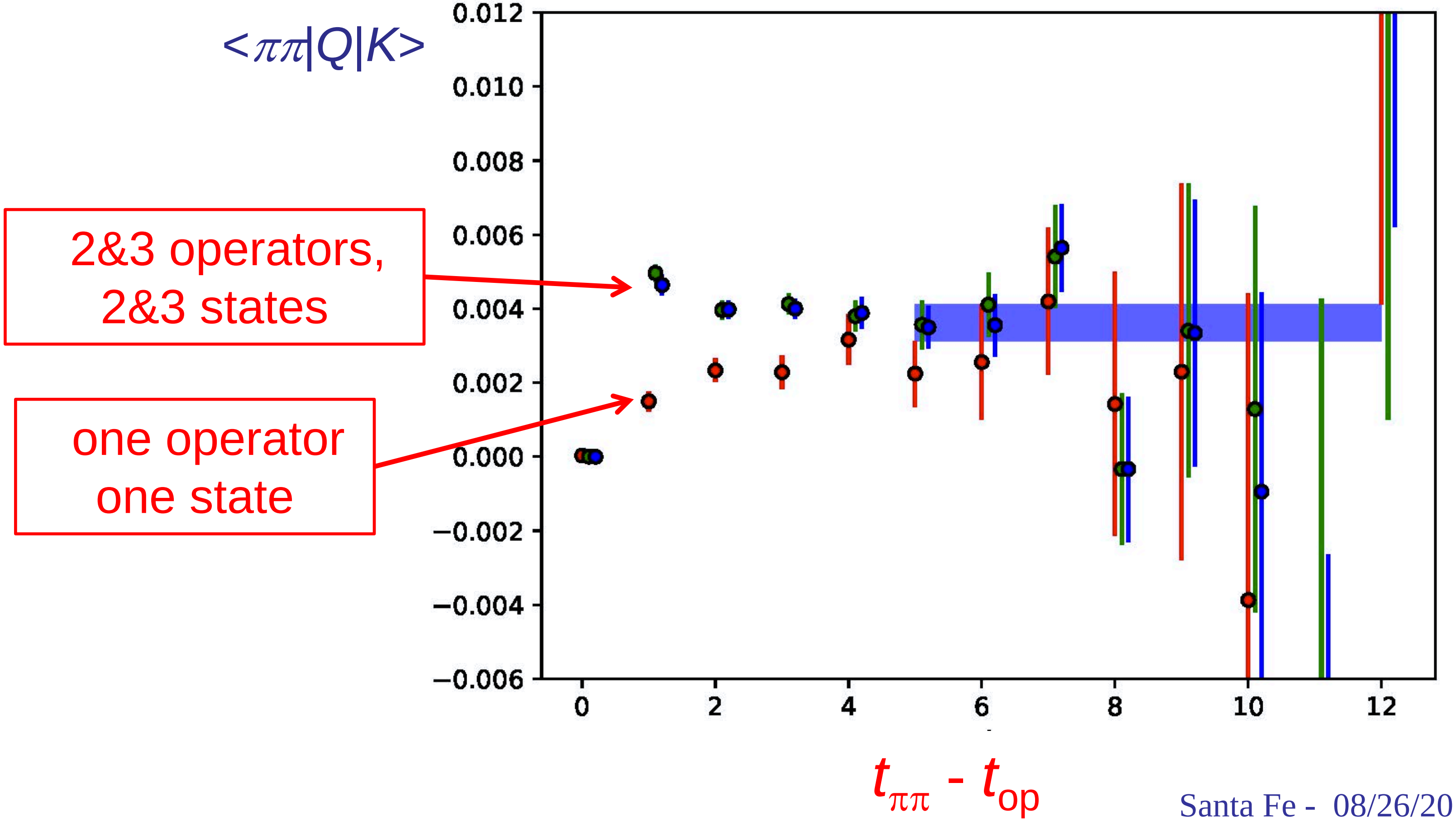
- Plateau does not extend to smaller t when extra operators are added.

$I = 0$ $\pi\pi$ scattering with $P_{\mathrm{cm}} \geq 0$

- Plateau does not extend to smaller *t* when extra operators are added.
- The matrix of amplitudes $A_{|a>,O_b}$ is largely diagonal.
- The fit to each operator is effectively a single-state fit with the same problems as those in 2015.
- Perhaps the result having no moving σ operator implemented?

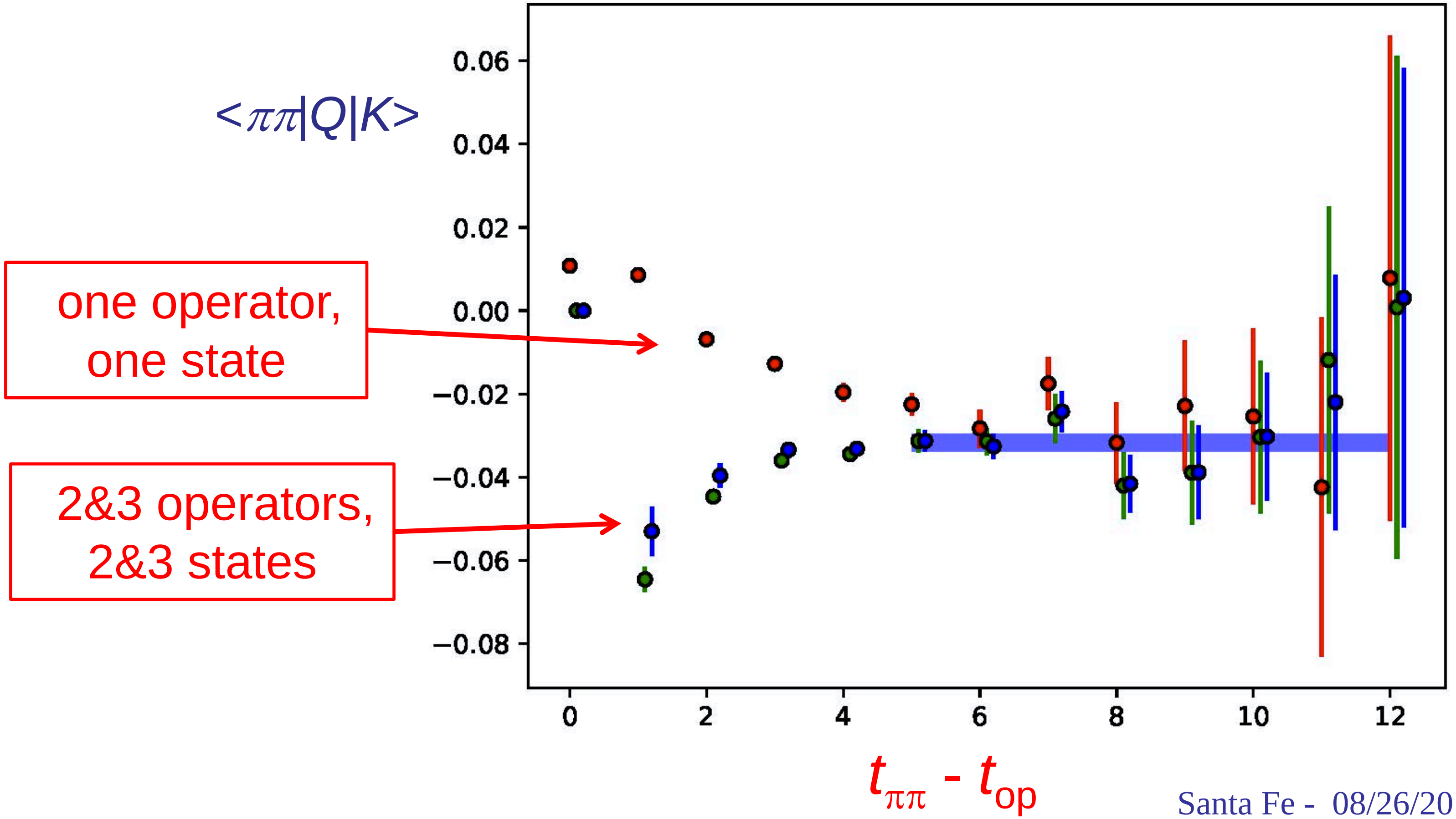
K → $\pi\pi$ from 3-operator fits (case I)

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



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

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



Two data analysis challenges

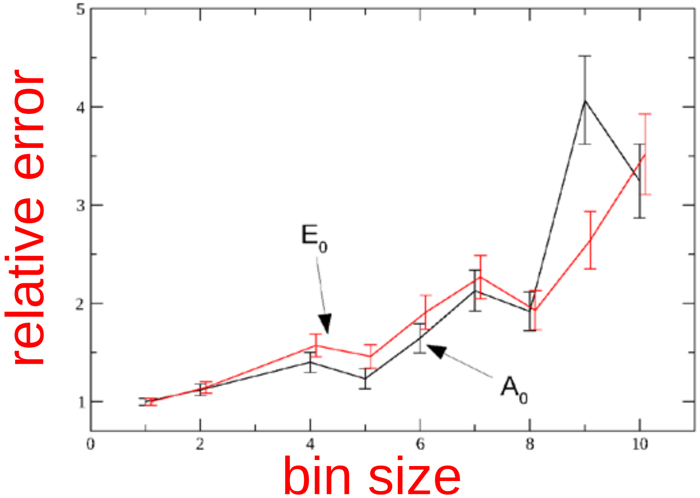
- Auto-correlations – we must be careful that our errors are accurate
- We need estimates of goodness of fit (p-values)
  - Demonstrate that our fits describe the data.
  - Decide if alternative fits used to estimate systematic errors are plausible.
  - However, our lattice QCD p-values are traditionally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

Auto-correlations

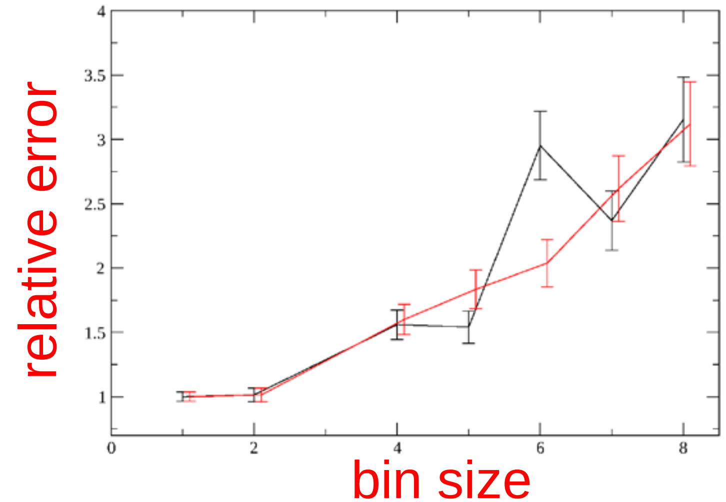
- Our measurements are made every 4 MD time units and are mildly correlated.
- While we have N=741 configurations, the covariance matrix for three operators and t = 5-15 time slices is 66 x 66!
- Noise grows as we bin the data and have fewer samples to measure the fluctuations.
- Solved by the *blocked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

I=0 $\pi\pi$ two-point function errors

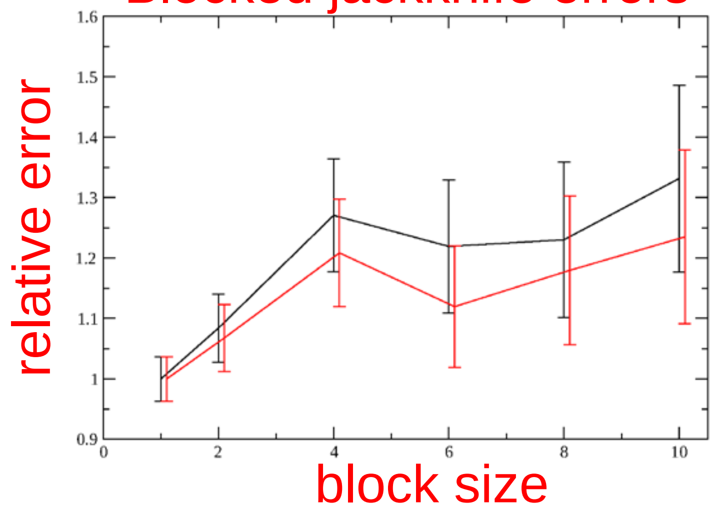
Binned data errors



Binned scrambled data errors



Blocked jackknife errors



Poor p-values

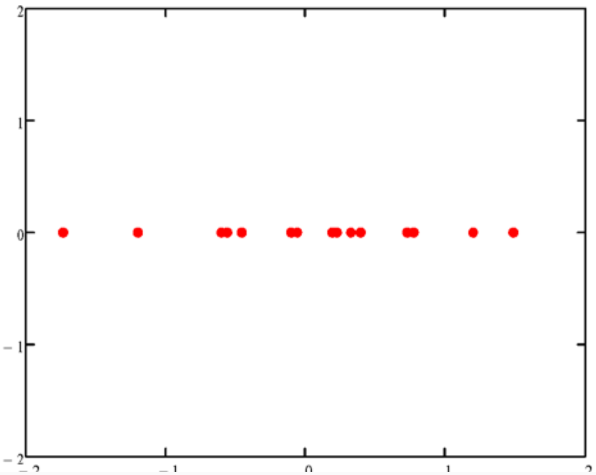
- After obtaining p-values of 0.1– 0.2 for most "best fits" consider a different line of work?
- Last spring, Tanmoy pointed out that this is often caused by ignoring fluctuations in the covariance matrix.
- This broadens the χ^2 distribution into the Hotelling T^2 distribution.
- Hotelling's is an analytically known distribution depending on the number of points being fit, the number of fit parameters (like χ^2) ***and*** on N.

Hotelling T^2 is insufficient

- Hotelling assumes that the data (not its averages) are Gaussian and uncorrelated.
- This is not true for our case.
- Abandon analytic methods and use a bootstrap analysis to determine the correct generalized χ^2 distribution from the data.
- Recall how the “sample with replacement” bootstrap method works.

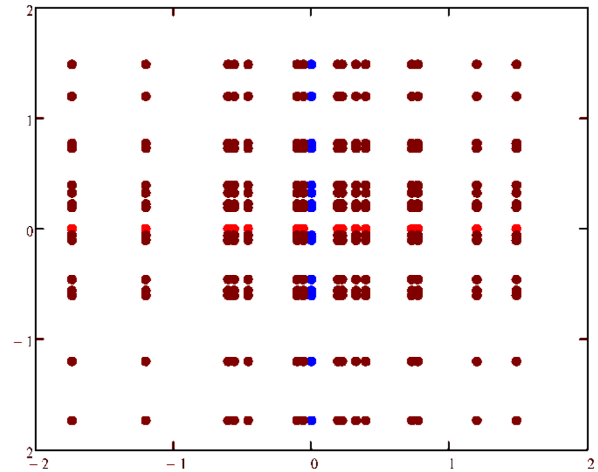
(Blocked) Bootstrap method

1 variable, N samples



$$\int dx\,\rho(x)f(x) = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

2 variables, N^2 samples



$$\int dx\,dx'\,\rho(x)\rho(x')f(x,x') = \frac{1}{N^2}\sum_{i,j=1}^{N} f(x_i,x_j)$$

N variables, N^N samples

Choose N_{boot} samples from these N^N points in N dimensions

$$\int dx_1\ldots dx_N\,\rho(x_1)\ldots\rho(x_N)f(x_1,\ldots,x_N) = \frac{1}{N^N}\overbrace{\sum_{i_1,\ldots i_N=1}^{N}}^{} f(x_1,\ldots x_N)$$

q^2 distribution

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

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

- Find $P(q^2)$ where

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

- Here $p_{int}(q^2)$ is the usual p-value
- Obtain $p(q^2)$ from our Monte Carlo data as follows:

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

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

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

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

q^2 distribution

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

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

- Thus

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

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

- $p(q^2) \approx N(q^2)/N_{boot}$ 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!

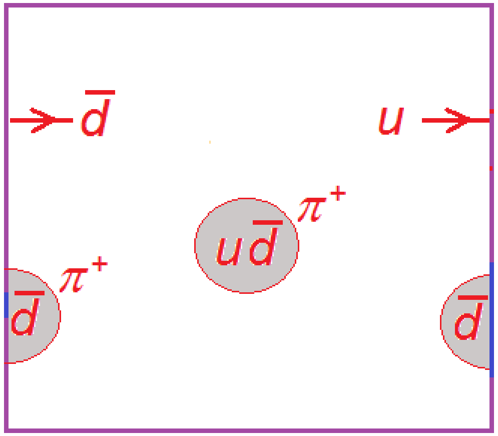
Conclusions

- Calculation of $K \rightarrow \pi\pi$ decay substantially improved over 2015 result.
- 216 → 741 configurations.
- Three $\pi\pi$ interpolating operators allow a careful discrimination between ground and excited states.
- Errors reduced by using correlated fits.
- Auto-correlations are taken into account
- Bootstrap q^2 distribution gives correct p-values.
- Final results available very soon.

Backup

$I = 0\ \ K \to \pi\,\pi$ with $E_{\pi\pi} = M_K$

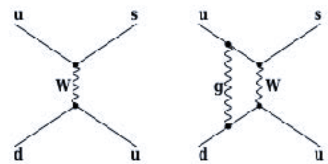
(Chris Kelly & Daiqian Zhang)



- Use **G-parity** BC to obtain p_π = 205 MeV (Changhoan Kim, hep-lat/0210003)
  - $G = C\, e^{i\pi I_y}$
  - Non-trivial: $\begin{pmatrix} u \\ d \end{pmatrix} \to \begin{pmatrix} \bar{d} \\ -\bar{u} \end{pmatrix}$
  - Gauge fields obey C BC
  - Extra I = 1/2, s' quark adds $e^{-m_K L}$ error
  - Must take non-local square root of s-s' determinant – non-locality also ~ $e^{-m_K L}$
  - Tests: f_K and B_K correct within errors.

Local four quark operators

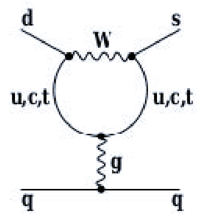
- **Current-current operators**



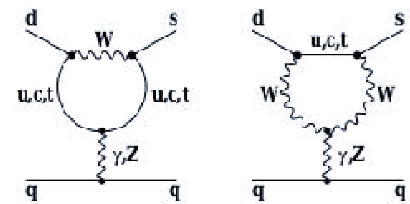
$$Q_1 \equiv (\bar{s}_\alpha d_\alpha)_{V-A}(\bar{u}_\beta u_\beta)_{V-A}$$

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

- **QCD Penguins**



- **Electro-Weak Penguins**



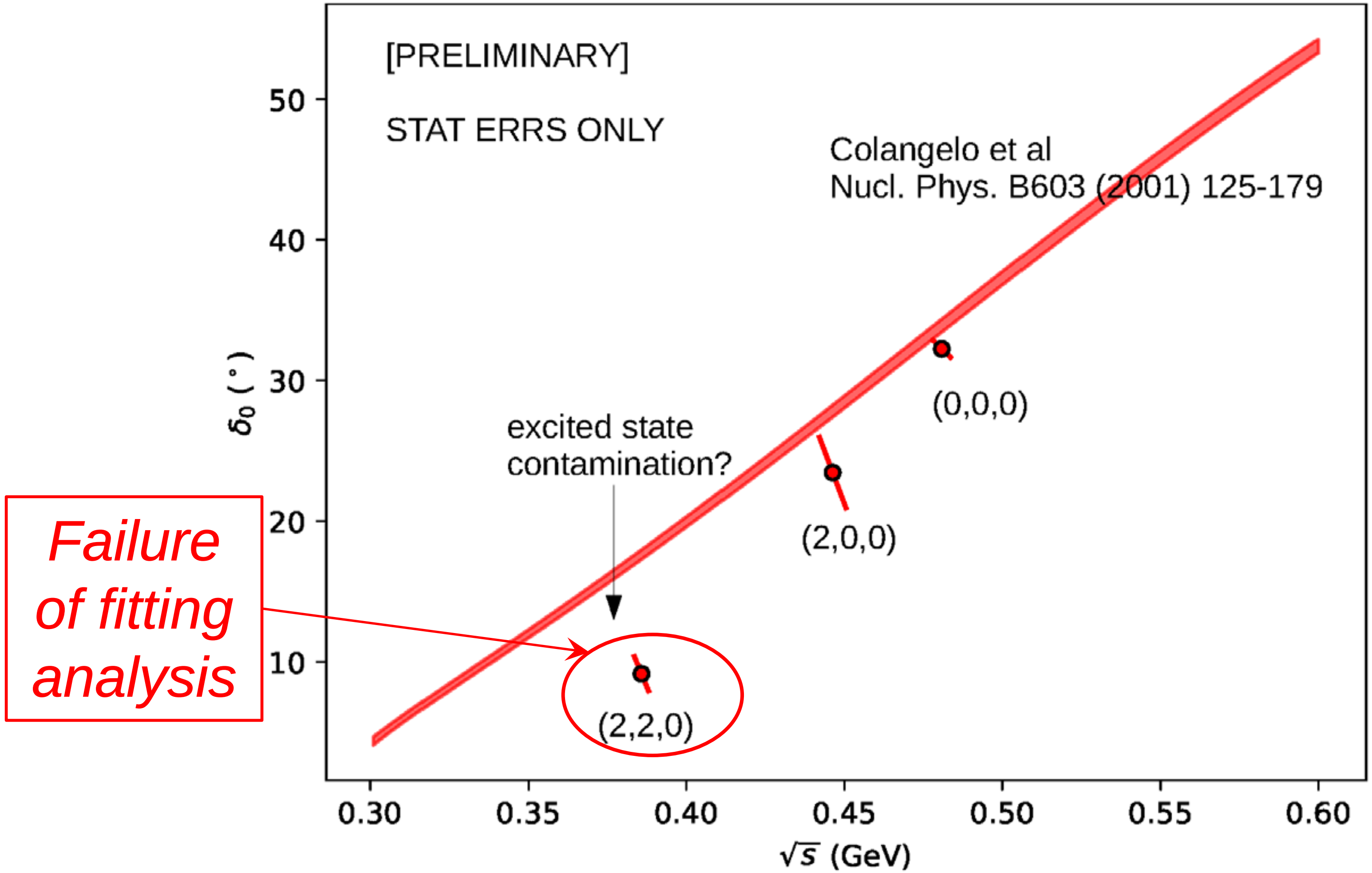
$$Q_7 \equiv \frac{3}{2}(\bar{s}_\alpha d_\alpha)_{V-A} \sum_{q=u,d,s} e_q(\bar{q}_\beta q_\beta)_{V+A}$$

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

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

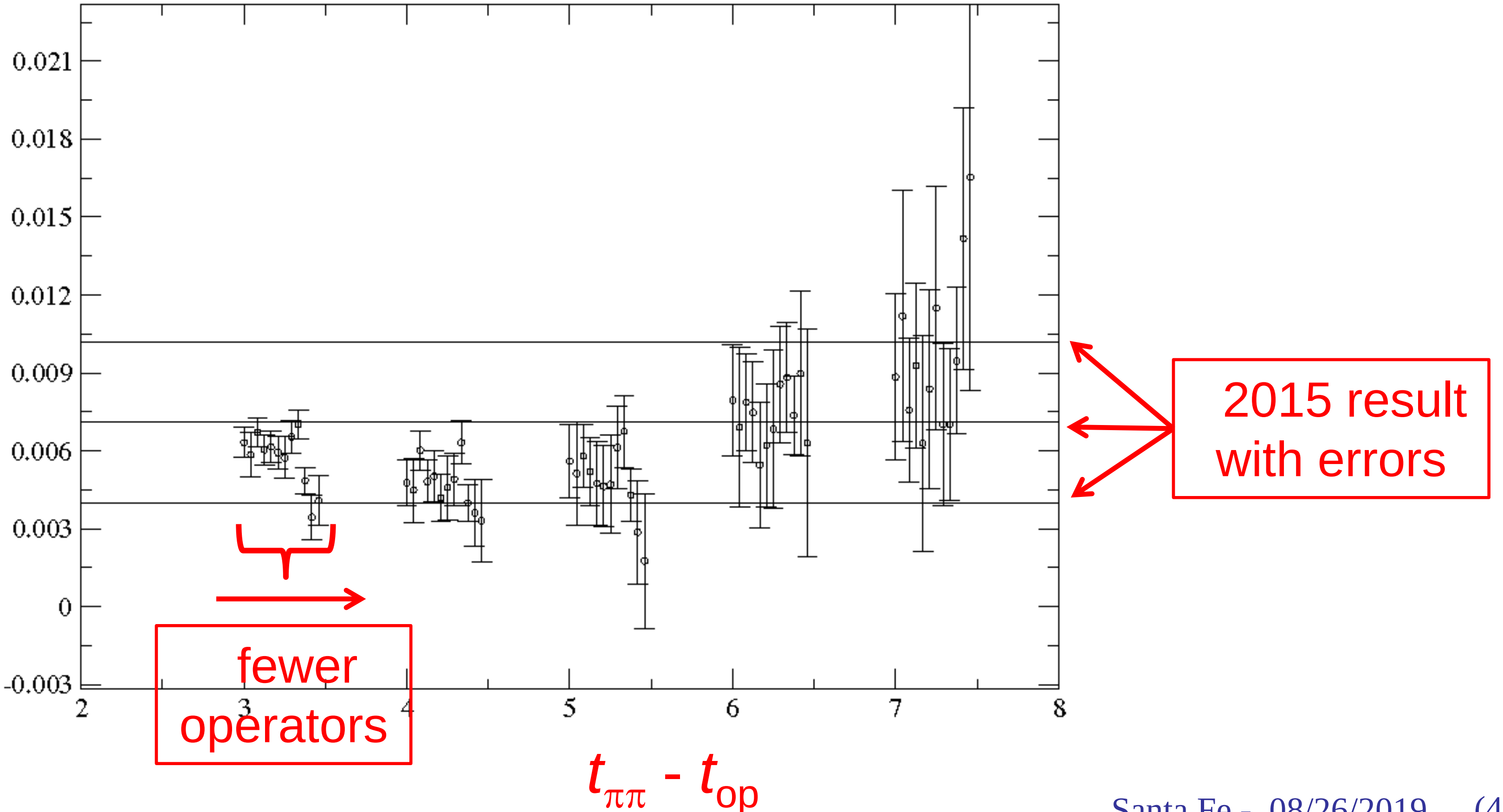
$$Q_{10} \equiv \frac{3}{2}(\bar{s}_\alpha d_\beta)_{V-A} \sum_{q=u,d,s} e_q(\bar{q}_\beta q_\alpha)_{V-A}$$

$I = 0$ $\pi\pi$ scattering with $P_{cm} \geq 0$



K → ππ from 3-operator fits (case I)

- Fit using up to 3 operators and 3 states with energies and amplitudes from ππ 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: