Update on the lattice calculation of direct CP-violation in K decays

(aka “Update on K=>pi pi & All That”)

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Lattice X IF 2019

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Motivation and previous result

Motivation

- Likely explanation for matter/antimatter asymmetry in Universe, baryogenesis, requires violation of CP.
- Amount of CPV in Standard Model appears too low to describe measured M/AM asymmetry: tantalizing hint of new physics.
- Direct CPV first observed in late 90s at CERN (NA31/NA48) and Fermilab (KTeV) in $K^0 \to \pi\pi$:

$$\eta_{00} = \frac{A(K_L \to \pi^0\pi^0)}{A(K_S \to \pi^0\pi^0)}, \qquad \eta_{+-} = \frac{A(K_L \to \pi^+\pi^-)}{A(K_S \to \pi^+\pi^-)}.$$

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

measure of direct CPV — measure of indirect CPV

- Small size of ε' makes it particularly sensitive to new direct-CPV introduced by many BSM models.
- In terms of isospin states: ΔI=3/2 decay to I=2 final state, amplitude A_2
  ΔI=1/2 decay to I=0 final state, amplitude A_0

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

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

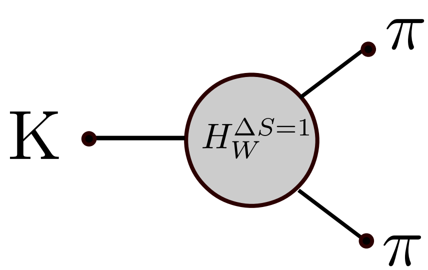
$$\boxed{\omega = \mathrm{Re}A_2/\mathrm{Re}A_0}$$

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

(δ_I are strong scattering phase shifts.)

Overview of calculation

- Hadronic energy scale << M_W – use weak effective theory.
- $K \to \pi\pi$ decays require single insertion of $\Delta S=1$ Hamiltonian:



10 effective four-quark operators

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

perturbative Wilson coeffs.

$$\tau = -\frac{V_{ts}^* V_{td}}{V_{us}^* V_{ud}} = 0.0014606 + 0.00060408i$$

Imaginary part solely responsible for CPV
(everything else is pure-real)

renormalization matrix (mixing)
Use RI-SMOM and convert to MSbar perturbatively

LL finite-volume correction

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

$M_j^{I,lat} = \langle (\pi\pi)_I | Q_j | K \rangle$ (lattice)

Summary of published results

[Phys.Rev. D91 (2015) no.7, 074502]

- A_2 computed on RBC/UKQCD 64^3x128 and 48^3x96 2+1f Mobius DWF ensembles with the Iwasaki gauge action and physical pion mass.
- a^{-1}= 2.36 GeV and 1.73 GeV resp - continuum limit taken.
- Statistical errors sub-percent, dominant systematic errors due to truncation of PT series in computation of RI-SMOM to MSbar matching and Wilson coefficients.
- 10% and 12% total errors on Re(A_2) and Im(A_2) resp.

[Phys.Rev.Lett. 115 (2015) 21, 212001]

- A_0 computed on 216cfgs of 32^3x64 Mobius DWF with Iwasaki+DSDR gauge action and physical pion mass.
- G-parity BCs in 3 directions to give physical kinematics.
- Single, coarse lattice with a^{-1}= 1.38 GeV but large physical volume to control FV errors.
- 21% and 65% stat errors on Re(A_0) and Im(A_0) due to disconn. diagrams and, for Im(A_0) a strong cancellation between Q_4 and Q_6.
- Dominant, 15% systematic error is due again to PT truncation errors exacerbated by low renormalization scale 1.53 GeV.

Result for ε'

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

$$\mathrm{Re}\left(\frac{\varepsilon'}{\varepsilon}\right) = \mathrm{Re}\left\{\frac{i\omega e^{i(\delta_2-\delta_0)}}{\sqrt{2}\varepsilon}\left[\frac{\mathrm{Im}A_2}{\mathrm{ReA}_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}\right]\right\}$$

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

- Error is dominated by that on A_0.
- Total error on Re(ε'/ε) is ~3x the experimental error.
- Result is in tension with Standard Model at 2.1σ level.

The “ππ puzzle” and multi-operator fits

On the importance of the ππ state

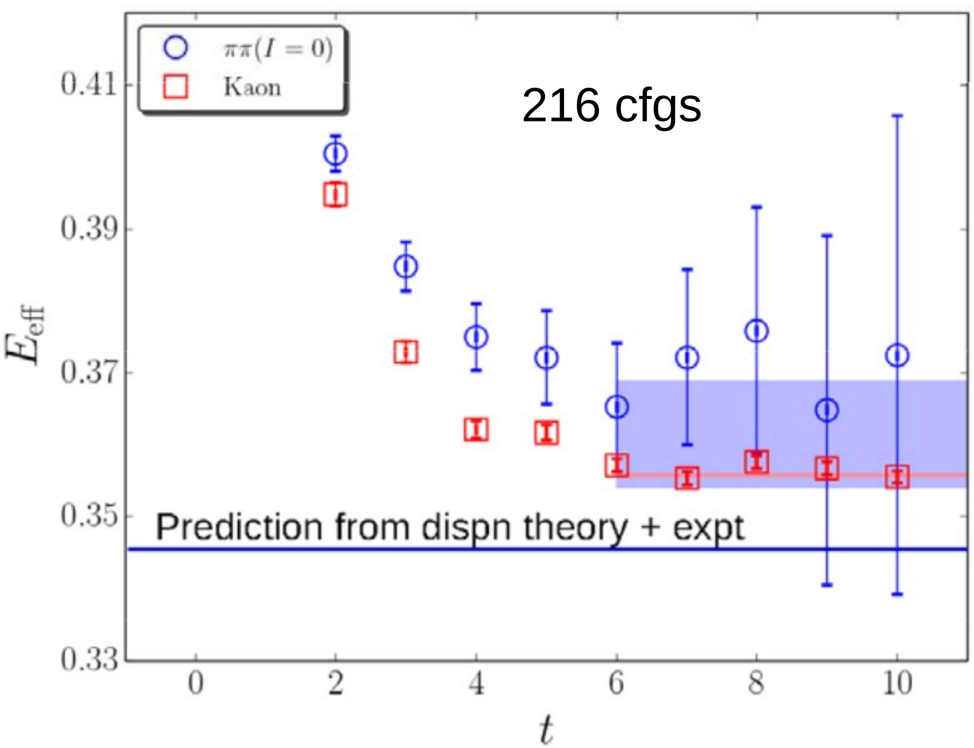
- Understanding I=0 ππ system is crucial:
  - Energy is needed for time dependence of correlation function from which we extract finite-volume $K \to \pi\pi$ matrix element.
  - Phase shift enters Lellouch-Luscher finite-volume correction to matrix element.
  - Phase shifts also enter in formula relating A_I to ε' itself
- 2015 calculation of δ_0 in 2σ tension with dispersion theory calculation:

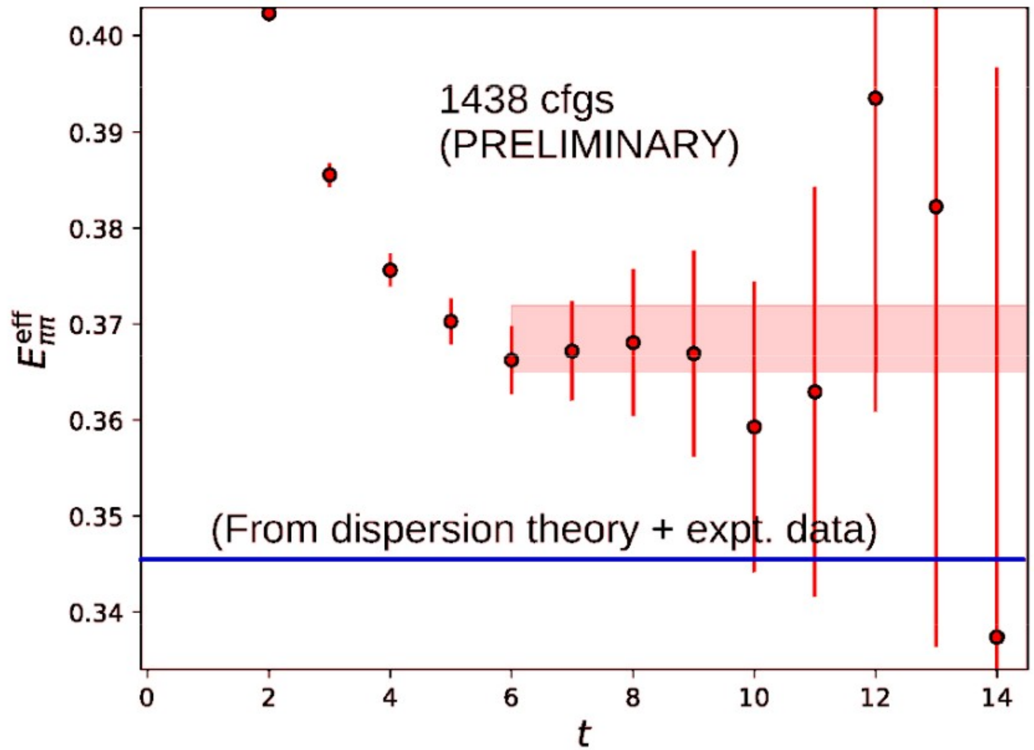
$$\begin{aligned}\delta_0 &= 23.8(4.9)(2.2)^\circ \ \ (\mathrm{latt}) \\ &= 34^\circ \ \ (\mathrm{G.Colangelo} \ \ et \ \ al)\end{aligned}$$

- This observation prompted increased focus on ππ system.

Increased statistics

- To resolve the “pi-pi puzzle” we increased statistics from 216 to 1438 (a 6.6x increase!).
  However this did not resolve the situation:





$$\delta_0 = 23.8(4.9)(2.2)^\circ \rightarrow 19.1(2.5)(1.2)^\circ$$

Resolving the pi-pi puzzle

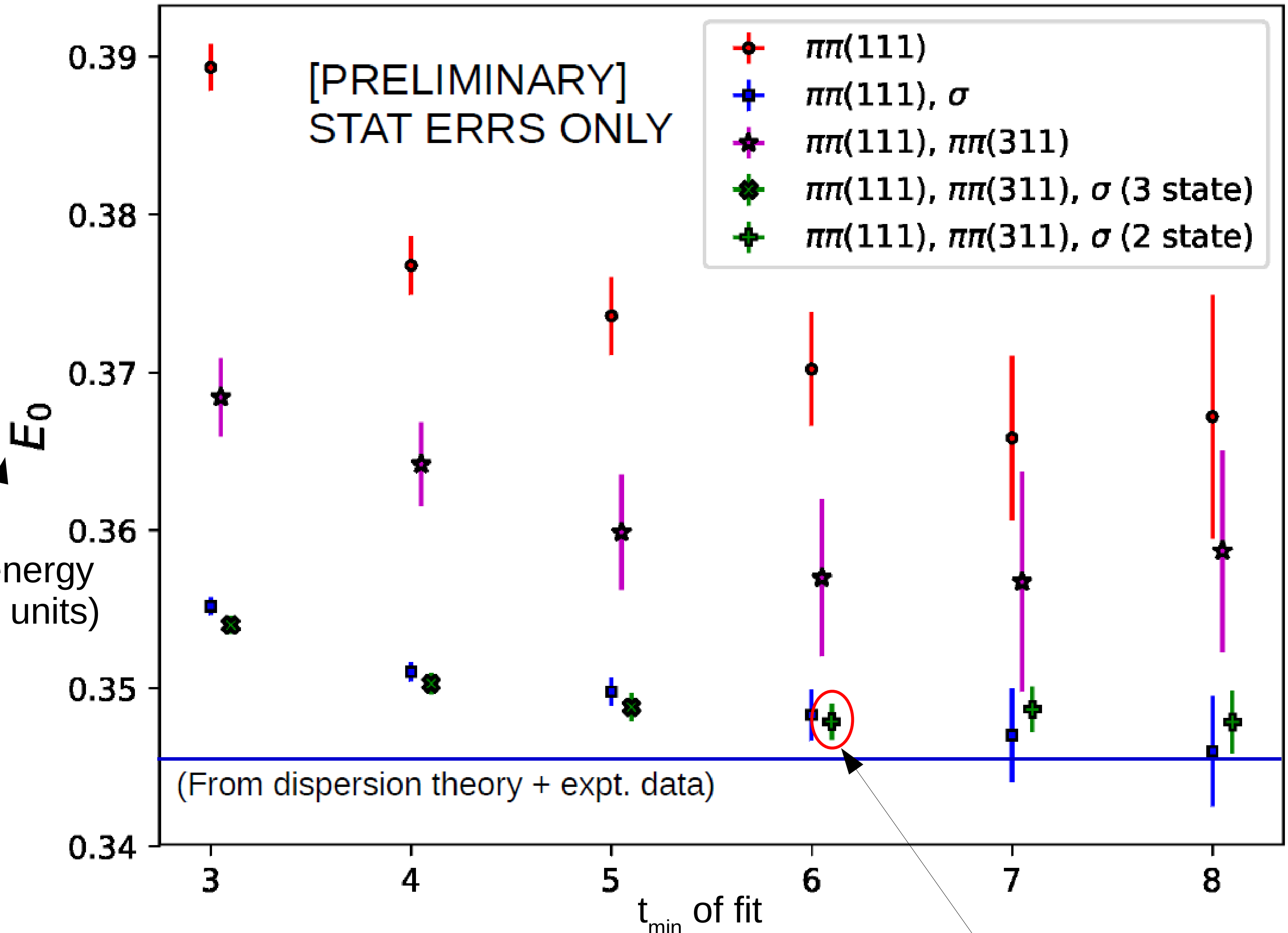
- Most likely explanation is excited state contamination masked by rapid growth of statistical errors.
- To resolve this we turned to multi-operator fits which provide much greater resolution on excited states time dependence alone.
- Obtain parameters by simultaneous fitting to matrix of correlation functions

$$C_{ij}(t) = \langle 0|O_i^\dagger(t)O_j(0)|0\rangle = C + \sum_\alpha A_{i,\alpha}A_{j,\alpha}e^{-E_\alpha t}$$

round-the-world single pion propagation small compared to errors - drop

- Increased from 1 → 3 operators: $\pi\pi(111)$ $\pi\pi(311)$ σ [cf T.Wang Monday]
- 741 configurations measured with 3 operators.

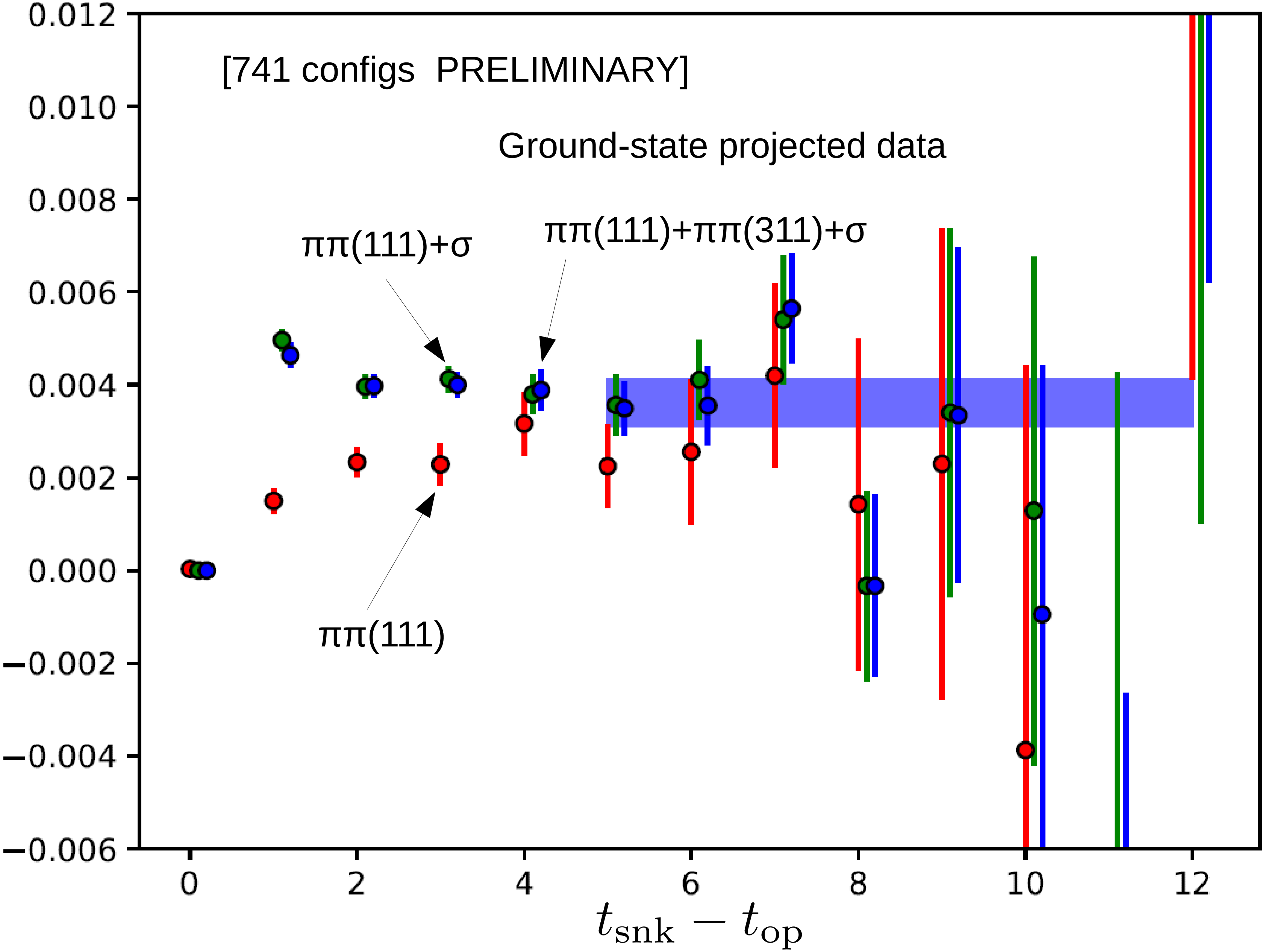
Effect of multiple operators on ππ



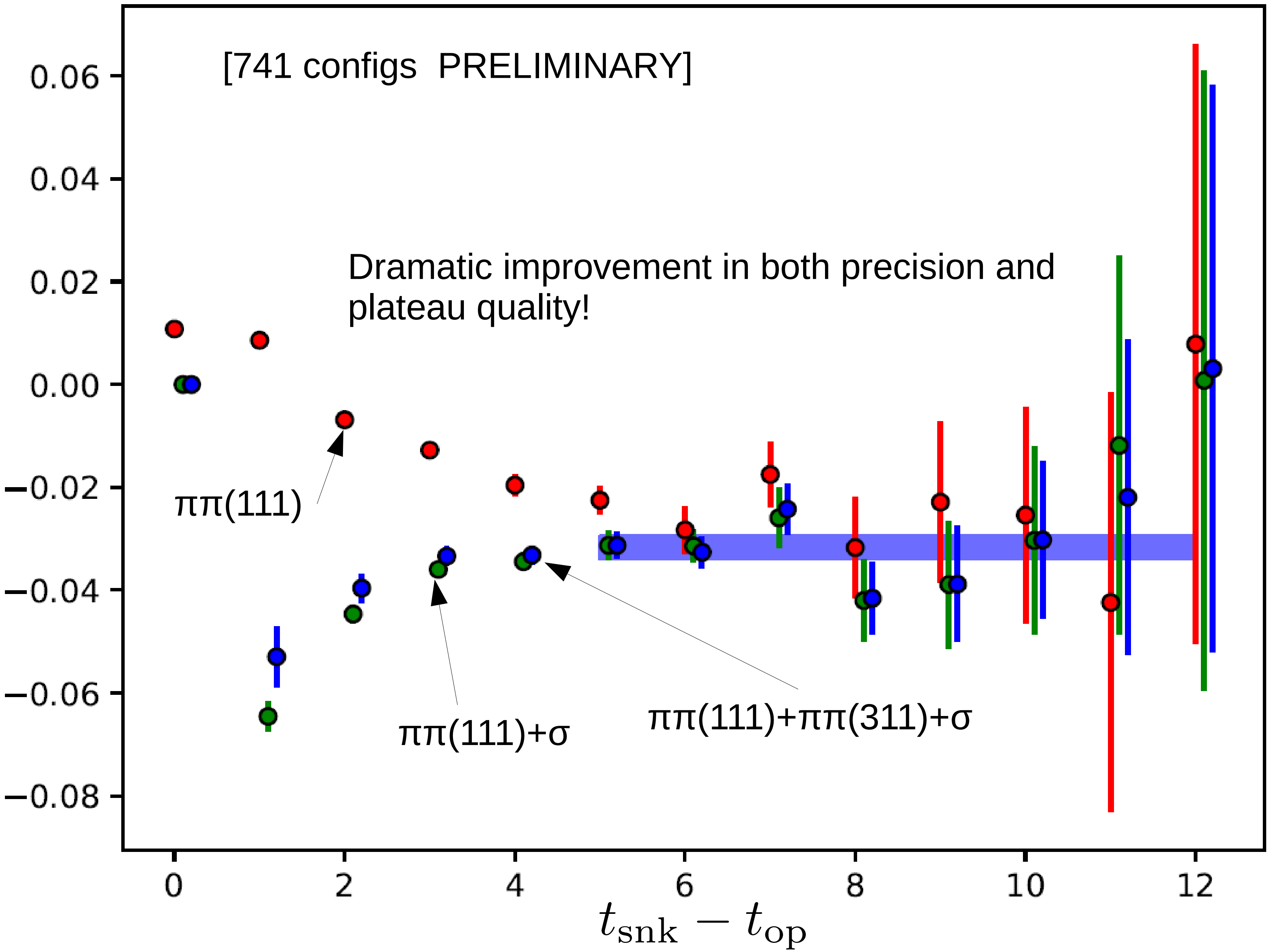
fitted energy
(lattice units)

Result compatible with dispersive value

Effect of multiple operators on K→ππ (case I)



Effect of multiple operators on K→ππ (case II)



Other systematic error improvements

Systematic error improvements

Description	Error	Description	Error
Finite lattice spacing	12%	Finite volume	7%
Wilson coefficients	12%	Excited states	$\leq 5\%$
Parametric errors	5%	Operator renormalization	15%
Unphysical kinematics	$\leq 3\%$	Lellouch-Lüscher factor	11%
Total (added in quadrature)			27%

[RBC&UKQCD PRL 115 (2015) 21, 212001]

NPR+Wilson Coefficients

- NPR error large due to use of 1-loop PT to match to MSbar at low, 1.53 GeV renormalization scale.
- Since 2015 have improved NPR error 15% → 8% (preliminary) by increasing scale to 2.29 GeV using step-scaling procedure. [PoS LATTICE2016 (2016) 308]
- Inclusion of dim.6 gauge-invariant operator G_1 which mixes with Q_i under renormalization, effects demonstrated to be %-scale as expected.

  [G. McGlynn arxiv:1605.08807]
- Do not expect significant improvement in Wilson coeffs error from scale increase as it is overshadowed by use of PT to cross the charm threshold (1.29 GeV).
- Working on circumventing this by computing 3→4 flavor matching non-perturbatively.
- Requires $\mu \ll m_c$. At these low energies, MOM-scheme NPR severely hampered by increased mixing with tower of gauge-noninvariant operators.
- Circumvent using position-space NPR which does not require gauge fixing. [cf Masaaki Tomii Tuesday]

- Also: Calculation of non-EW NNLO Wilson coefficients is close to being published. [Cerdà-Sevilla, Gorbahn, Jäger, Kokulu]
- Results suggest only small NNLO corrections to PT matching over charm threshold. Depending on publication timing our quoted WC systematic may be smaller! [cf. M. Cerdà-Sevilla Kaon 2019 talk]

Discretization error

- Currently have results only on single lattice with coarse lattice spacing a^{-1}=1.38(1) GeV.
- Require second lattice spacing. Going to finer lattice requires more lattice sites; prohibitively expensive for current gen. computers.
- Plans for repeating calculation on multiple lattices on next-Gen machines (Aurora, Perlmutter). Extensive code preparation in progress to support GPU port.

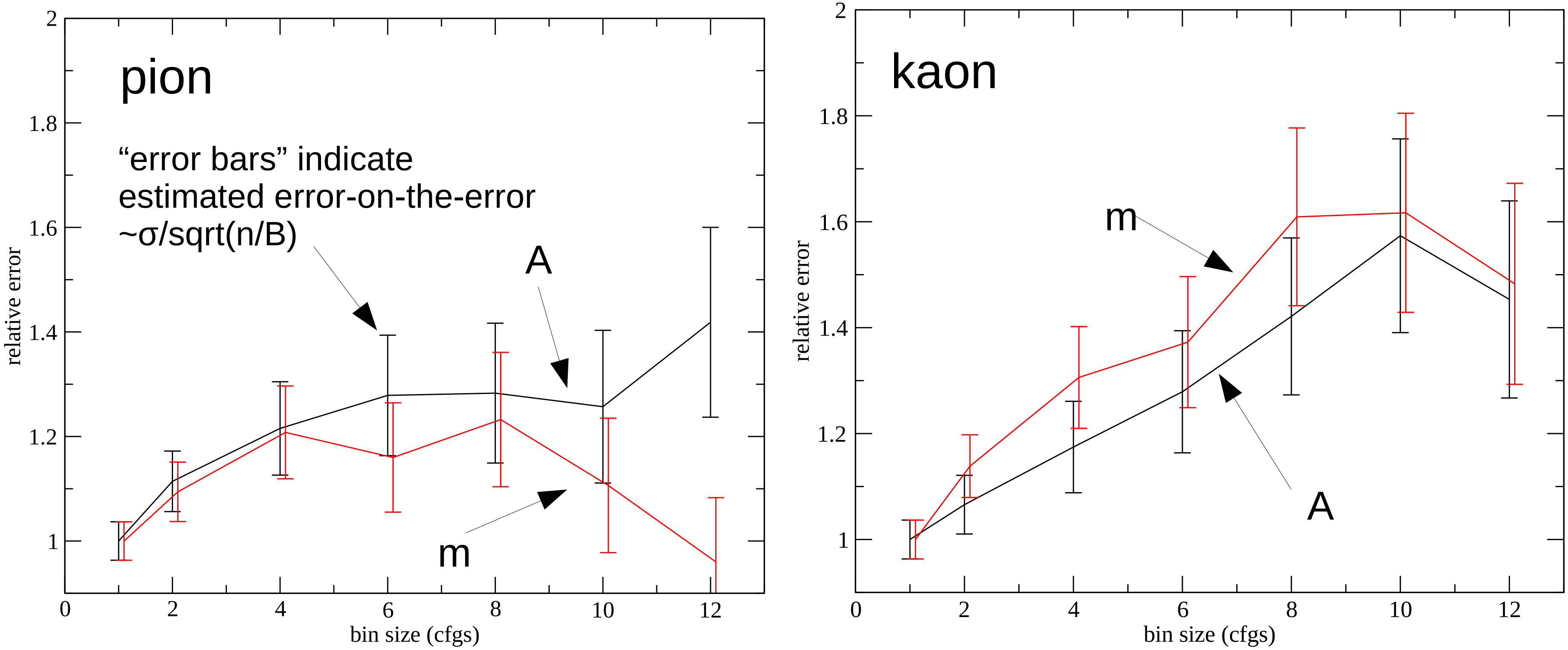
Related projects on the horizon:

- Performing calculation taking advantage of modern multi-operator techniques to fit excited-state $\pi\pi$ contributions directly, without G-parity BCs. [cf. D. Hoying Lattice 2019 talk]
- Laying the groundwork for non-perturbatively computing the effects of isospin breaking and electromagnetism. [EPJ Web Conf. 175 (2018) 13016]
- Study of complete, non-perturbative calculation of Wilson coefficients [EPJ Web Conf. 175 (2018) 13014, arXiv:1711.05768]

Advances in statistical techniques

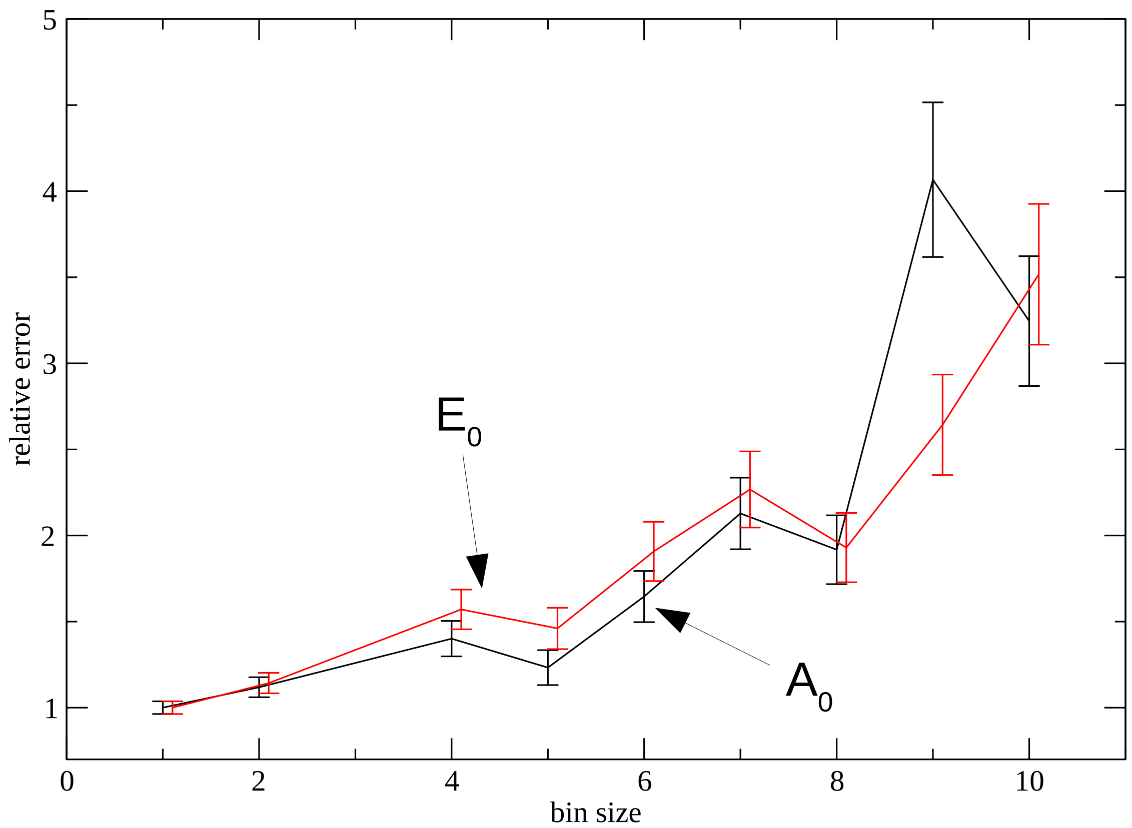
Dealing with autocorrelations

- With increased statistics we now have evidence for (limited) autocorrelation effects: $\tau_{int} \sim 4$ MDTU (1 cfg).
- Naively expect ~1.4x larger errors.
- Standard approach is to bin (average) data over blocks sufficiently large to make the blocks independent.



- Pion and kaon energies behave as expected with binning

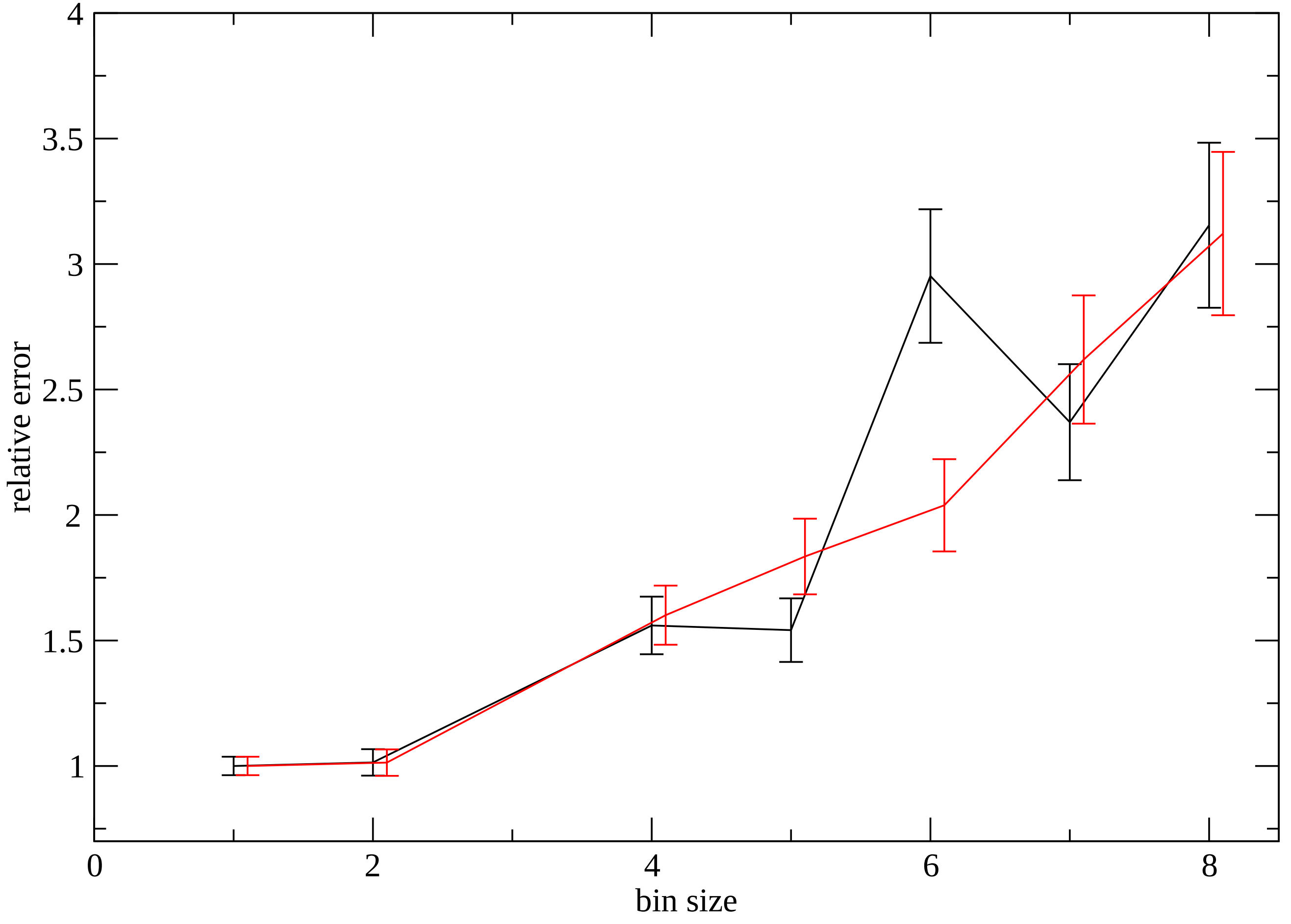
I=0 ππ 2pt function



- ππ errors continue growing with bin size and do not stabilize. Why?
- Covariance matrix is 66x66 here!
- As bin size increased, fewer data points enter determination of covariance matrix $\Rightarrow$ matrix becomes less and less well resolved.
- Fluctuations of low eigenvalues increase, causing error growth unrelated to autocorrelation

Scrambled data

- Isolate effect of loss of resolution of covariance matrix by randomly scrambling data to destroy autocorrelations

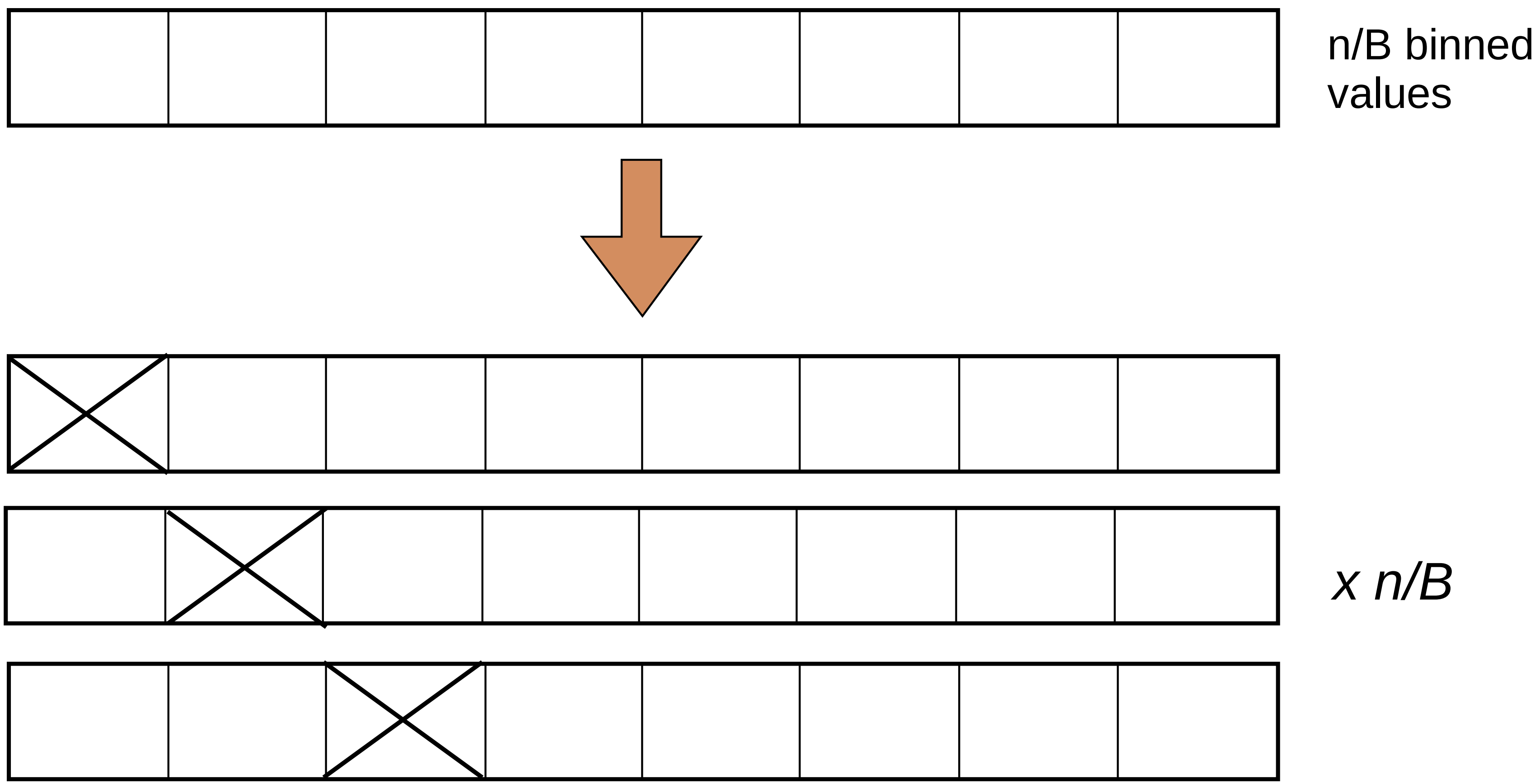


- Error growth essentially the same!

Block jackknife

- To prevent loss of resolution of covariance matrix while still taking into account autocorrelations, we perform **block jackknife**

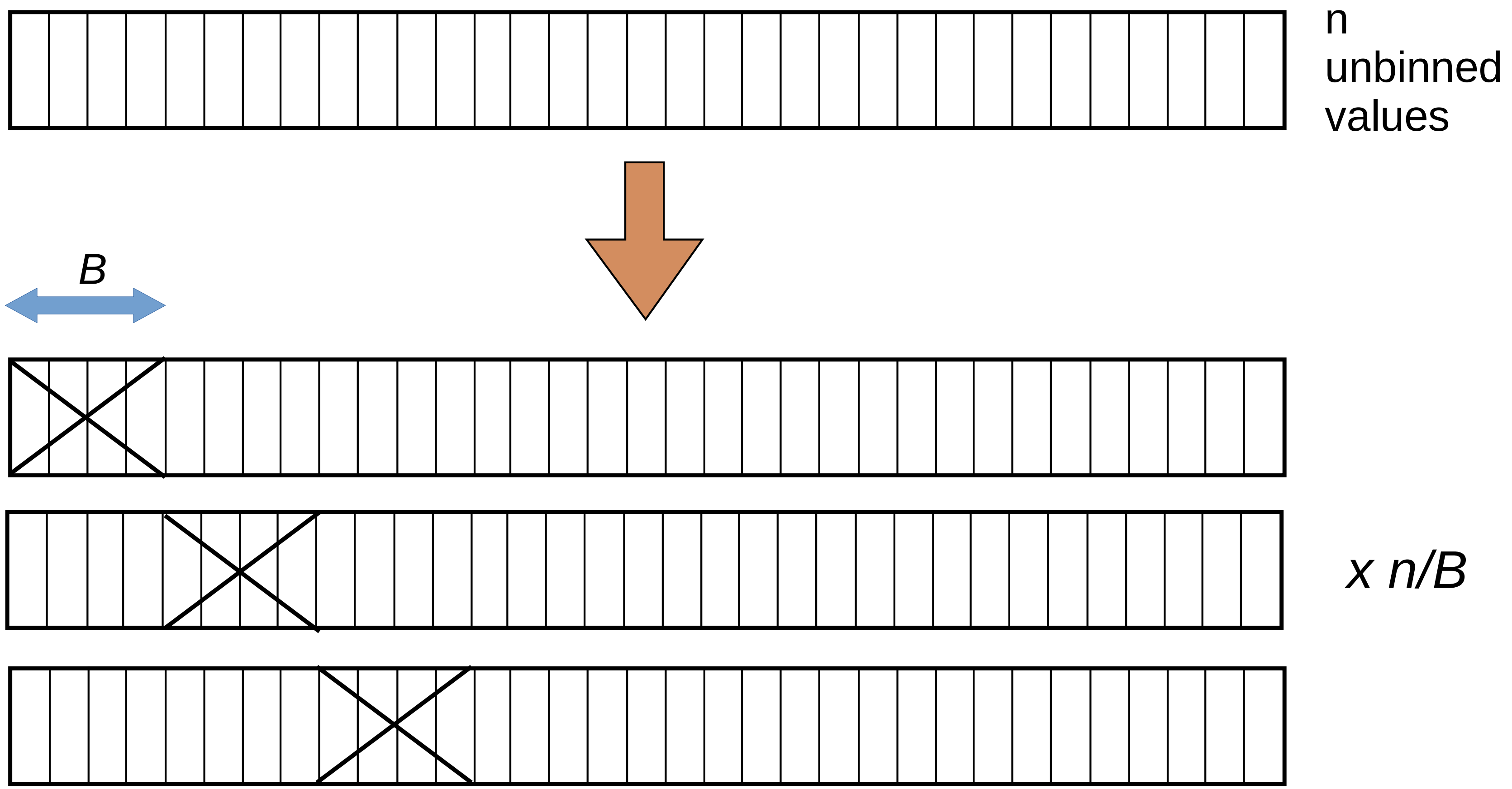
Regular, binned jackknife: generate *n/B* “reduced ensembles” of *n/B-1* numbers by successively dropping values



- With binning, covariance matrix obtained from just *n/B-1* numbers

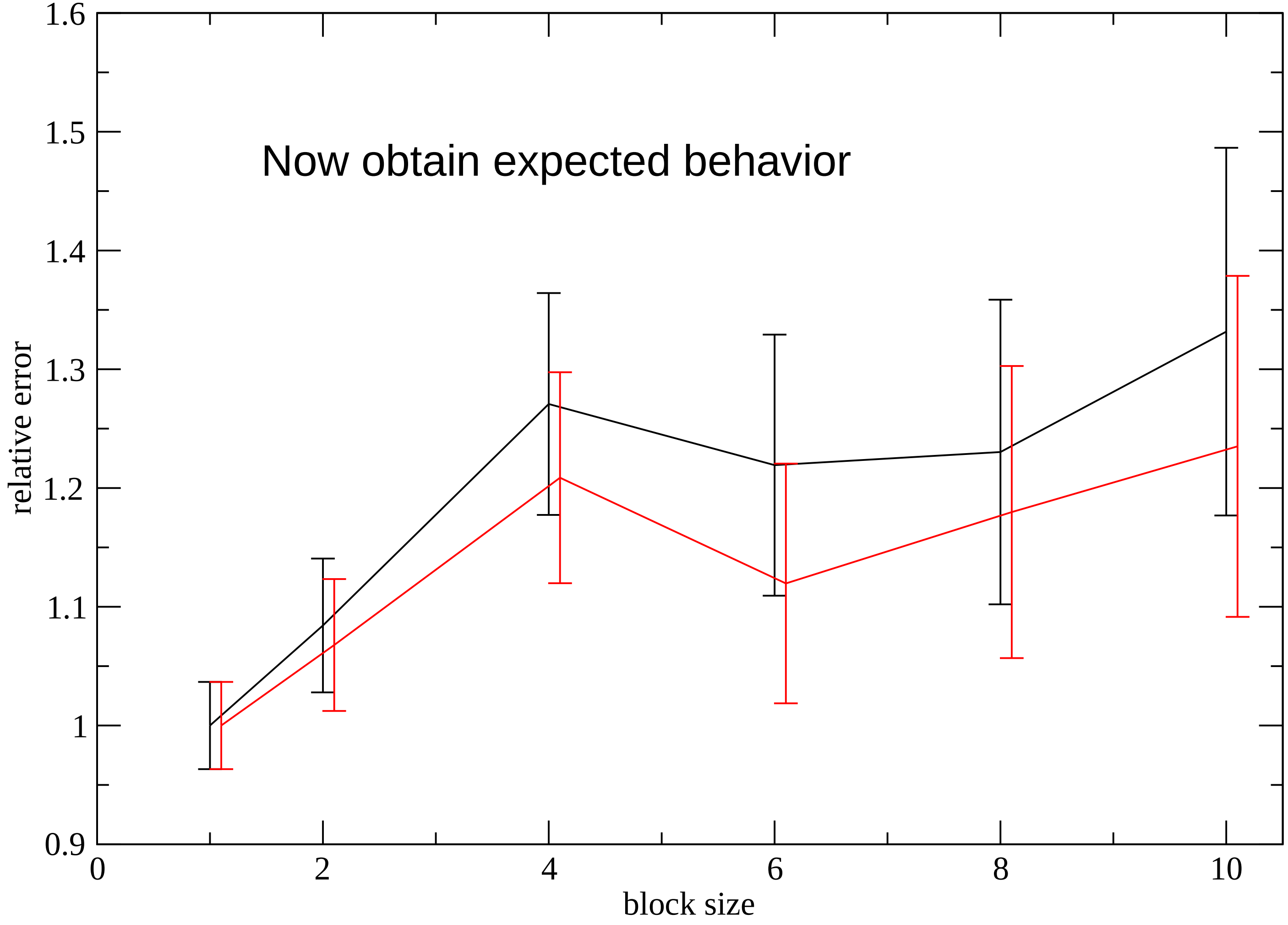
Block jackknife II

block jackknife: From *unbinned* data generate *n/B* reduced ensembles but of size *n-B* values by throwing away successive **blocks** of size *B*



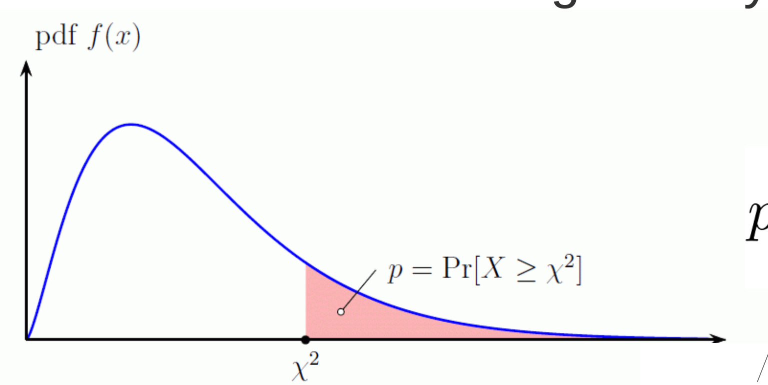
- Covariance matrix obtained from *n-B* values !
- Jackknife procedure ensures correct statistical error

I=0 ππ 2pt function with block jackknife



Goodness of fit

- Large number (741) of configurations encourages more sophisticated statistical techniques.
- In particular, well-controlled correlated fits allow for reliable goodness-of-fit metrics which aid fitting and systematic error estimation.
- Goodness-of-fit described by a p-value - the probability of getting a *worse* fit allowing for only statistical fluctuations.



degrees of freedom

$$p(q^2, k) = \int_{q^2}^{\infty} dx \; \mathrm{PDF}_{\chi^2}(x, k)$$

χ^2 distribution

measurement at t

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

fit function evaluated at t

With covariance matrix obtained from sample covariance:

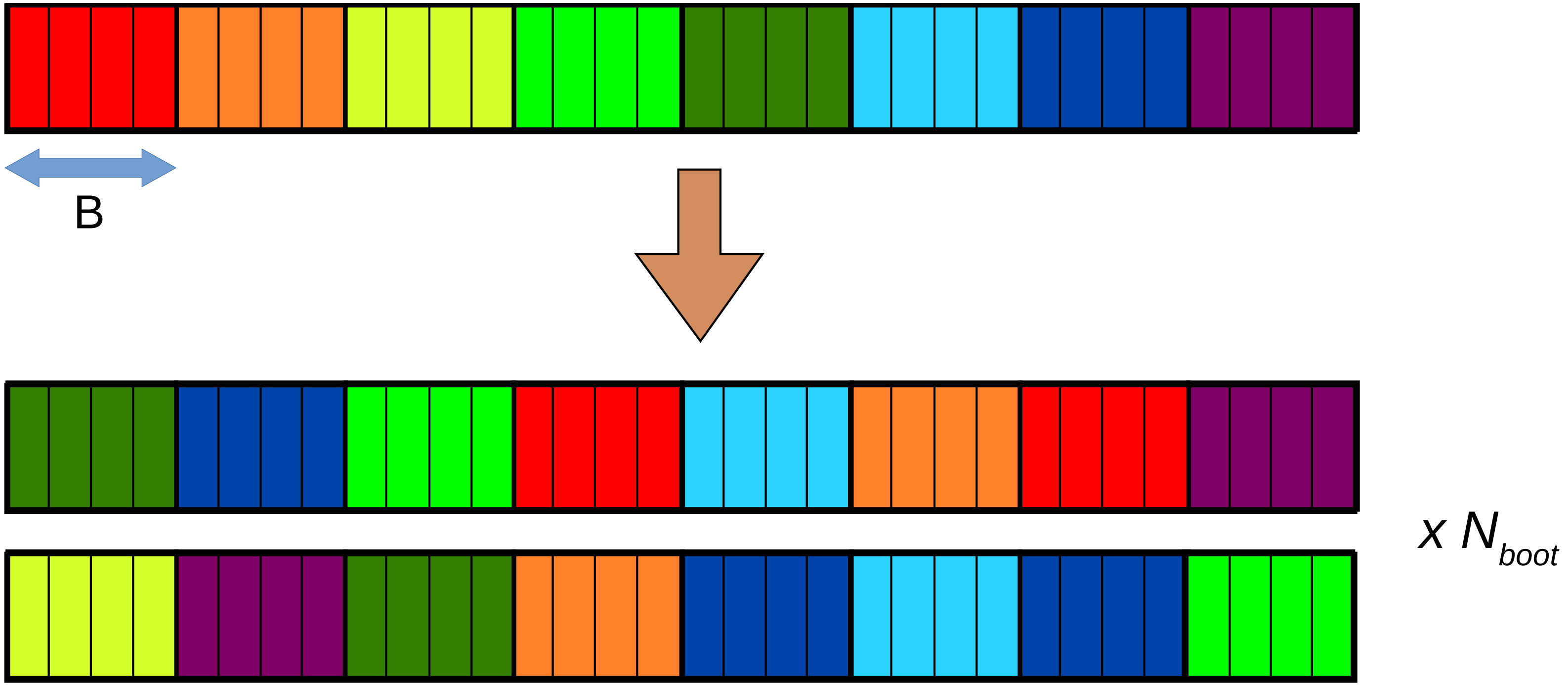
$$C_{tt'} = \frac{1}{n(n-1)} \sum_{i=1}^{n} \left[v_{i,t} - \bar{v}_t\right] \left[v_{i,t'} - \bar{v}_{t'}\right]$$

P-value issues

- Despite high degree of stability under changing fit ranges, goodness of fit for $\pi\pi$ typically quite poor.
- Importance of reliable $\pi\pi$ fits strongly motivates resolving this issue.
- Key is to recognize that the χ^2 distribution does not account for fluctuations in the *covariance matrix* over the population.
- When cov. mat. is determined from data, finite statistics effects broaden the distribution of q^2 as the matrix fluctuates along with the data.
- For ensembles of *uncorrelated Gaussian data* (not QCD path integral-distributed!) the corrected distribution can be determined analytically:
  It is the Hotelling T^2 distribution, $T^2(k, n-1)$ for n samples.
- However in general there is no analytic result.
- Even if we assume Gaussian data, numerical tests indicate strong autocorrelation effects that can only be removed by binning to large bin sizes (a no-go for us!).

Non-overlapping block bootstrap (NBB)

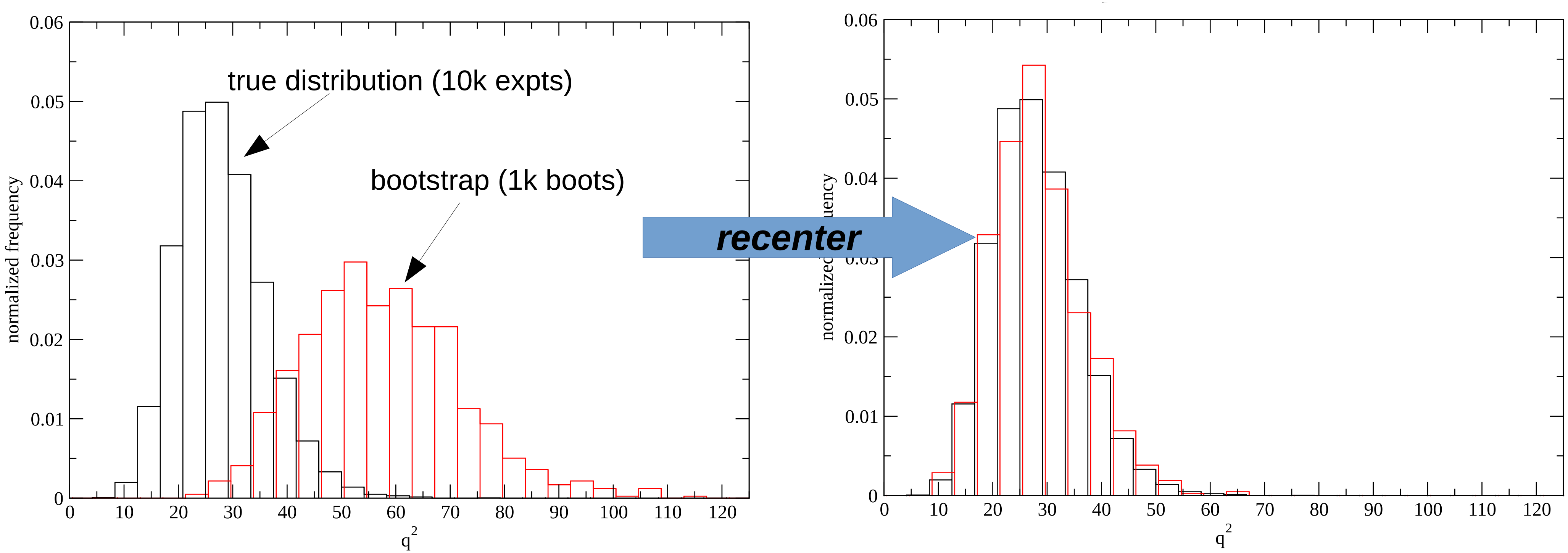
- The **bootstrap** technique allows us to estimate properties of the population from just one ensemble, by randomly resampling (with replacement).
- The (non-overlapping) block variant resamples blocks rather than single configurations, much like block jackknife, in order to account for autocorrelations:



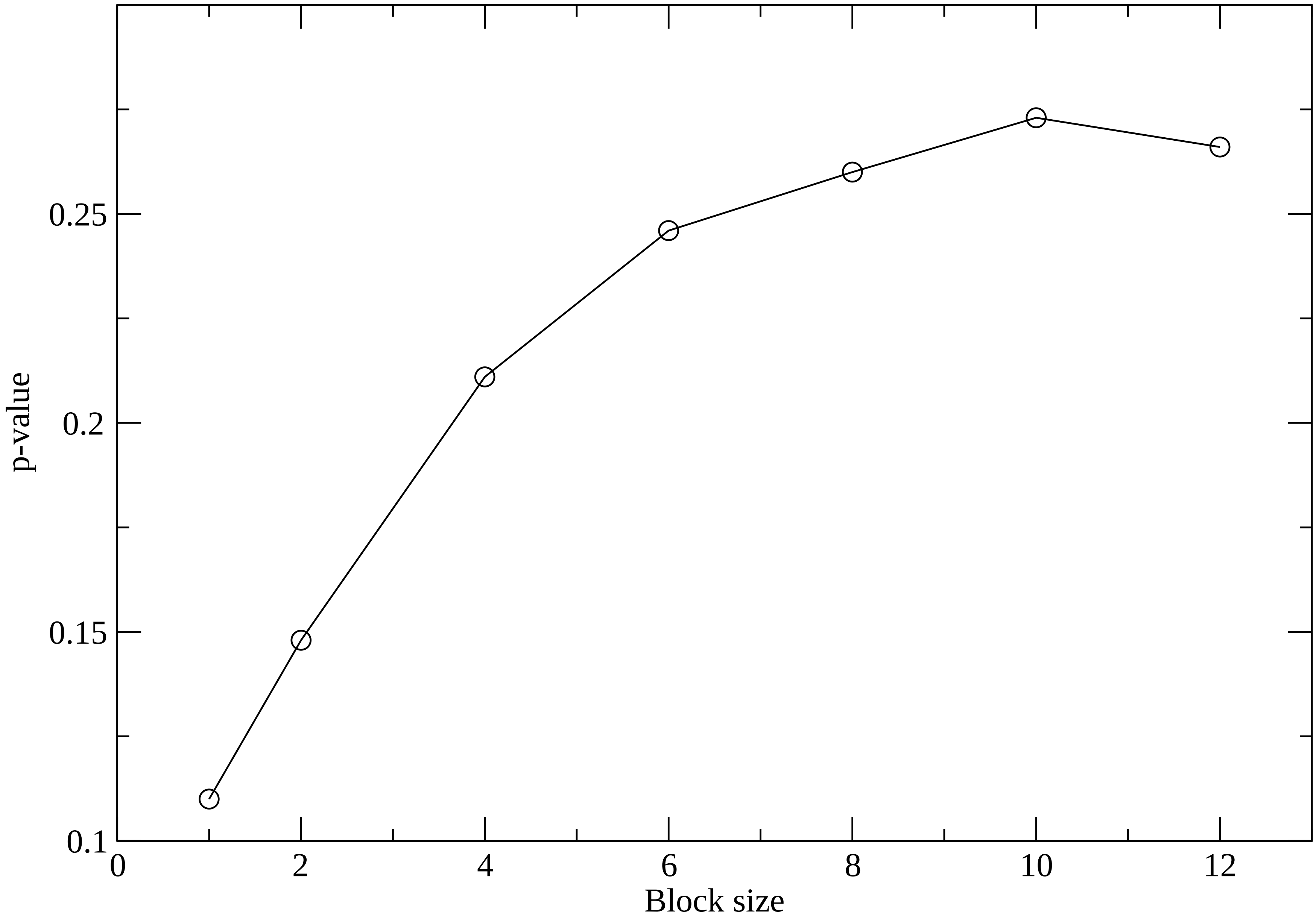
Computing p-values via bootstrap

- Use NBB to directly compute the distribution of q^2!
  - ✓ No normality assumption
  - ✓ Blocking accounts for autocorrelations without binning
- Minor subtlety: bootstrap ensemble means $\bar{b}^{\alpha}$ distributed about ensemble mean $\bar{v}$ ***not population mean***
- Results in broader distribution of q^2 with larger mean
- Correct by “recentering”: $\bar{b}^{\alpha}(t) \rightarrow \bar{b}^{\alpha}(t) + [f(t,\vec{p}) - \bar{e}(t)]$

gaussian data, no autocorrelations, 400 samples

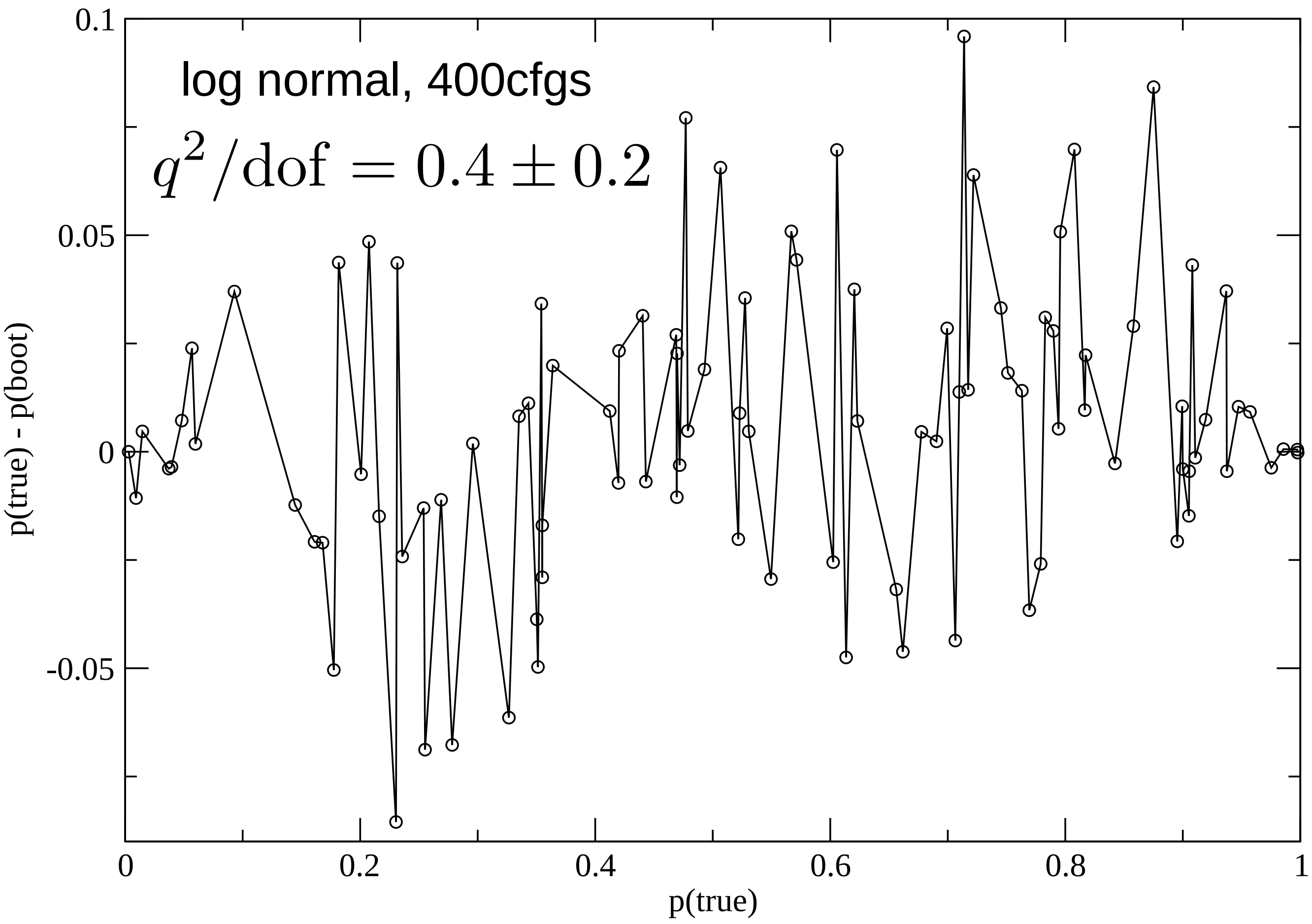


I=0 ππ fit bootstrap p-value



p-values for uncorrelated fits!

- Conventional wisdom is that one cannot obtain the goodness-of-fit for uncorrelated fits. Using the bootstrap technique we can!



Conclusions

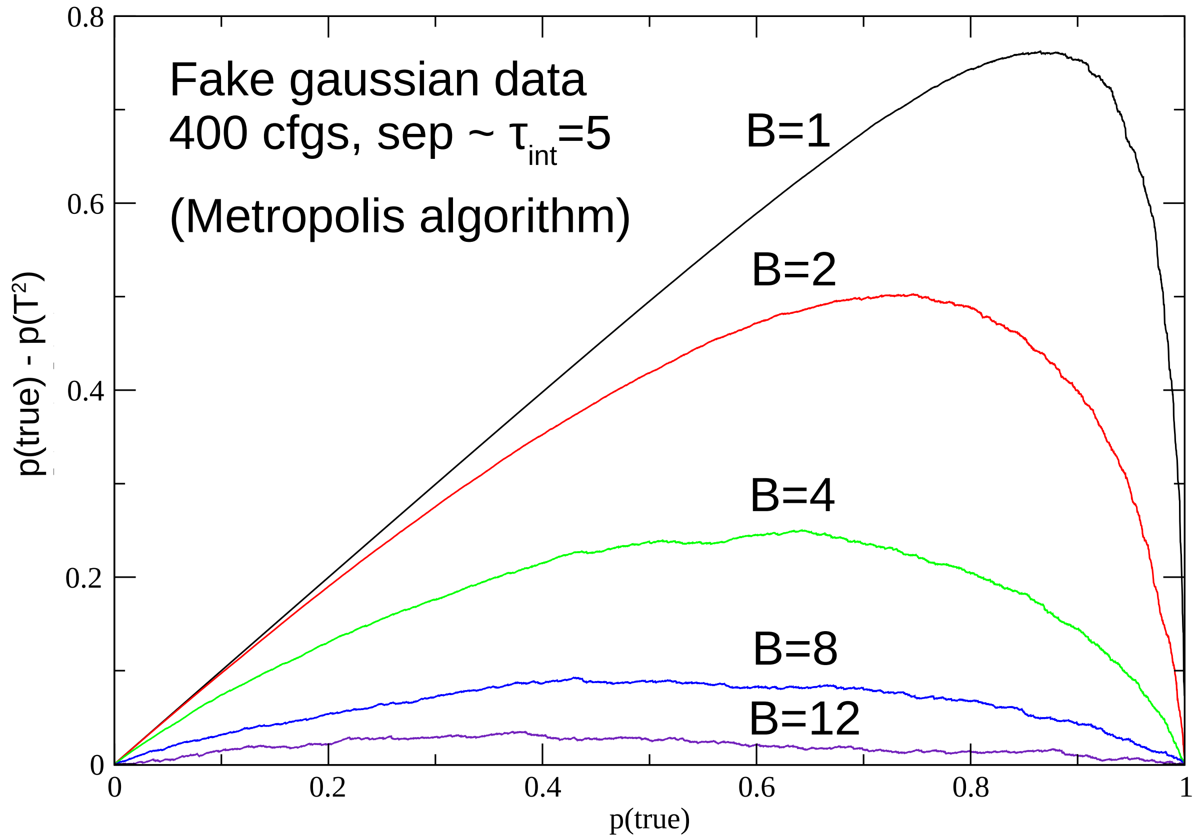
Conclusions

- Multi-operator techniques appear to resolve discrepancy with dispersive prediction for I=0 $\pi\pi$ phase shift.
- Marked improvement in quality of plateaus in $K\to\pi\pi$, better control over excited state systematics.
- Programmes for reducing other systematic errors in progress.
- Already achieved 2x improvement in NPR error via step scaling.
- Potential near-term reduction in Wilson coeff. systematic through NNLO PT calculation. In longer term we aim for a non-perturbative matching through the charm threshold.
- Advanced statistical techniques allow for more reliable p-values and enable us to account for mild autocorrelation effects without exploding our statistical error through binning.
- Expect no further hurdles to completion of project and we aim to publish within the next few months.

Thank you!

Is the Hotelling distribution sufficient?

- Numerical experiments with fake data show Hotelling T^2 relatively tolerant of non-normality.
- **However** T^2 relies on independent configurations: *extremely* sensitive to autocorrelations.
- Even with binning, slow convergence to true distribution:

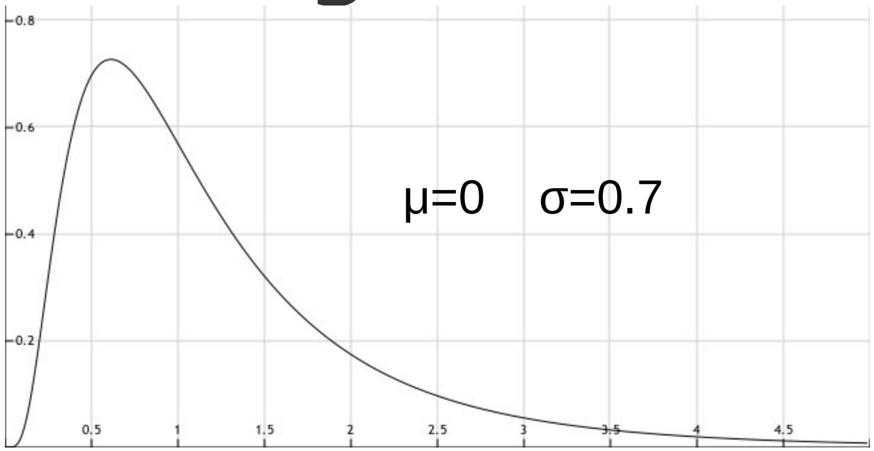


dramatically underestimates p

- Wish to avoid binning due to explosion in statistical error from reduced resolution of covariance matrix

Demonstration II - log-normal

400 cfgs, log-normal



Stat error and bias fall as $n, B \to \infty \quad (B \ll n)$