I=0 ππ scattering at physical masses on the lattice

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Motivation

- Significant goal of RBC & UKQCD is physical lattice calculation of ε', the measure of direct CP-violation in $K \to \pi\pi$ decays.
- Direct CPV heavily suppressed in Standard Model hence ε' is very sensitive to BSM sources of CPV.
- When compared to experiment, any deviations may help shed light on origin of matter/antimatter asymmetry.
- Understanding ππ system is crucial:
  - Energy is needed for time dependence of correlation function from which extract finite-volume $K \to \pi\pi$ matrix element.
  - Phase shift enters Lellouch-Luscher finite-volume correction to matrix element.

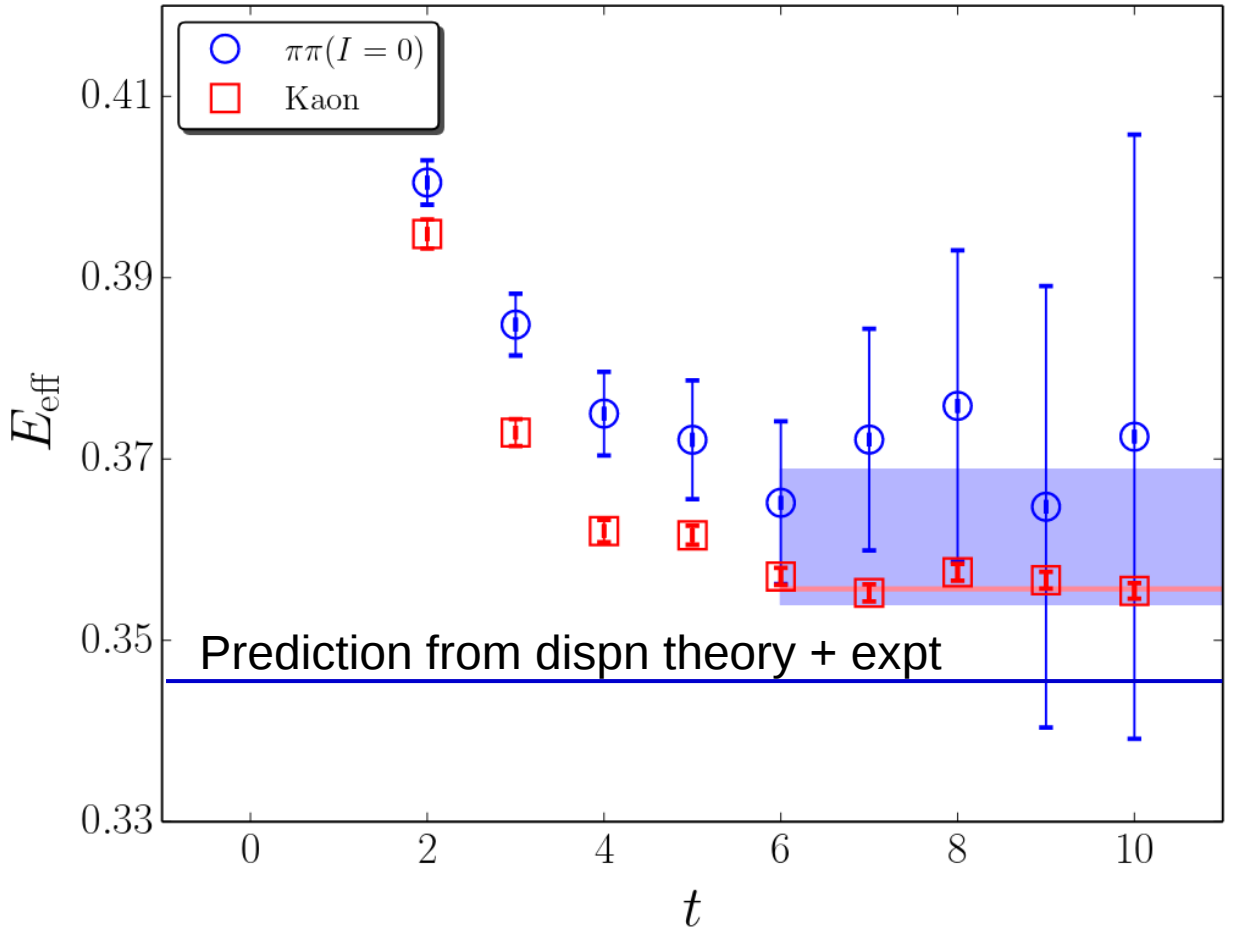
2015 calculation

[Phys.Rev.Lett. 115 (2015) no.21, 212001]

- First result published in 2015.
- 216 configurations.
- 32^3x64 lattice volume.
- (Mobius) domain wall fermions with physical quark masses.
- Iwasaki+DSDR action allowing coarse lattice spacing of a^{-1}=1.38 GeV and correspondingly large physical volume $(4.6\ \text{fm})^3$ while keeping chiral symmetry breaking under control.
- G-parity boundary conditions on quarks such that pions obey antiperiodic BCs : $p_\pi = \pm\pi/L,\ \pm 3\pi/L, \ldots$
- Lattice size L chosen to make ground-state ππ energy match kaon mass to ensure physical decay.

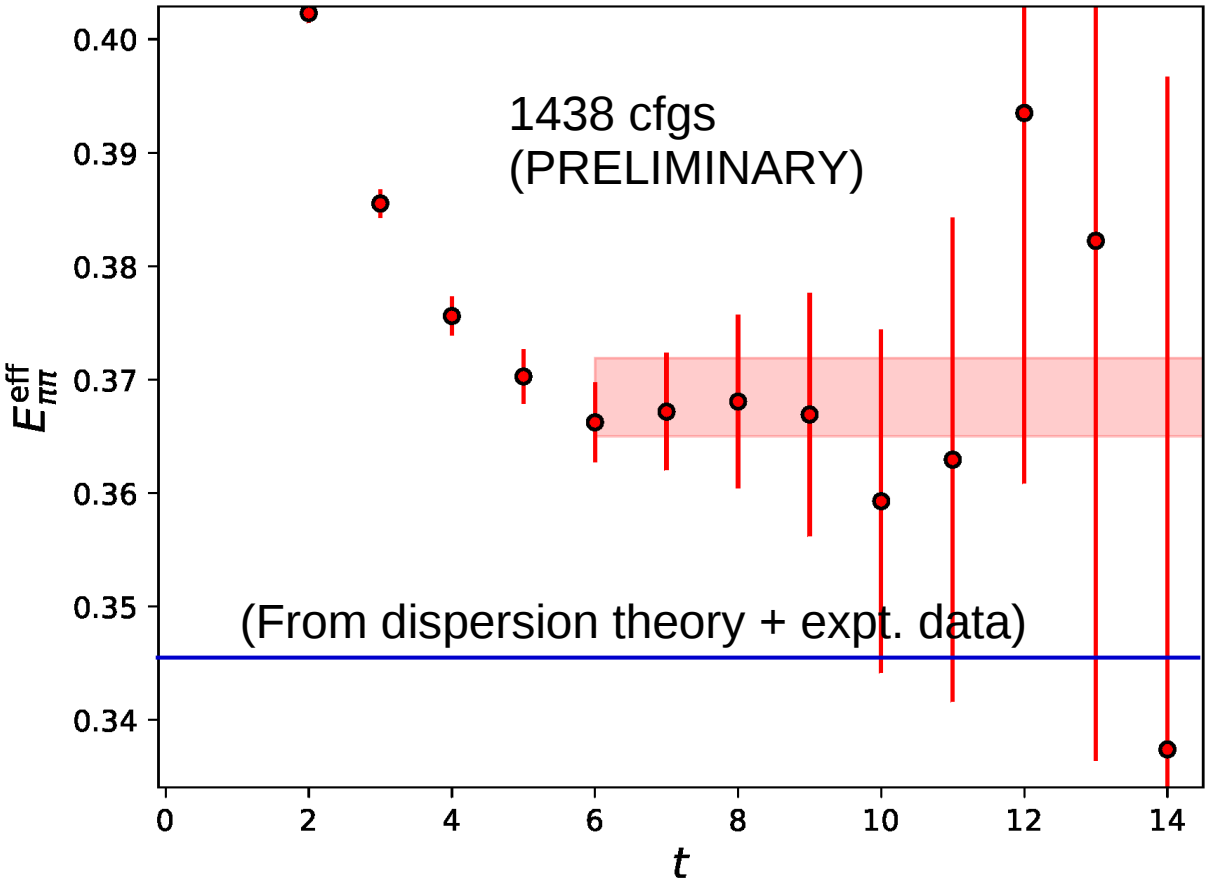
2015 calculation - ππ energy

- Pions generated with momenta (±1,±1,±1)π/L
- From these construct operator "ππ(111,111)" with total momentum zero (back to back moving pions)
- The two single-pion sources are placed on timeslices separated by 4 which significantly reduces vacuum contribution.



2015 calculation - ππ energy

- Despite showing good stability under changes of t_{min} and between 1 and 2 state fits, our energy is several σ larger than predicted by dispersion theory.
- Manifests in phase-shift (obtained via Luscher formula from energy): δ_0=23.8(4.9)(1.2)° vs ~34°
- Persists when data set enlarged by almost 7x!



Resolution of ππ puzzle

- Shortly after 2015 publication we began a program to investigate this discrepancy in more detail.
- Most likely explanation is excited state contamination from a nearby state that the fitter is unable to isolate from the time dependence alone.
- Solution is to add additional operators.
- Matrix of correlators:

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

- This is very powerful as evidenced by fact that multiple operators can distinguish the presence of excited states even from a single timeslice:

  If, e.g 2 operators and only one state

$$\det(C(t)) = \left(A_{00}^2 \times A_{10}^2 - A_{10}A_{00} \times A_{00}A_{10}\right) e^{-E_0 t} = 0$$

Stationary ππ

Extra operators

- We added two additional operators with same quantum numbers:
  - Scalar “σ” operator ~ $\bar{u}u + \bar{d}d$
  - “ππ(311,311)” operator comprising back-to-back pions with momenta (±3,±1,±1)π/L + cyclic perms.
- We now have 741 measurements with these new operators.
- We perform 3-operator 3-state fits. The correlator matrix is symmetric and comprises 6 independent correlation functions.
- Note that around-the-world effects are expected in these correlators where one pion propagates forwards in time and the other backwards:

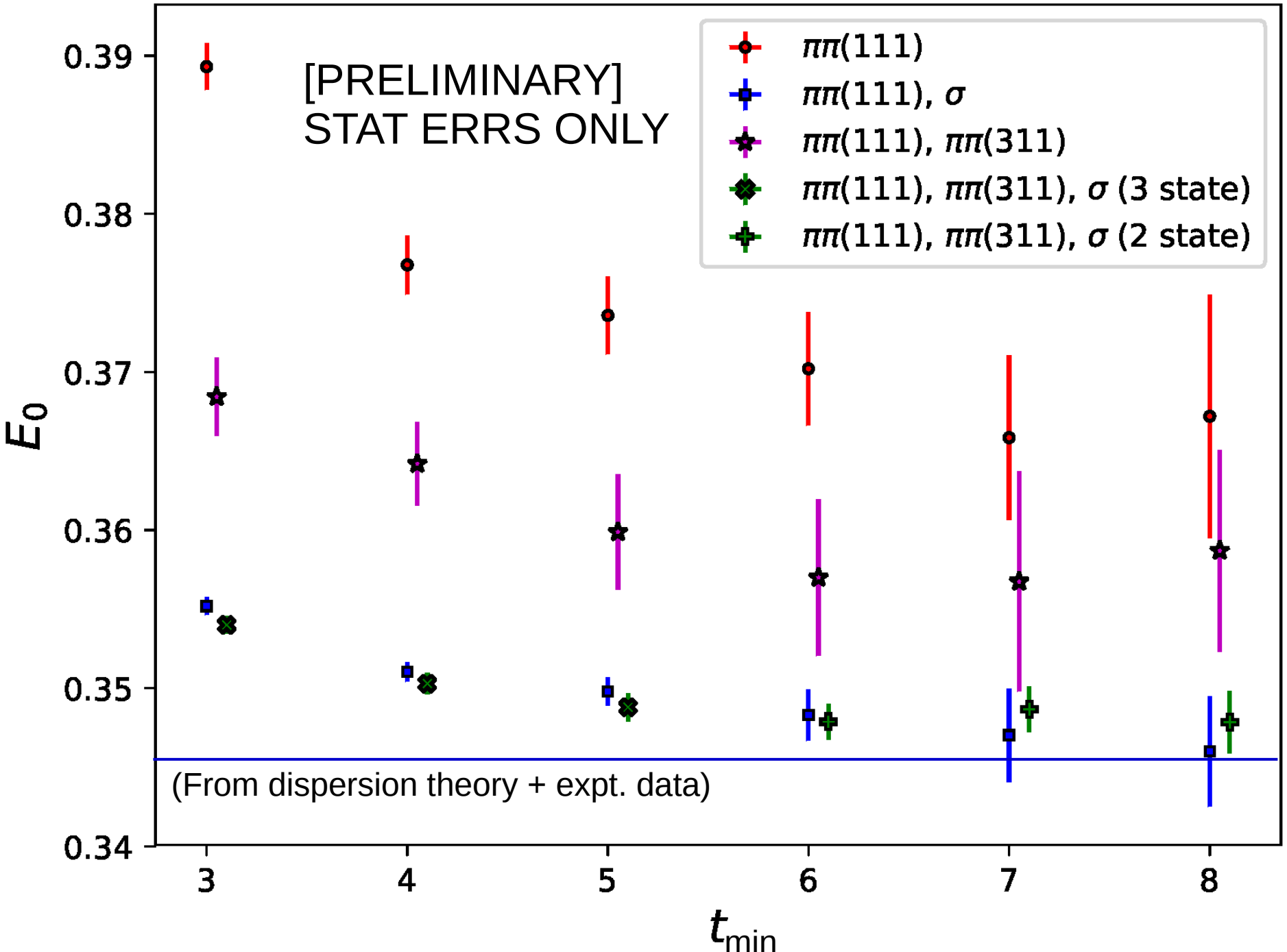
2*4 from split-sources

$$Ae^{-E_\pi t}e^{-E_\pi (L_T - t - 8)} \sim \text{constant}$$

- For ππ(111,111), ππ(111,111) correlator can estimate constant from single-pion correlator: constant ~ 5×10^{-5} vs O(1) amplitude.

  ~10% contribution at t=15 (most precise data has 25% errs at t=15)

Effect of additional operators



Effect of additional operators (contd.)

- Extra operators have significant impact on ground-state energy resulting in much better agreement with dispersive prediction.
- Phase shift 31.7(6)° vs ~34° prediction (5-15, stat errs only).
- Fits are quite tricky however: data are highly correlated and thus correlated fits are desired to minimize errors and provide goodness-of-fit information.
- Covariance matrices are 66x66 for a fit from 5-15! Obtain using double-jackknife procedure.
- Not clear how reliable covariance matrices are given 15 orders-of-magnitude between lowest and highest eigenvalue.
- Number of fit parameters is large: 3x3 amplitudes, 3 energies and 6 constants = 18 parameters.
- Rapid decay of signal/noise, especially for ππ(311,311), ππ(311,311) correlator which has 100% errors at t=8.

Constant terms and p-values

- For these fits the constants all come out as zero within errors, e.g. 5-15 fit with 3 states:

$C_{\pi\pi(111),\pi\pi(111)}$	$-6(12) \times 10^{-5}$
$C_{\pi\pi(111),\pi\pi(311)}$	$-11(33) \times 10^{-6}$
$C_{\pi\pi(111),\pi\pi(311)}$	$-27(34) \times 10^{-8}$
$C_{\pi\pi(311),\pi\pi(311)}$	$-5(95) \times 10^{-7}$
$C_{\pi\pi(311),\sigma}$	$-37(95) \times 10^{-9}$
$C_{\sigma,\sigma}$	$-10(11) \times 10^{-10}$

- We can therefore ignore the constants here.

	5-15 (3 state)	6-15 (2-state)	7-15 (2-state)
χ^2/dof	1.37	1.37	1.17
p-value	0.04	0.06	0.2

- χ^2/dof look good but p-values (essentially probability data agrees with model) quite poor, particularly for small t: dof ~ O(50), hence χ^2 distribution strongly peaked.
- Not clear how meaningful given knowledge of covariance matrix: 1.37 → 1.17 requires $\Delta\chi^2 \sim 10$ in context where contribution of each of the ~65 eigenmodes varies significantly in range 1×10^{-4} up to 6.5×10^{0}.

Systematic errors

- Despite difficulties, agreement between fit parameters is very good.

Param	6 minus 5	7 minus 6
$A^0_{\pi\pi(111)}$	$-0.0028(59)$	$0.0065(80)$
$A^0_{\pi\pi(311)}$	$0.062(69)$	$-0.132(95)$
A^0_σ	$-0.0044(57)$	$-0.0042(82)$
E_0	$-0.0026(21)$	$0.0023(29)$
$A^1_{\pi\pi(111)}$	$-0.027(41)$	$-0.120(77)$
$A^1_{\pi\pi(311)}$	$-0.026(50)$	$-0.025(85)$
A^1_σ	$-0.068(56)$	$0.052(86)$
E_1	$-0.019(21)$	$-0.010(32)$

Relative differences between fit parameters at consecutive t_{min}

- Variation indicates systematic error associated with fitting strategy is small, possibly negligible.
- Possibility of further excited state contamination cannot be ruled out and should be estimated.
- Discretization effects and remnant finite-volume errors require estimation.

Comoving ππ

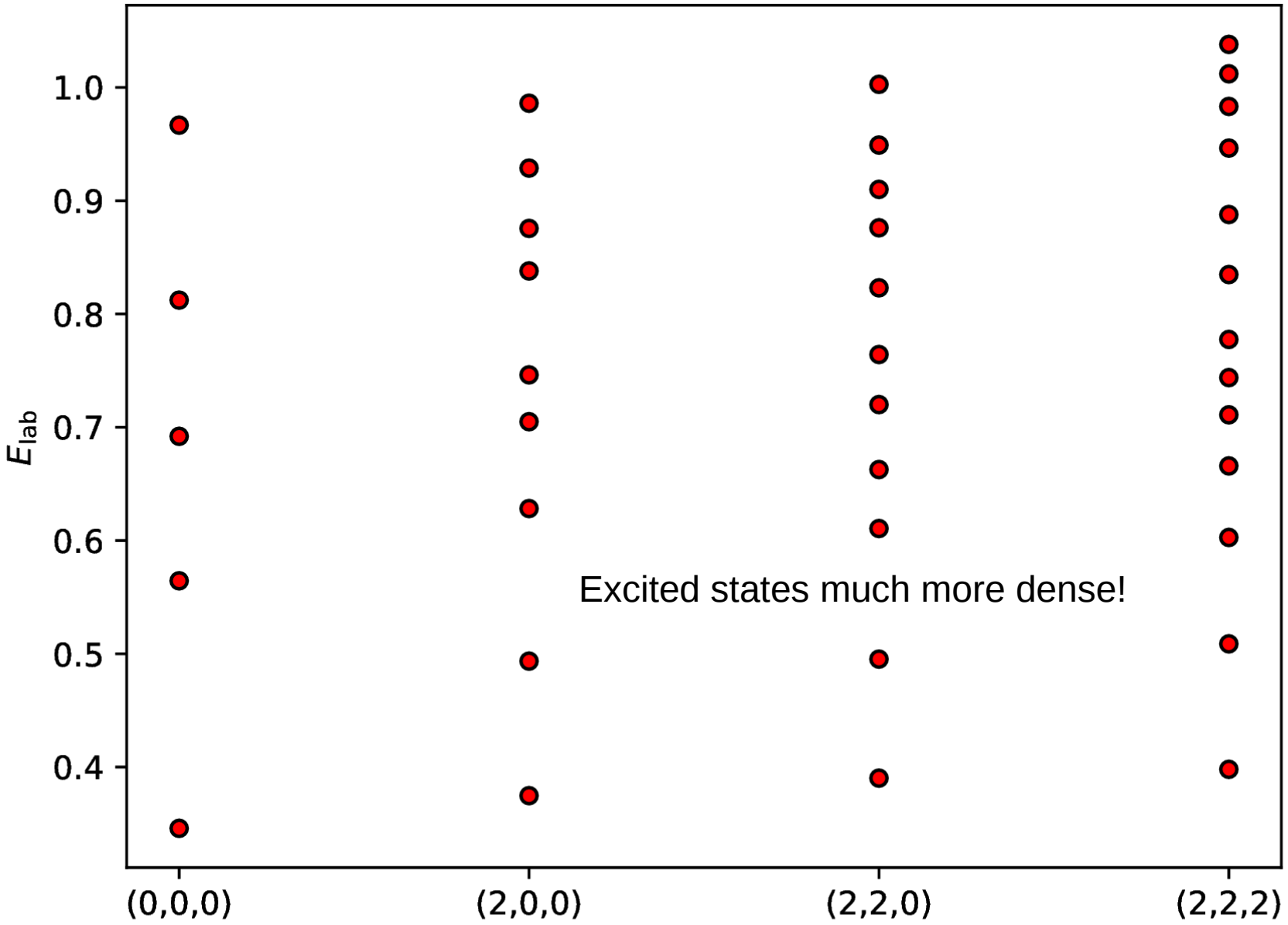
Comoving ππ

- Due to use of “all-to-all propagator” framework we are also able to compute ππ correlation functions for states of non-zero total momentum for minimal extra cost.
- Combining our pions in p_π=(±3,±1,±1)π/L and (±1,±1,±1)π/L momentum sets we can access ππ total momenta (±2,0,0)π/L, (±2,±2,0)π/L and (±2,±2,±2)π/L
- For each we can construct 3 independent operators: ππ(111,111), ππ(311,111) and ππ(311,311) that contain 0,1 and 2 pion operators in the (±3,±1,±1)π/L, resp.
- This allows us to compute the I=0 ππ phase shift at 3 additional (lower) center-of-mass energies and thus map out the energy dependence of the phase shift.
- Lellouch-Luscher factor for K→ππ actually needs the *derivative* of the phase shift wrt. energy: we can now compute this from first principles.
- Potentially improve 11% systematic error on K→ππ.

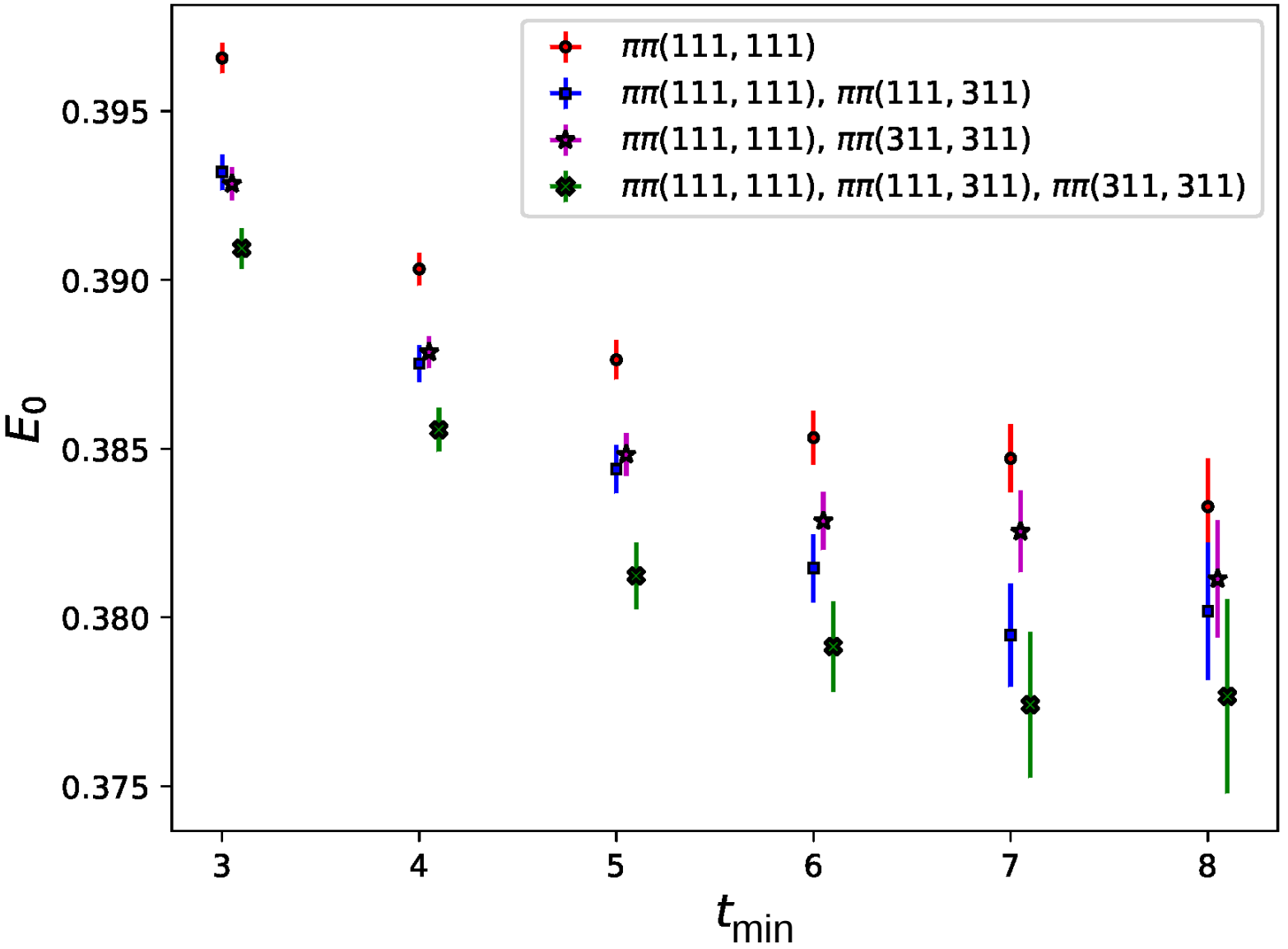
[Using Colangelo et al Nucl. Phys. B603 (2001) 125-179]

Predicted energies

By (numerically) matching dispersion theory curve of δ(E) and Luscher's δ(E; L) we can predict allowed finite volume energies



$p_{tot}=(2,0,0)\pi/L$ ground state energy



$p_{tot}=(2,0,0)\pi/L$ discussion

7-15

$C_{gnd,gnd}$	$-40(57)\times10^{-6}$
$C_{gnd,exc1}$	$-39(28)\times10^{-6}$
$C_{gnd,exc2}$	$-16(14)\times10^{-6}$
$C_{exc1,exc1}$	$-24(15)\times10^{-6}$
$C_{exc1,exc2}$	$-110(70)\times10^{-7}$
$C_{exc2,exc2}$	$-51(37)\times10^{-7}$

- Constants have wrong sign yet resolvable from 0 at 1.5σ
- Likely just fit artefact: fit without constants as before

Quantity	$t_{\min}=6$	7	8
χ^2/dof	1.00	0.96	0.87
p-value	0.47	0.55	0.69

- Fits without constants, χ^2/dof and p-values both very good.

- Why is this so much better behaved than the stationary case? Perhaps it is due to the nature of the operators:

(2,0,0)

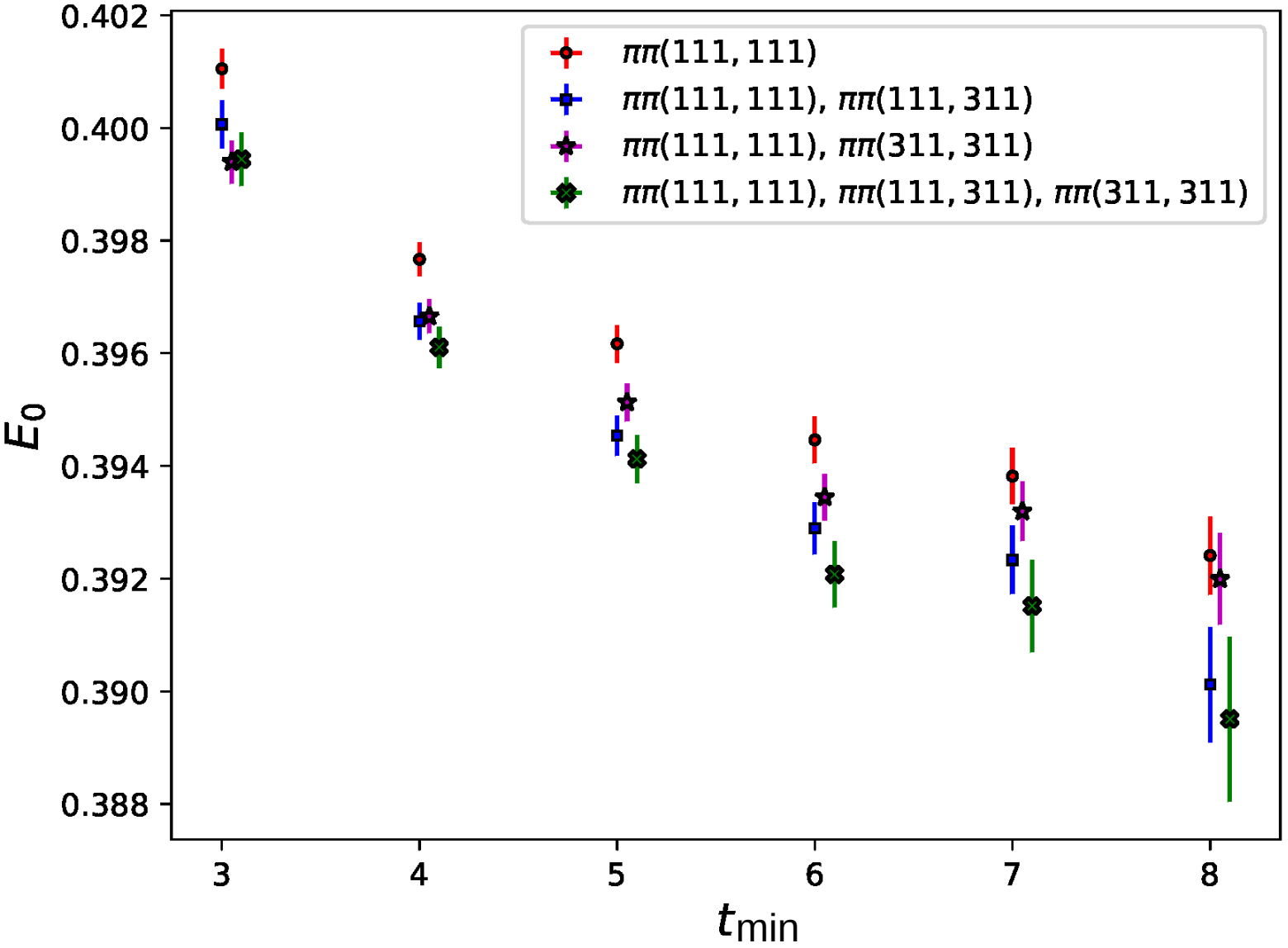
	Param	7-15
ππ(111,111)	A^0_{gnd}	1.0(0.0)
	A^1_{gnd}	−0.306(45)
	A^2_{gnd}	−0.138(18)
ππ(311,111)	A^0_{exc1}	0.086(21)
	A^1_{exc1}	1.0(0.0)
	A^2_{exc1}	−0.30(10)
ππ(311,311)	A^0_{exc2}	0.013(12)
	A^1_{exc2}	0.092(46)
	A^2_{exc2}	1.0(0.0)

(0,0,0)

Param	4-15
$A^0_{\pi\pi(111)}$	1.0(0.0)
$A^1_{\pi\pi(111)}$	0.470(20)
$A^2_{\pi\pi(111)}$	0.311(73)
$A^0_{\pi\pi(311)}$	0.0528(86)
$A^1_{\pi\pi(311)}$	−0.84(12)
$A^2_{\pi\pi(311)}$	1.0(0.0)
A^0_{σ}	1.0(0.0)
A^1_{σ}	−0.830(28)
A^2_{σ}	−0.87(22)

- Relative couplings (to favored) indicate considerably less intercoupling between states and operators
- More diagonal amplitude matrix suggests simpler covariance matrix.
- Also perhaps more exposure to excited state contamination?

$p_{tot}=(2,2,0)\pi/L$ ground state energy



$p_{tot}=(2,2,0)\pi/L$ discussion

- Adding operators does not appear to improve almost-linear dependence of energy on t_{min}
  - excited state contamination?

6-15

$C_{gnd,gnd}$	$90(41)\times10^{-6}$
$C_{gnd,exc1}$	$8(19)\times10^{-6}$
$C_{gnd,exc2}$	$10(89)\times10^{-7}$
$C_{exc1,exc1}$	$-17(94)\times10^{-7}$
$C_{exc1,exc2}$	$-30(44)\times10^{-7}$
$C_{exc2,exc2}$	$-24(22)\times10^{-7}$

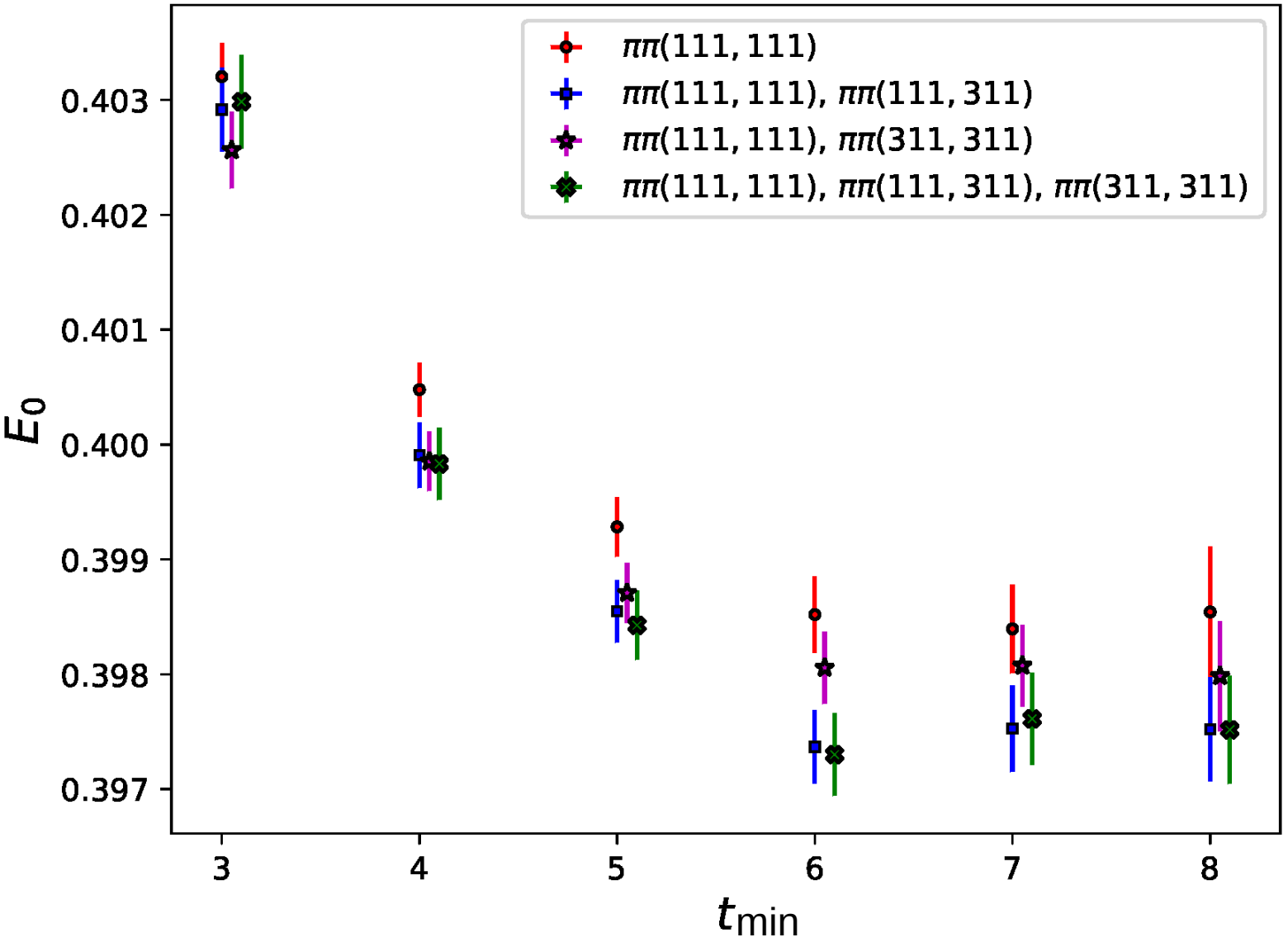
- Constants unresolved from 0 apart from in one case where it has correct sign and is consistent with expectation.
- p-value strongly supports including constants, eg. 6-15: p=0.1 (with) vs 3×10^{-7} (without).

- Nevertheless I will *not* include constants as I believe that these extra 6 parameters are spurious and just act to absorb some excited state contamination.
  (supported by the (2,2,2) case as we will see)
- Why is (2,2,0) worse than (2,0,0) or (0,0,0)? Again this appears due to the nature of the operators:

	Param	6-15
ππ(111,111)	A^0_{gnd}	$1.0(0.0)$
	A^1_{gnd}	$-0.160(15)$
	A^2_{gnd}	$-0.0790(64)$
ππ(311,111)	A^0_{exc1}	$0.0173(76)$
	A^1_{exc1}	$1.0(0.0)$
	A^2_{exc1}	$-0.186(43)$
ππ(311,311)	A^0_{exc2}	$-0.0082(33)$
	A^1_{exc2}	$0.045(20)$
	A^2_{exc2}	$1.0(0.0)$

- Amplitude matrix is much more diagonal, little intercoupling between operators and states.
- Suggests a 4th state could easily be present that couples strongly only to 1st operator.
- Would explain fact that adding operators does not seem to improve t_{min} dep.

$p_{tot}=(2,2,2)\pi/L$ ground state energy



p_{tot}=(2,2,2)π/L discussion

- Results appear to plateau at t_{min}=6.

6-15

$C_{gnd,gnd}$	$-6(60) \times 10^{-6}$
$C_{gnd,exc1}$	$-41(25) \times 10^{-6}$
$C_{gnd,exc2}$	$-21(11) \times 10^{-6}$
$C_{exc1,exc1}$	$-18(11) \times 10^{-6}$
$C_{exc1,exc2}$	$-117(52) \times 10^{-7}$
$C_{exc2,exc2}$	$-62(26) \times 10^{-7}$

- p-values strongly favor including constants: 6-15 p=0.25 (with), p=3x10^{-8} (without)
- However values have the wrong sign.
- Despite apparent plateau, amplitude matrix is again very close to diagonal

Param	6-15
A^0_{gnd}	1.0(0.0)
A^1_{gnd}	−0.073(11)
A^2_{gnd}	−0.0352(80)
A^0_{exc1}	−0.0125(57)
A^1_{exc1}	1.0(0.0)
A^2_{exc1}	−0.189(49)
A^0_{exc2}	−0.0151(27)
A^1_{exc2}	0.049(24)
A^2_{exc2}	1.0(0.0)

(relative couplings)

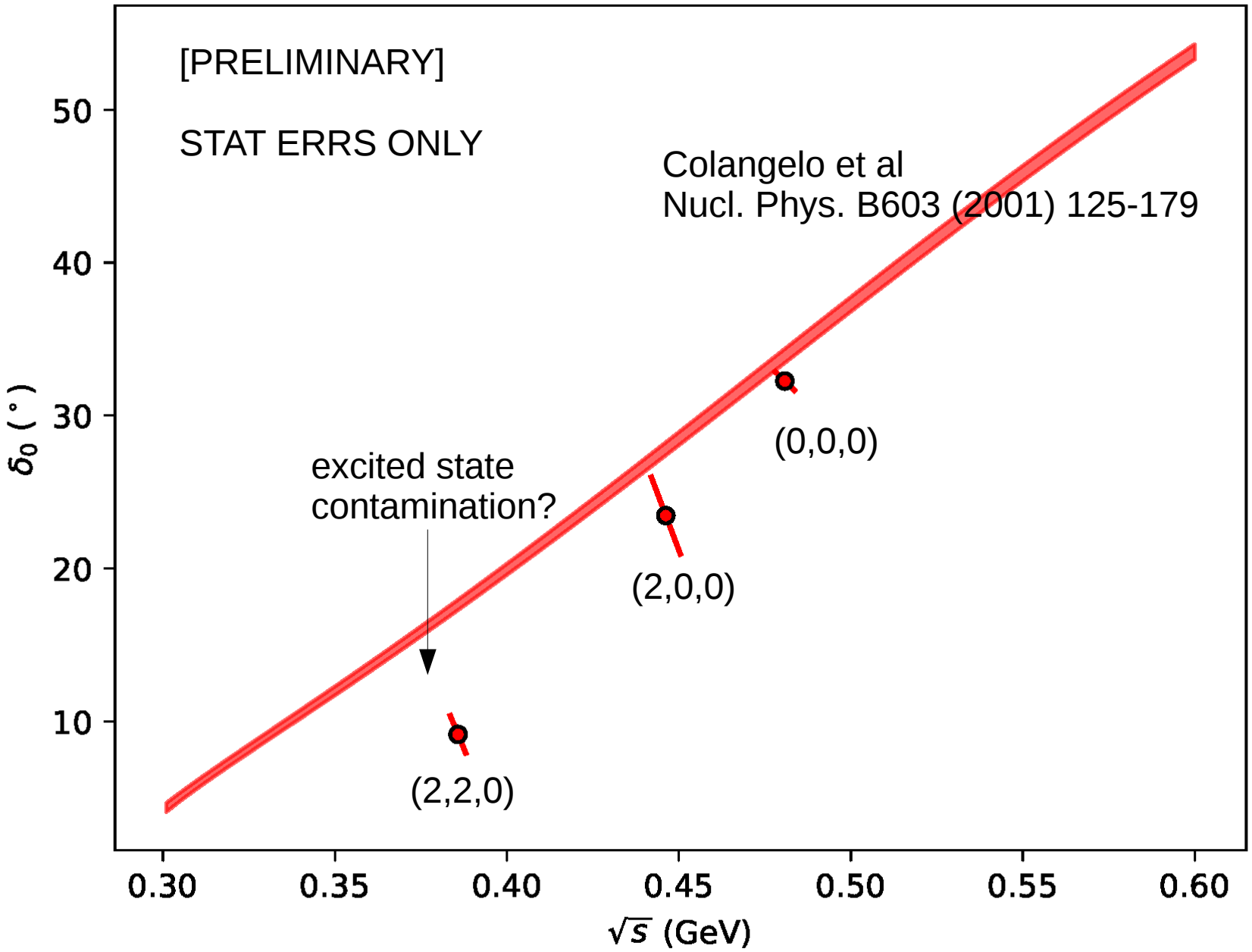
(relative diffs. const/no const)

Param	6-15
A^0_{gnd}	0.00151(82)
A^0_{exc1}	−0.18(31)
A^0_{exc2}	−0.09(13)
E_0	0.00099(63)
A^1_{gnd}	0.061(93)
A^1_{exc1}	−0.0021(69)
A^1_{exc2}	0.61(44)
E_1	−0.0010(43)
A^2_{gnd}	−0.04(13)
A^2_{exc1}	0.25(16)
A^2_{exc2}	−0.010(14)
E_2	−0.0074(74)

- Likelihood then is constants are spurious and just help account for breakdown of 3-state model.
- This lends support for dropping the constants for the (2,2,0) case where the amplitude matrix is similarly near-diagonal.
- Ultimately a sys. error will be required to account for the excited state contamination that will likely be larger than any difference we see between including/excluding constants.

Phase shift energy dependence

Phase shift energy dependence



Conclusions

Conclusions

- For stationary ππ, adding 2 more operators significantly reduces excited state contamination and improves agreement with dispersive result.
  - Vastly improved understanding of ππ system at ~500 MeV
- Comoving ππ allow direct measurement of energy dependence of phase-shift: Potentially improve 11% Lellouch-Luscher systematic on $K \to \pi\pi$.
- For comoving ππ, particularly at larger total momenta, our 3 operators appear to only weakly intercouple between the 3 states.
- Excited state systematic errors on comoving ππ energies likely remain significant, reducing their value in mapping out the phase-shift energy dependence.
- Multi-state correlated fits to noisy data are very difficult. However varying the fit strategy appears to have little effect on the results.
- GEVP may allow us to circumvent many of these difficulties, and is under active consideration. Correct treatment of constants acts as stumbling block here.

Conclusions (contd.)

- Impact of significant improvement in understanding of stationary ππ system upon $K \to \pi\pi$ is under examination.
- Matrix elements with all 3 operators have been computed and therefore we expect to be able to isolate the ground-state contribution much more effectively.
- Expect results in the next few months.

Thank you!