S-wave $\pi\pi$ I=0 and I=2 scattering with physical pion mass

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Motivation

- Important component in $K \to \pi\pi$ calculation
  - Energy and amplitude are needed in determining lattice matrix element
  - Phase shift and its derivative are necessary in LL factor
- First lattice calculation on $\pi\pi$ scattering with **physical pion mass** around kaon mass with **disconnected** diagram included in I=0
- 2015 results gives $\pi\pi$ energy which is 3σ(7σ with more statistics) higher than the phenomenological prediction(Pi-Pi puzzle)

$$\begin{aligned}\delta_0 &= 23.8(4.9)(1.2)^\circ(PRL, 2015)\\ &= 19.1(2.5)(1.2)^\circ(1386 confs)\\ &\approx 34^\circ(Dispersion)\end{aligned}$$

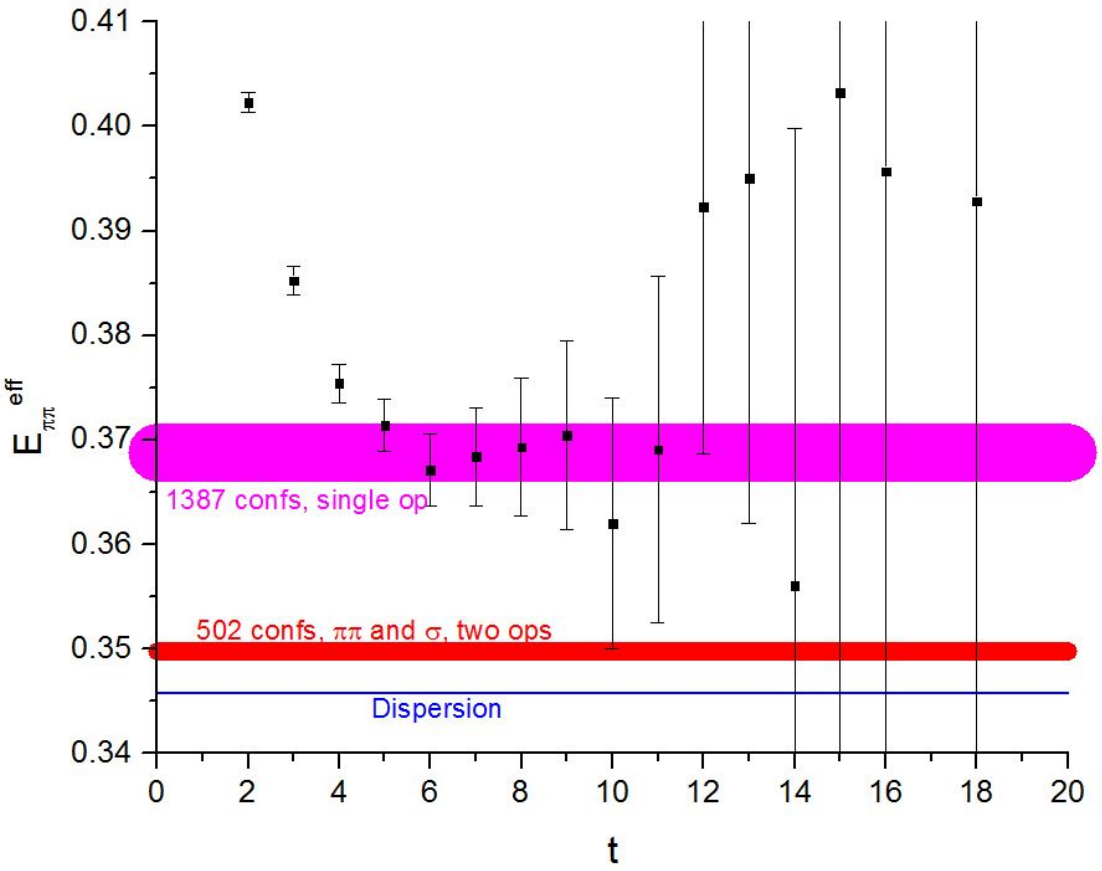
Possible reason could be excited state contamination for $\pi\pi$ state.
Solution: introducing more operators.

Calculation details and techniques

- G-parity boundary condition
  Helps with $K \to \pi\pi$ calculation, ground state π has momentum $(\pm\frac{\pi}{L}, \pm\frac{\pi}{L}, \pm\frac{\pi}{L})$
- All to all propagator
  Better overlap between interpolating operator and meson ground state, 900 low modes plus 1536 random modes from time/flavor/color/spin dilution, 1s hydrogen wave function smearing. We use mesonfield with different choices of momentum for each pion
- Time separated pipi operator
  Two pions are time separated by 4
- Adding more operators
  In I=0 calculation, we add sigma operators which looks like $(\bar{u}u + \bar{d}d)$ with zero momentum.
  In both I=0 and I=2 calculation, we add "311" π operator with momentum $(\pm\frac{3\pi}{L}, \pm\frac{\pi}{L}, \pm\frac{\pi}{L})$
- Using Non-overlapping blocked bootstrap to calculate p-value more reliably (cf Chris Kelly Wednesday)

Multiple operators

- We introduced sigma operator on 2018 which hugely suppresses the excited state contamination error.
- Adding more operators (e.g. $\pi\pi(311,311)$) to suppress remaining excited state contamination?



Stationary $\pi\pi$ I=2

Two operators: S-wave $\pi\pi$(111,111) and $\pi\pi$(311,311)

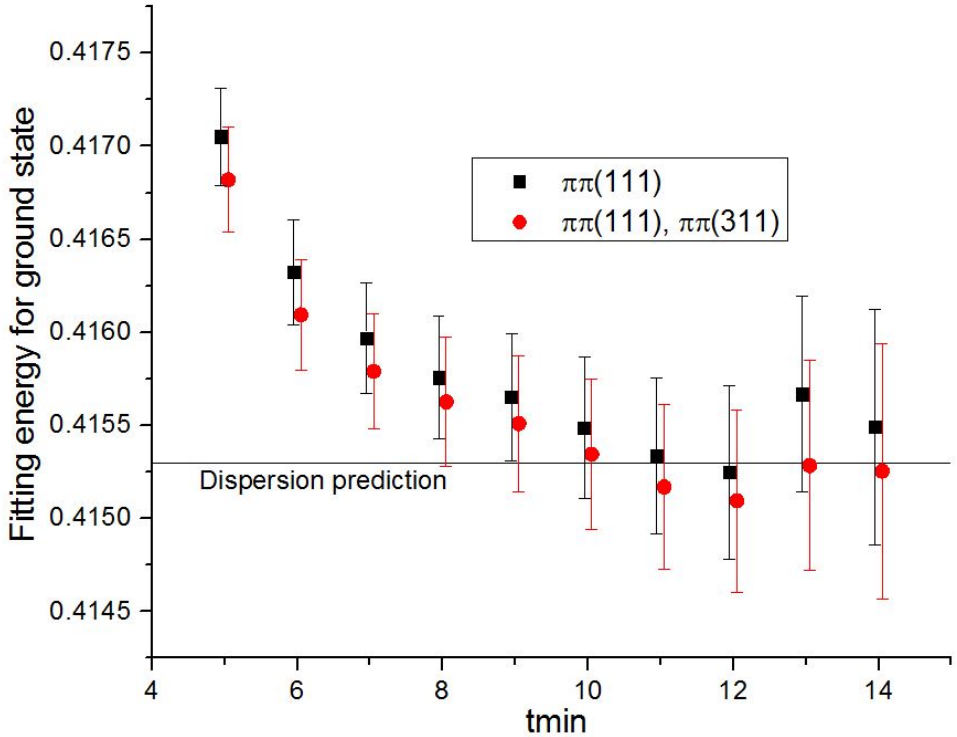


Figure: Stationary $\pi\pi_{I=2}$, fitting energy as a function of fitting tmin

Correlated fit is performed with one/two operators and one/two states so that number of states matches number of operators. Form of fitting function is

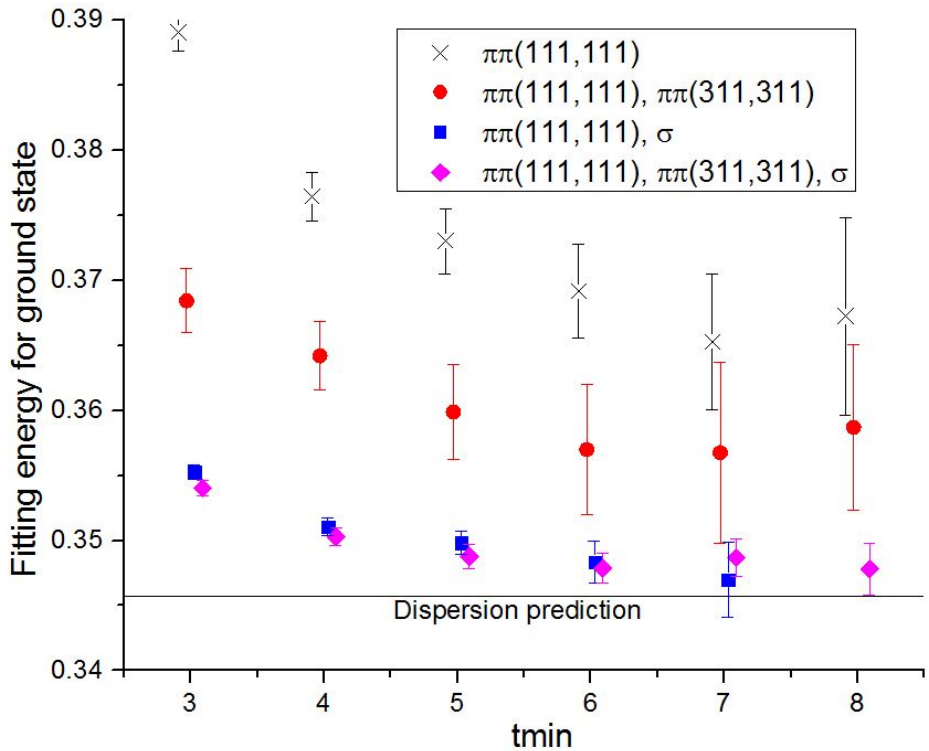
$$C_{ij}(t) = C + \sum_s A_{is} A_{js} (e^{-E_s t} + e^{-E_s (T-t)}) \quad (1)$$

Stationary $\pi\pi$ I=2

- Introducing the second operator slightly lowers the ground state energy, suggesting this operator only has a small effect in $\pi\pi_{I=2}$ case.
- There is a constant term describing the around the world effect. This term is significantly resolvable from 0 (about 60σ) therefore necessary in fitting. Without including this term significantly ruins p-value.
- All fitting has extremely good p-value (about 0.5).

Stationary $\pi\pi$ I=0

Three operators: S-wave $\pi\pi(111, 111)$, $\pi\pi(311, 311)$, σ



Correlated fit is performed with 1/2/3 operators and 1/2/3 states.
Fitting function is almost the same as stationary I=2, with the difference that we neglect the constant since it is statistically consistent with 0 from a fitting with it. That gives us better statistical error.

Stationary $\pi\pi$ I=0

- In stationary I=0, introducing the σ operator helps a lot in suppressing excited state error, $\pi\pi(311)$ operator is also good since it also suppresses the excited state error, but not as good as σ operator.
- Normalized overlap matrix also supports this argument

	state_0	state_1	state_2
$\pi\pi(111, 111)$	1.0(0.0)	0.47(2)	0.31(7)
σ	1.0(0.0)	-0.83(3)	-0.87(22)
$\pi\pi(311, 311)$	0.053(9)	-0.84(12)	1.0(0.0)

- We believe that with three (or only two) operator, we now have a good control of excited state contamination error with current level of statistics, since
  - The introduction of an extra somewhat useful operator doesn't improve the result.
  - Clear plateau
  - p-value of more than 0.3 suggests it is a good fit, with tmin$>$ 5.
- We will justify that later with recently developed technique of analysing systematic error.

Moving frame calculation

Intro

- We can recombine π operators with different momenta to do calculation with different CM momentum
- Three CM momenta: $(\pm 2, 0, 0)\pi/L$, $(\pm 2, \pm 2, 0)\pi/L$, $(\pm 2, \pm 2, \pm 2)\pi/L$ and their permutation.
- Three operators: $\pi\pi(111, 111)$, $\pi\pi(311, 311)$ and $\pi\pi(111, 311)$.
- Together with stationary case, it allows us to calculate phase shift at four different energies.
- Moving frame calculation is more vulnerable to excited state contamination error due to the denser spectrum of states.

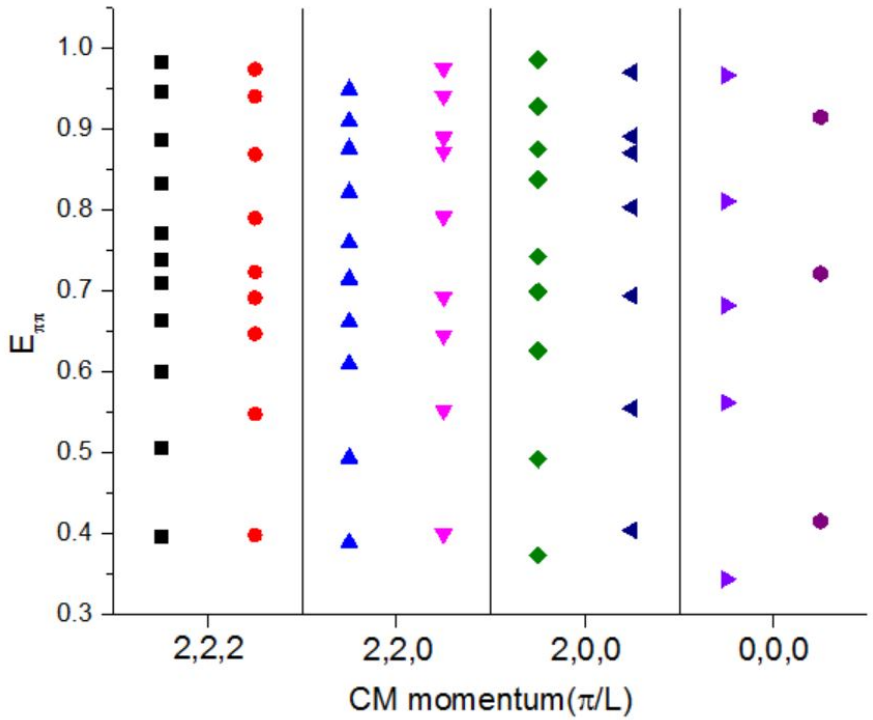


Figure: Spectrum of $\pi\pi$ state. Left: I=0; Right: I=2

Moving $\pi\pi$ I=2

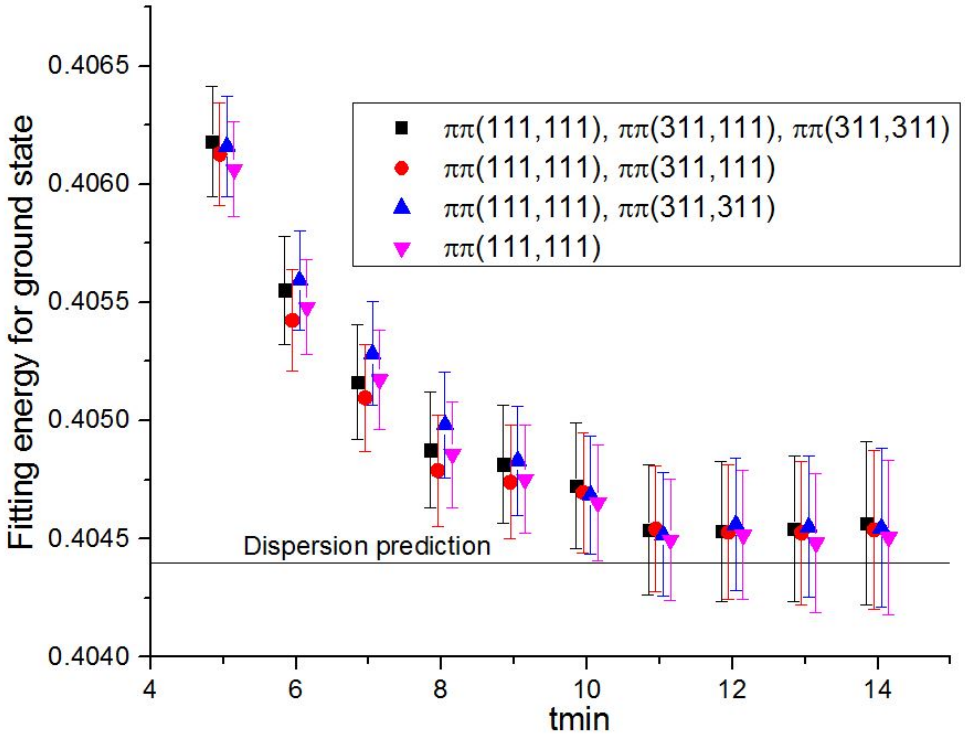


Figure: Moving $\pi\pi_{I=2}$ with CM momentum $(2,0,0)\frac{\pi}{L}$, fitting energy as a function of fitting tmin

Correlated fit is performed with 1/2/3 operators and 1/2/3 states so that number of states matches number of operators. Fitting function is the same as stationary I=2

Moving $\pi\pi$ I=2

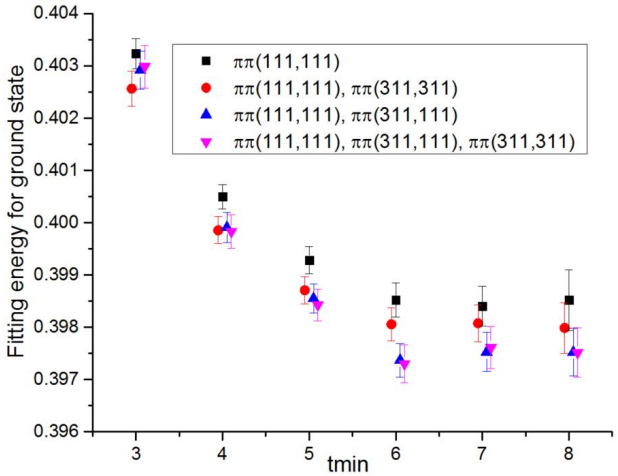
- Introducing the second and third operator has almost no effect in moving frame!

$P_{CM} = (0,0,0)$	state_0	state_1
op_0	1.0(0.0)	0.072(56)
op_1	-0.068(3)	1.0(0.0)

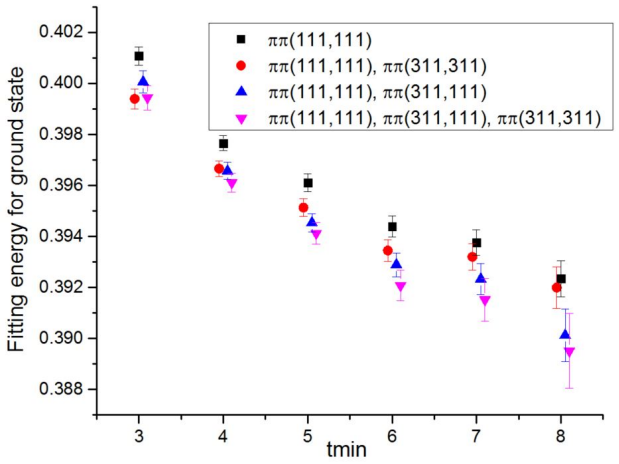
$P_{CM} = (2,0,0)$	state_0	state_1	state_2
op_0	1.0(0.0)	0.049(3)	0.037(8)
op_1	0.032(0.000)	1.0(0.0)	0.043(11)
op_2	0.00(0.00)	0.069(2)	1.0(0.0)

- Overlap matrix is more diagonal than stationary case, which suggests our current choice of extra operators give us little information about the excited state that couples to ground state operator, which is possibly the fourth state.
- Constant term is significantly resolvable from 0 (about 60σ) therefore necessary in fitting, just like stationary I=2 case.
- The results of other two CM momentum shows similar behavior.
- All fitting has extremely good p-value (about 0.5).

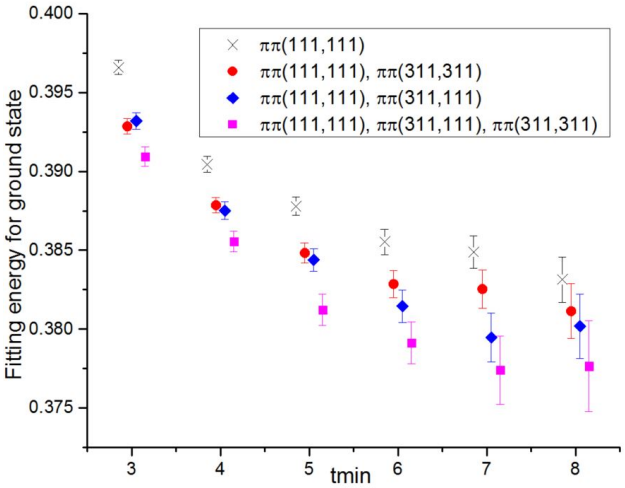
Moving $\pi\pi$ I=0



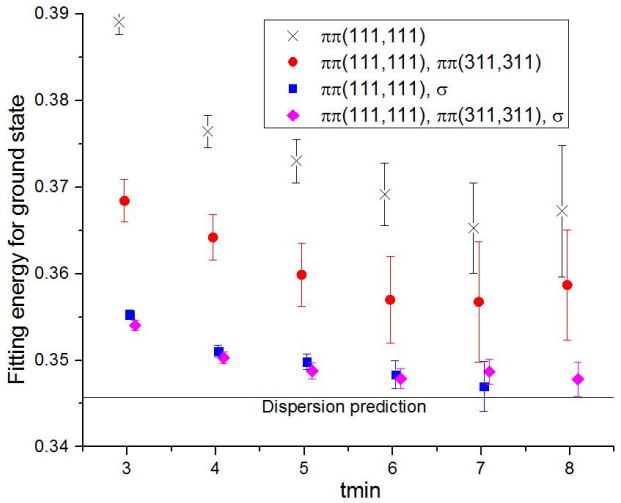
(a) Moving $\pi\pi_{I=2}$ with CM momentum $(2,2,2)\frac{\pi}{L}$



(b) Moving $\pi\pi_{I=2}$ with CM momentum $(2,2,0)\frac{\pi}{L}$



(c) Moving $\pi\pi_{I=2}$ with CM momentum $(2,0,0)\frac{\pi}{L}$



(d) Stationary $\pi\pi_{I=2}$ with CM momentum $(0,0,0)\frac{\pi}{L}$

Moving $\pi\pi$ I=0

- In moving I=0, introducing the second and third operator lowers the energy by roughly 1.5σ, which has smaller effect comparing with stationary I=0, suggesting there might be observable excited state contamination error.
- The overlap matrix of moving cases are all highly diagonal, and as CM momentum goes down (more similar to stationary case), the overlap matrix becomes less diagonal

$P_{CM} = (2,2,2)$	state_0	state_1	state_2
$\pi\pi(111,111)$	1.0(0.0)	-0.07(1)	-0.035(8)
$\pi\pi(111,311)$	-0.013(6)	1.0(0.0)	-0.19(5)
$\pi\pi(311,311)$	-0.015(2)	0.05(2)	1.0(0.0)

$P_{CM} = (2,2,0)$	state_0	state_1	state_2
$\pi\pi(111,111)$	1.0(0.0)	-0.16(2)	-0.080(6)
$\pi\pi(111,311)$	0.017(8)	1.0(0.0)	-0.19(4)
$\pi\pi(311,311)$	-0.008(3)	0.05(2)	1.0(0.0)

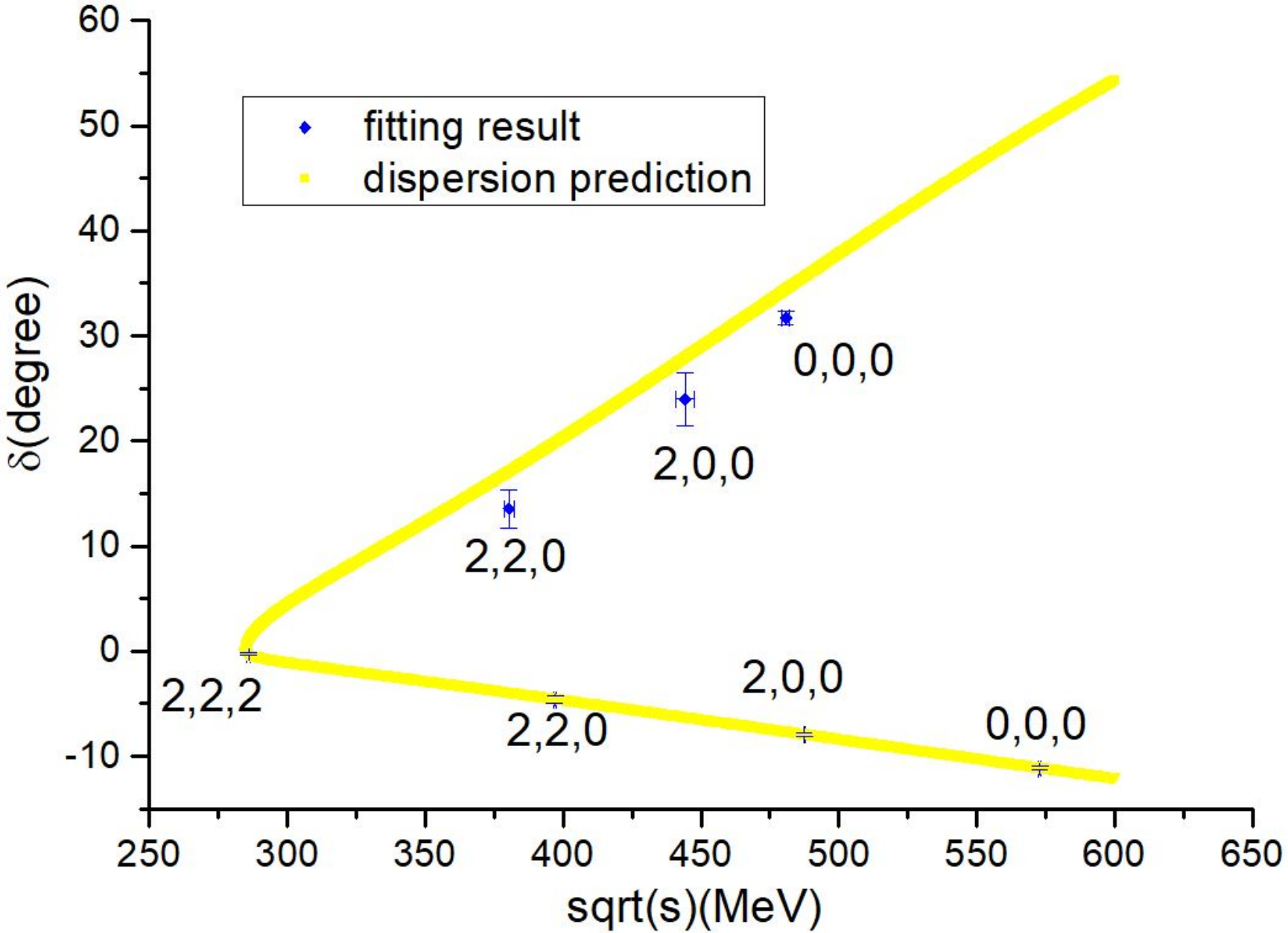
$P_{CM} = (2,0,0)$	state_0	state_1	state_2
$\pi\pi(111,111)$	1.0(0.0)	-0.31(5)	0.14(2)
$\pi\pi(111,311)$	0.09(2)	1.0(0.0)	-0.30(20)
$\pi\pi(311,311)$	0.01(1)	0.09(5)	1.0(0.0)

$P_{CM} = (0,0,0)$	state_0	state_1	state_2
$\pi\pi(111,111)$	1.0(0.0)	0.47(2)	0.31(7)
$\pi\pi(311,311)$	0.053(9)	-0.84(12)	1.0(0.0)
σ	1.0(0.0)	-0.83(3)	-0.87(22)

Summary of multiple operators

- Extra states and operators significantly increase the number of fitting parameter: from 3(2) to 9(6) to 18(12).
- Multiple operators are not always helpful, for example multiple operators in moving frame with large CM momentum are not as useful as they are in stationary case.
- Choose operator carefully. One reason multiple operators are helpful in stationary I=0 is because we introduce the σ operator.
- Sometimes multiple operators might make fitting less stable. For example the size of covariance matrix in moving frame calculation can be 6 times bigger than single operator.

Summary of multiple operators



Systematic error

Possible source of systematic error:

- Finite lattice spacing error
- Finite volume effect
- Excited state contamination

Due to the small off-diagonal terms in overlap matrix, there could be large excited state contamination remains for state which mainly couples to one operator.

Develop a new technique to estimate the error of third kind.

Excited state contamination error

Step 1: Fit our data to the initial model (e.g. 3 states model).
Step 2: Fit $\pi\pi(111, 111)$ data to a model where an extra state (e.g. 4th state) is included, we freeze the energy of that extra state based on some model (e.g. from dispersion prediction), and also the parameter related to other excited state based on initial fit.
Step 3: The jackknife difference between step 2 and step 1 can be viewed as systematic error from excited state contamination.

Only including systematic error from excited state contamination, we have results for 3ops in stationary $\pi\pi_{I=0}$

$$\delta_0 = 31.7(0.6)(0.1)^\circ(741 confs, 3 ops) \tag{2}$$

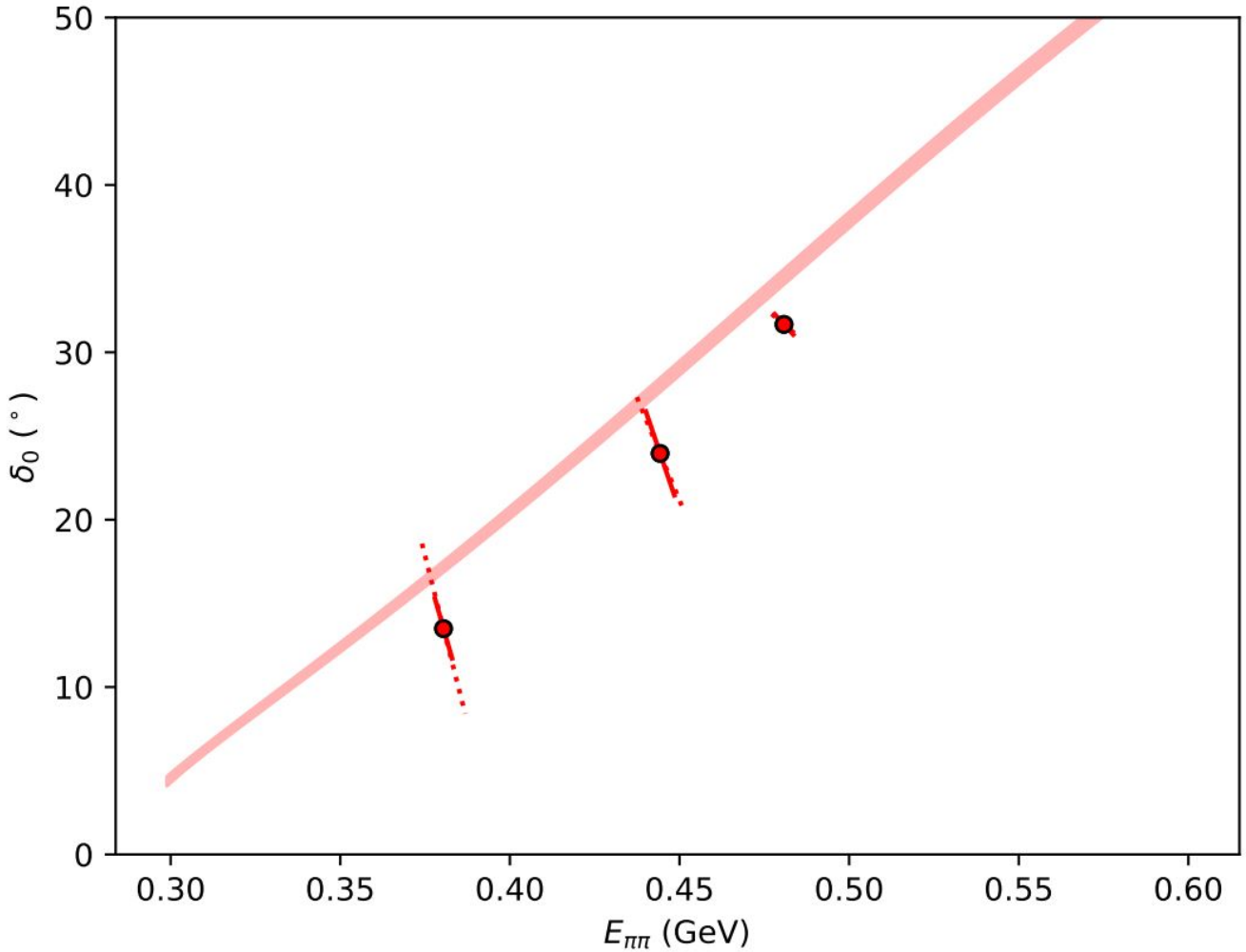
We can also use this technique to update systematic error of $\pi\pi_{I=0}$ phase shift with old, single operator data

$$\delta_0 = 19.1(2.5)(1.2)^\circ \textit{(1386 confs, old sys error)} \tag{3}$$
$$= 19.1(2.5)(6.8)^\circ \textit{(1386 confs, new sys error, one extra state)} \tag{4}$$
$$\approx 34^\circ(\textit{Dispersion}) \tag{5}$$

We hugely under estimate the systematic error in 2015 PRL when we have a single operator.

Excited state contamination error

After including systematic error from excited state contamination, our results in moving frame are now consistent with dispersion predictions.



We can do the same thing for I=2, but the results suggests that in that case, this systematic error are very small so that can be neglected.

Conclusion

What do we get:

- A solid stationary $\pi\pi_{I=0}$ phase shift is obtained.
- Extra operators plays a large role in reducing the excited state contamination error in stationary $\pi\pi_{I=0}$ calculation, but offer less advantage in other cases. A more thorough investigation of other operators may yield better choices that couples more strongly with the states of interest.
- A new technique of analysing remaining excited state contamination error.

Outlook:

- Adding moving σ operators into moving frame calculation.
- Finish k$\rightarrow \pi\pi$ calculation with k$\rightarrow \sigma$ diagrams included (cf Chris Kelly, Wednesday).