

Handling complicated Wick contractions in lattice QCD

– $K \rightarrow \pi\pi$ part 3 –

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BNL HET Lunch Seminar

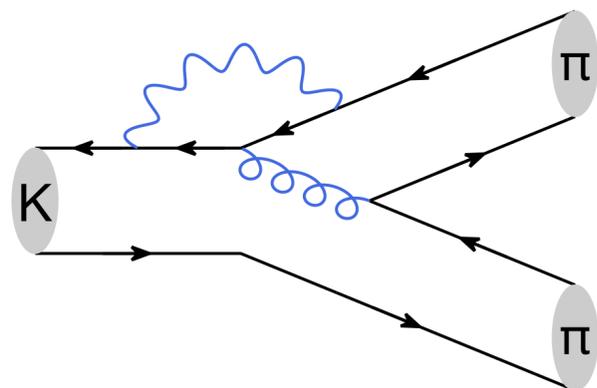
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$K \rightarrow \pi\pi$ & CP violation

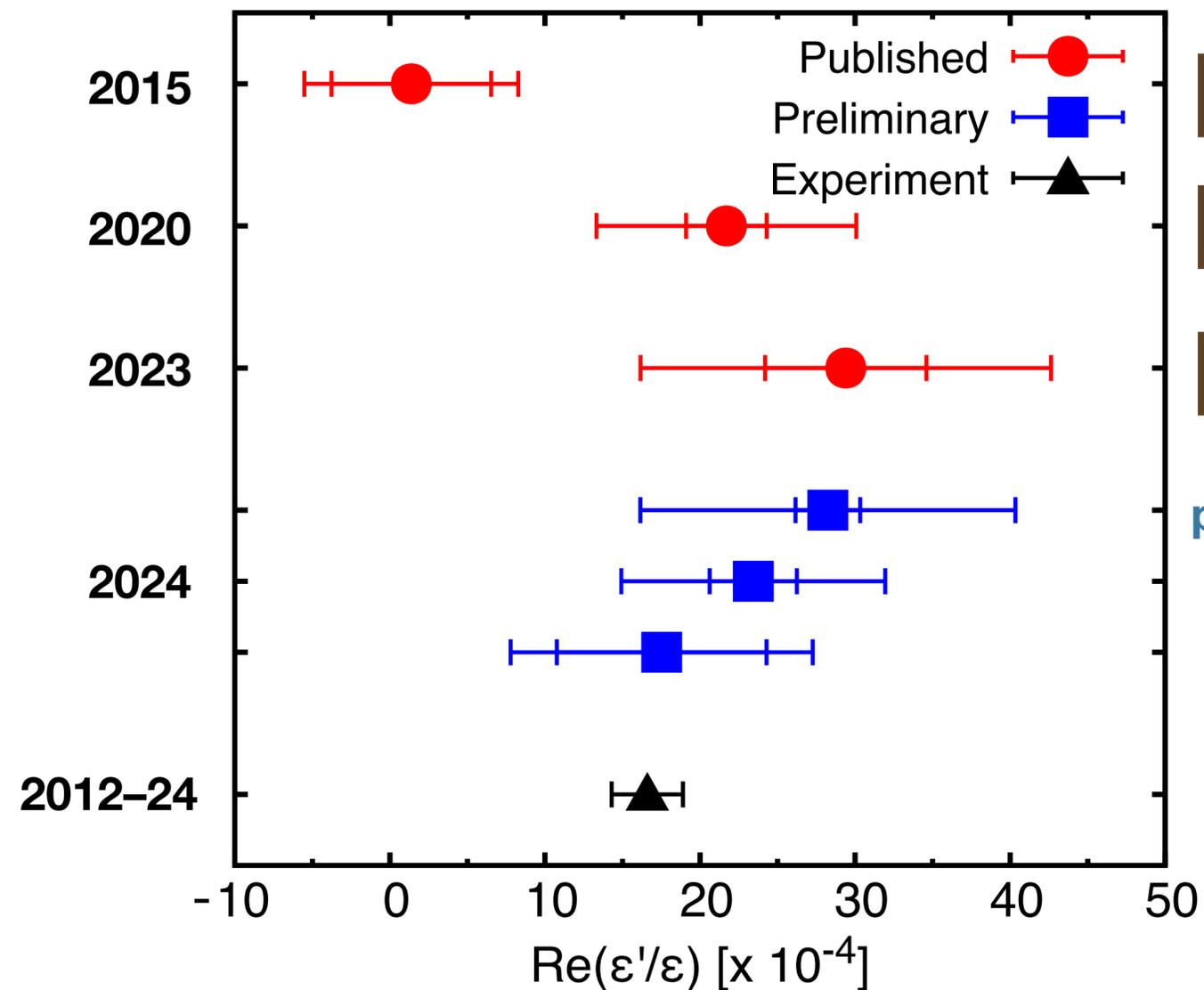
$$|K_L\rangle = |K_2\rangle + \varepsilon |K_1\rangle$$

CP odd $|K_2\rangle$ and CP even $|K_1\rangle$ are combined to form $|K_L\rangle$.
 The transition to $|\pi\pi\rangle$ (CP even) is dominated by $|K_1\rangle$ (indirect CPV, ε) and $|K_2\rangle$ (direct CPV, ε').

$$\frac{\Gamma(K_L \rightarrow \pi^0\pi^0)}{\Gamma(K_S \rightarrow \pi^0\pi^0)} \bigg/ \frac{\Gamma(K_L \rightarrow \pi^+\pi^-)}{\Gamma(K_S \rightarrow \pi^+\pi^-)} = 1 - 6\text{Re}(\varepsilon'/\varepsilon)$$



RBC/UKQCD vs Experiment



Challenges

- **Operator mixing**

- ◆ 10 four-quark operators
- ◆ desired to prevent extra mixing
- ◆ chiral symmetry with domain wall fermions preferable

- **On-shell kinematics in euclidean space**

- ◆ final two-pion state with $E = m_K \approx 500 \text{ MeV}$ needed

- **Computational cost/
Statistics**

- ◆ disconnected diagrams

- **Charm-loop effects**

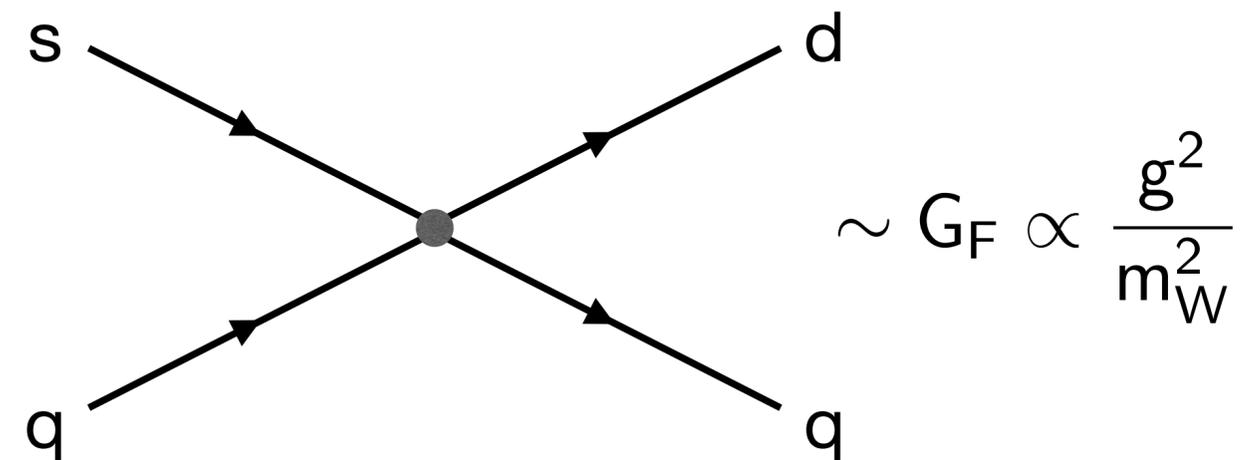
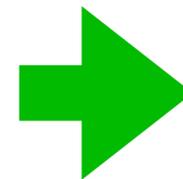
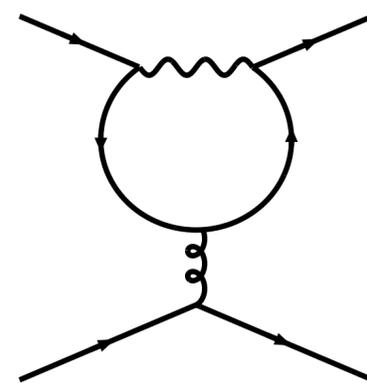
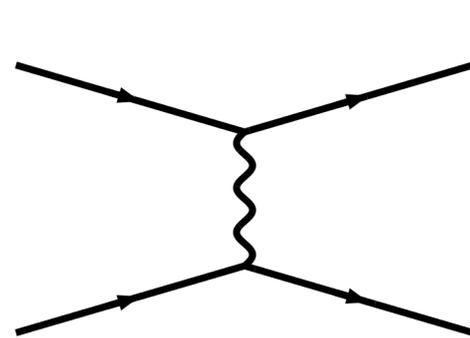
- ◆ expected significant
- ◆ lattices still not fine enough to introduce charm with physical m_π

- **Overall complexity**

- ◆ requires significant human time & effort

Approach to weak matrix elements

- Two typical scales
 - Electroweak scale: $m_W = 80 \text{ GeV}$, $m_Z = 91 \text{ GeV}$
 - QCD scale: $\Lambda_{\text{QCD}} \sim 300 \text{ MeV}$
- Low-energy effective interactions @ QCD scale



▸ $H_W = \sum_i \underline{c_i(\mu)} \underline{O_i(\mu)}$

Wilson coefficients **Effective operators**

$\Delta S = 1$ effective operators

- $(\bar{s}q)_{V-A}(\bar{q}'q'')_{V\pm A} = \bar{s}\gamma_\mu(1 - \gamma_5)q' \cdot \bar{q}'\gamma_\mu(1 \pm \gamma_5)q''$
- α, β : color indices

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

$$Q_2 = (\bar{s}u)_{V-A} (\bar{u}d)_{V-A} ,$$

$$Q_3 = (\bar{s}d)_{V-A} \sum_q (\bar{q}q)_{V-A} ,$$

$$Q_4 = (\bar{s}_\alpha d_\beta)_{V-A} \sum_q (\bar{q}_\beta q_\alpha)_{V-A} ,$$

$$Q_5 = (\bar{s}d)_{V-A} \sum_q (\bar{q}q)_{V+A} ,$$

$$Q_6 = (\bar{s}_\alpha d_\beta)_{V-A} \sum_q (\bar{q}_\beta q_\alpha)_{V+A} ,$$

$$Q_7 = \frac{3}{2} (\bar{s}d)_{V-A} \sum_q e_q (\bar{q}q)_{V+A} ,$$

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

$$Q_9 = \frac{3}{2} (\bar{s}d)_{V-A} \sum_q e_q (\bar{q}q)_{V-A} ,$$

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

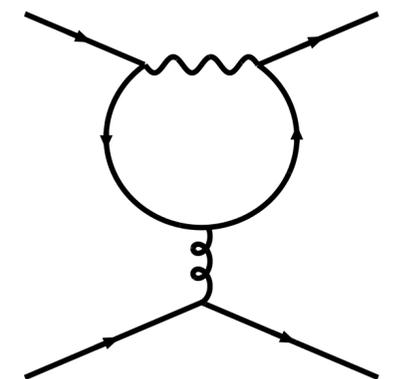
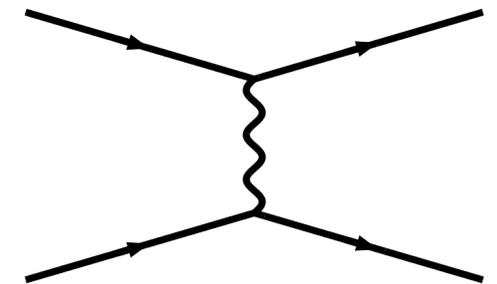
Current-current operators

- $Q_1^c = (\bar{s}_\alpha c_\beta)_{V-A} (\bar{c}_\beta d_\alpha)_{V-A}$ & $Q_2^c = (\bar{s}c)_{V-A} (\bar{c}d)_{V-A}$
enter when $n_f \geq 4$

QCD penguin operators

- sum over q runs for all active quarks

EW penguin operators



$K \rightarrow \pi\pi$ Amplitude and ε'

$\pi\pi$ phase shifts at m_K

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

$$A_I = \frac{G}{\sqrt{2}} V_{us}^* V_{ud} \sum_i \frac{[z_i(\mu) + \tau y_i(\mu)] M_{I,i}(\mu)}{\text{Wilson coefs.}} \quad \text{pQCD}$$

$$M_{I,i}(\mu) = \lim_{a \rightarrow 0} \sum_j Z_{ij}(\mu, a) \left\langle (\pi\pi)_I \left| \underline{Q_j^{\text{lat}}(a)} \right| K \right\rangle$$

Bare Matrix elements
LQCD

$K \rightarrow \pi\pi$ Amplitude and ε'

$\pi\pi$ phase shifts at m_K

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

$$A_I = \frac{G}{\sqrt{2}} V_{us}^* V_{ud} \sum_i \underbrace{[z_i(\mu) + \tau y_i(\mu)]}_{\substack{\text{Wilson coefs.} \\ \text{pQCD}}} M_{I,i}(\mu)$$

$$M_{I,i}(\mu) = \lim_{a \rightarrow 0} \underbrace{\sum_j Z_{ij}(\mu, a)}_{\substack{\text{Renormalization} \\ \text{LQCD+pQCD} \\ \text{(my previous talk)}}} \underbrace{\left\langle (\pi\pi)_I \left| Q_j^{\text{lat}}(a) \right| K \right\rangle}_{\substack{\text{Bare Matrix elements} \\ \text{LQCD}}}$$

Outline

- Role of correlation functions (for calculation of bare matrix elements)
 - Basics and some complications for the $K \rightarrow \pi\pi$ case
- Basics of how to calculate correlation functions
- Handling complicated calculations – Automated Wick contractor
- Detailed strategy for $K \rightarrow \pi\pi$ calculation

Role of correlation functions for calculation of bare matrix elements

3pt function

want ME of this

$$\left\langle \underbrace{O_{\text{sink}}(t_1 + t_2)}_{\text{annihilates the final state}} \underbrace{Q(t_1)}_{\text{want ME of this}} \underbrace{O_{\text{src}}(0)}_{\text{generates the initial state}}^\dagger \right\rangle$$

source & sink operators usually projected to

- specific quantum numbers, e.g. isospin, parity, strangeness, ...
 - specific (total) spatial momentum
- exclude extra states that are out of interest

3pt function

$$\left\langle O_{\text{sink}}^{\varphi}(t_1 + t_2) Q(t_1) O_{\text{src}}^{\varphi'}(0)^{\dagger} \right\rangle$$

$$= \sum_{m,n} \left\langle 0 \left| O_{\text{sink}}^{\varphi} \right| E_m^{\varphi} \right\rangle \left\langle E_m^{\varphi} \left| Q \right| E_n^{\varphi'} \right\rangle \left\langle E_n^{\varphi'} \left| O_{\text{src}}^{\varphi'} \right| 0 \right\rangle e^{-E_m^{\varphi} t_2} e^{-E_n^{\varphi'} t_1}$$

**ME w ground
initial & final states**

large t_1 & t_2 \longrightarrow

$$\left\langle 0 \left| O_{\text{sink}}^{\varphi} \right| E_0^{\varphi} \right\rangle \left\langle E_0^{\varphi} \left| Q \right| E_0^{\varphi'} \right\rangle \left\langle E_0^{\varphi'} \left| O_{\text{src}}^{\varphi'} \right| 0 \right\rangle e^{-\underline{E_0^{\varphi}} t_2} e^{-\underline{E_0^{\varphi'}} t_1}$$

$\left\langle 0 \left| O_{\text{sink}}^{\varphi} \right| E_0^{\varphi} \right\rangle$ & E_0^{φ} obtained from 2pt function

$$\left\langle O_{\text{sink}}^{\varphi}(t) O_{\text{sink}}^{\varphi}(0)^{\dagger} \right\rangle \xrightarrow{\text{large } t} \left\langle 0 \left| O_{\text{sink}}^{\varphi} \right| E_0^{\varphi} \right\rangle \left\langle E_0^{\varphi} \left| O_{\text{sink}}^{\varphi} \right| 0 \right\rangle e^{-E_0^{\varphi} t}$$

$K \rightarrow \pi\pi$ case

$$\begin{aligned} & \langle O^{\pi\pi}(t_1 + t_2) Q_i(t_1) O_K(0)^\dagger \rangle \\ \rightarrow & \langle 0 | O^{\pi\pi} | E_0^{\pi\pi} \rangle \langle \underbrace{E_0^{\pi\pi} (\approx 2m_\pi)}_{\text{energy not conserved!}} | Q_i | m_K \rangle \langle m_K | O_K^\dagger | 0 \rangle e^{-E_0^{\pi\pi} t_2} e^{-m_K t_1} \end{aligned}$$

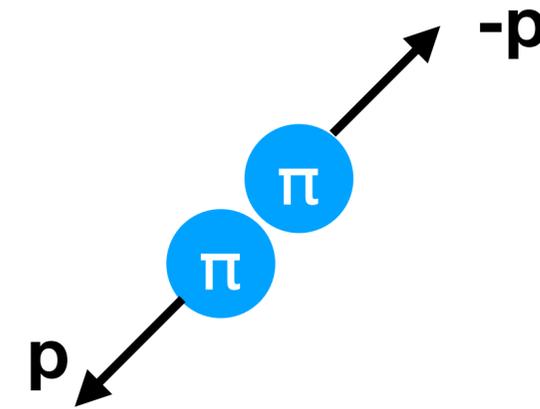
- Need a $\pi\pi$ state with back-to-back momentum
 - ▶ G-parity boundary conditions \rightarrow pions anti-periodic and must move in a finite box
 - ▶ Periodic boundary conditions with variational method (my earlier talk)
 - ▶ Moving frame also possible in a finite box (1 pion same mom as kaon)

Various $\pi\pi$ operators

- $\pi\pi$ -like operators

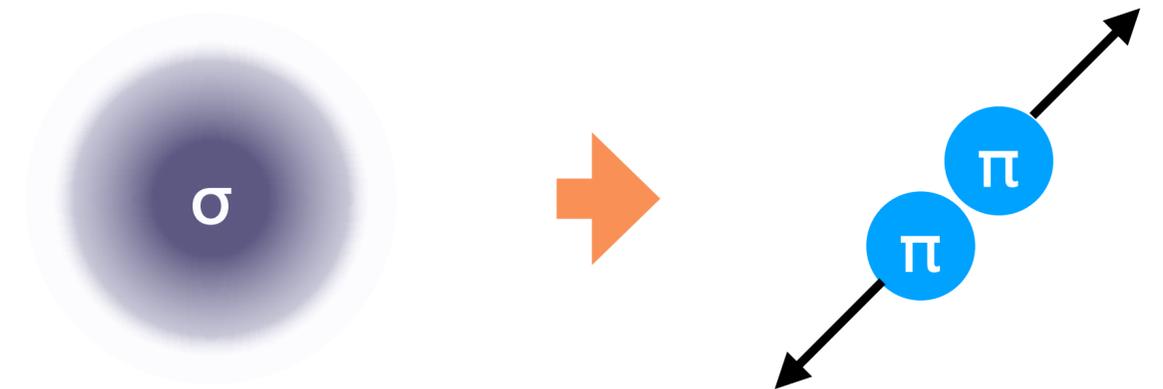
$$O^{\pi\pi}(\vec{p}) = \sum_{\vec{x}, \vec{y}} e^{i\vec{p}\cdot(\vec{x}-\vec{y})} O_{\pi}(\vec{x}, t) O_{\pi}(\vec{y}, t)$$

- ▶ $\vec{p} = \vec{0}$: couples well with ground state
- ▶ $\vec{p} = (0, 0, \frac{2\pi}{L}), (0, \frac{2\pi}{L}, \frac{2\pi}{L}), (\frac{2\pi}{L}, \frac{2\pi}{L}, \frac{2\pi}{L}) \dots$
control excited states



When isospin is 0:

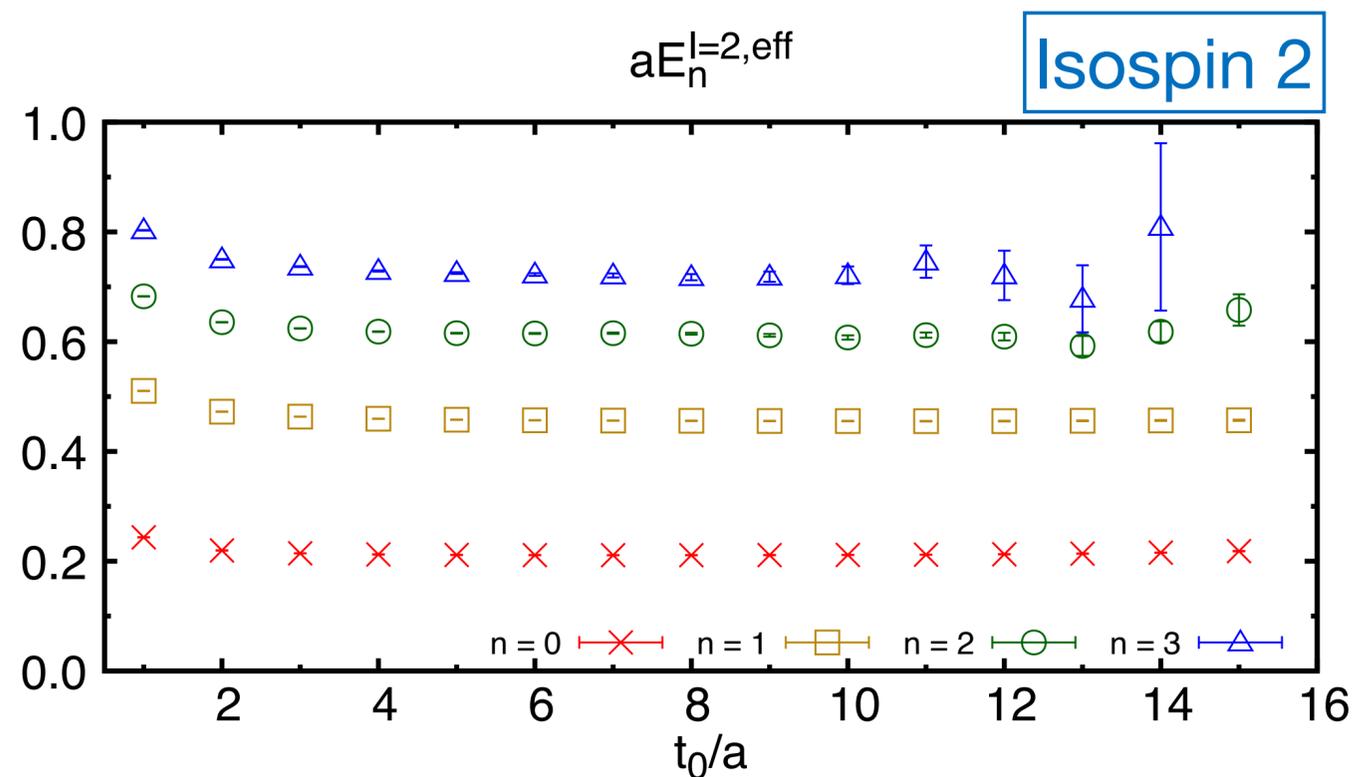
- σ -like operator to control $\pi\pi$ states near $f_0(500)$ resonance
- $$O_{\sigma} \sim \frac{\bar{u}u + \bar{d}d}{\sqrt{2}}$$



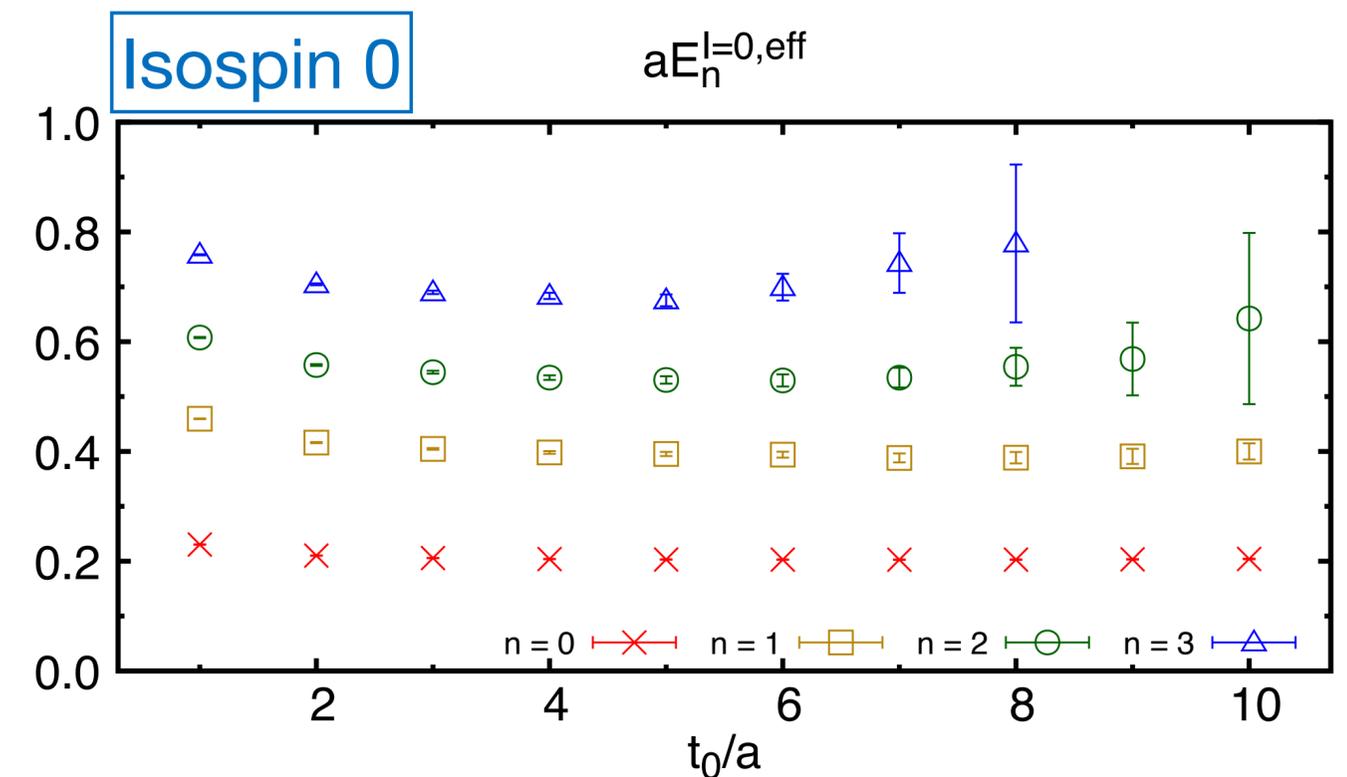
Variational method

$$C_{ab}(t) = \left\langle O_a(t) O_b(0)^\dagger \right\rangle : \text{matrix of correlation functions of } \pi\pi \text{ operators}$$

GEVP \longrightarrow $O_n = \sum_a v_{n,a} O_a$: couple mostly with the E_n state, not with other states



$\pi\pi$ energies
from GEVP



What to calculate

- Single Kaon 2pt function

$$\langle O_K(t) O_K(0)^\dagger \rangle \rightarrow \langle 0 | O_K | 0 \rangle \langle 0 | O_K^\dagger | 0 \rangle e^{-m_K t}$$

- $\pi\pi$ 2pt functions

$$\langle O_a^{\pi\pi}(t) O_b^{\pi\pi}(0)^\dagger \rangle \xrightarrow{\text{GEVP}} v_{n,a}, \langle 0 | O_n^{\pi\pi} | E_n^{\pi\pi} \rangle, E_n^{\pi\pi}$$

- $K \rightarrow \pi\pi$ 3pt functions

$$\langle O_a^{\pi\pi}(t_1 + t_2) Q_i(t_1) O_K(0)^\dagger \rangle$$

$$\xrightarrow[\text{large } t_1 \& t_2]{\sum_a v_{n,a} \times} \langle 0 | O_n^{\pi\pi} | E_n^{\pi\pi} \rangle \langle E_n^{\pi\pi} | Q_i | m_K \rangle \langle m_K | O_K^\dagger | 0 \rangle e^{-E_n^{\pi\pi} t_2} e^{-m_K t_1}$$

ME with $\pi\pi$ excited state

What to calculate

- Single Kaon 2pt function

$$\langle O_K(t) O_K(0)^\dagger \rangle \rightarrow \langle 0 | O_K | 0 \rangle \langle 0 | O_K^\dagger | 0 \rangle e^{-m_K t}$$

- $\pi\pi$ 2pt functions

$$\langle O_a^{\pi\pi}(t) O_b^{\pi\pi}(0)^\dagger \rangle \xrightarrow{\text{GEVP}} v_{n,a}, \langle 0 | O_n^{\pi\pi} | E_n^{\pi\pi} \rangle, E_n^{\pi\pi}$$

Today's topic
How to calculate these
correlation functions

- $K \rightarrow \pi\pi$ 3pt functions

$$\langle O_a^{\pi\pi}(t_1 + t_2) Q_i(t_1) O_K(0)^\dagger \rangle$$

$$\xrightarrow[\text{large } t_1 \& t_2]{\sum_a v_{n,a} \times} \langle 0 | O_n^{\pi\pi} | E_n^{\pi\pi} \rangle \langle E_n^{\pi\pi} | Q_i | m_K \rangle \langle m_K | O_K^\dagger | 0 \rangle e^{-E_n^{\pi\pi} t_2} e^{-m_K t_1}$$

ME with $\pi\pi$
excited state

Calculation of correlation functions

How to calculate correlation functions

- Ensemble average \rightarrow Monte Carlo method

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\bar{q} \mathcal{D}q \mathcal{D}U \mathcal{O}(\bar{q}, q, U) e^{-S(\bar{q}, q, U)} \quad \mathcal{O} = O_1(x_1) O_2(x_2) \dots O_n(x_n)$$

Wick contraction,
correlator with given
background gauge field

$$= \frac{1}{Z} \int \mathcal{D}U \underbrace{\hat{\mathcal{O}}(D(U)^{-1}, U)}_{\text{Boltzmann weight}} \underbrace{\det D(U) e^{-S_G(U)}}_{\text{Boltzmann weight}} \xrightarrow{\text{Monte Carlo sampling}} \frac{1}{N} \sum_{i=1}^N \hat{\mathcal{O}}(D(U_i)^{-1}, U_i)$$

Integrating out fermion fields

- Flow of computation
 - Ensemble generation : U_1, U_2, \dots, U_N based on the Boltzmann weight
 - Measurement: Calculate observable $\hat{\mathcal{O}}(D(U_i)^{-1}, U_i)$ for each configuration U_i **[today's topic]**
 - Statistical analysis

Measurements

$$\widehat{\mathcal{O}}(D(U_i)^{-1}, U_i) = \mathcal{O} \left(\frac{\partial}{\partial \theta}, \frac{\partial}{\partial \bar{\theta}}, U_i \right) \exp \left[-\bar{\theta} D(U_i)^{-1} \theta \right] \Big|_{\theta, \bar{\theta}=0}$$

- $\theta, \bar{\theta}$: Grassmann variables with spin, color, flavor and position indices

↑
space-time

- Example: 2pt function of π^+

$$O_1(x_1) = \bar{u}(x_1) i\gamma_5 d(x_1), \quad O_2(x_2) = O_1(x_2)^\dagger = \bar{d}(x_2) i\gamma_5 u(x_2)$$

$$\mathcal{O} = \bar{u}(x_1) i\gamma_5 d(x_1) \bar{d}(x_2) i\gamma_5 u(x_2)$$

$$\mathcal{O} \rightarrow \widehat{\mathcal{O}} : \quad \bar{u}(x_1) \rightarrow \frac{\partial}{\partial \theta_{(u,x_1)}} \quad d(x_1) \rightarrow \frac{\partial}{\partial \bar{\theta}_{(d,x_1)}} \quad \bar{d}(x_2) \rightarrow \frac{\partial}{\partial \theta_{(d,x_2)}} \quad u(x_2) \rightarrow \frac{\partial}{\partial \bar{\theta}_{(u,x_2)}}$$

$$\longrightarrow \widehat{\mathcal{O}}(D(U_i)^{-1}, U_i) = \frac{\partial}{\partial \theta_{(u,x_1)}} i\gamma_5 \frac{\partial}{\partial \bar{\theta}_{(d,x_1)}} \frac{\partial}{\partial \theta_{(d,x_2)}} i\gamma_5 \frac{\partial}{\partial \bar{\theta}_{(u,x_2)}} \exp \left[-\bar{\theta} D(U_i)^{-1} \theta \right] \Big|_{\theta, \bar{\theta}=0}$$

Hand exercise of π^+ 2pt func

$$\widehat{\mathcal{O}}(D(U_i)^{-1}, U_i) = \frac{\partial}{\partial \theta_{(u,x_1)}} i\gamma_5 \frac{\partial}{\partial \bar{\theta}_{(d,x_1)}} \frac{\partial}{\partial \theta_{(d,x_2)}} i\gamma_5 \frac{\partial}{\partial \bar{\theta}_{(u,x_2)}} \exp \left[-\bar{\theta} D(U_i)^{-1} \theta \right] \Big|_{\theta, \bar{\theta}=0}$$

$$= \frac{1}{2} \frac{\partial}{\partial \theta_{(u,x_1)}} i\gamma_5 \frac{\partial}{\partial \bar{\theta}_{(d,x_1)}} \frac{\partial}{\partial \theta_{(d,x_2)}} i\gamma_5 \frac{\partial}{\partial \bar{\theta}_{(u,x_2)}} \bar{\theta} D^{-1} \theta \cdot \bar{\theta} D^{-1} \theta$$

$$= \frac{\partial}{\partial \theta_{(u,x_1)}} i\gamma_5 \frac{\partial}{\partial \bar{\theta}_{(d,x_1)}} \frac{\partial}{\partial \theta_{(d,x_2)}} i\gamma_5 \bar{\delta}_{(u,x_2)} D^{-1} \theta \cdot \bar{\theta} D^{-1} \theta$$

$$\bar{\delta}_{(u,x_2)} = \frac{\partial \bar{\theta}}{\partial \bar{\theta}_{(u,x_2)}}$$

$$= \frac{\partial}{\partial \theta_{(u,x_1)}} i\gamma_5 \frac{\partial}{\partial \bar{\theta}_{(d,x_1)}} \frac{\partial}{\partial \theta_{(d,x_2)}} \bar{\theta} D^{-1} \theta \cdot i\gamma_5 \bar{\delta}_{(u,x_2)} D^{-1} \theta$$

$$= -\frac{\partial}{\partial \theta_{(u,x_1)}} i\gamma_5 \frac{\partial}{\partial \bar{\theta}_{(d,x_1)}} \bar{\theta} D^{-1} \delta_{(d,x_2)} \cdot i\gamma_5 \bar{\delta}_{(u,x_2)} D^{-1} \theta$$

$$= -\frac{\partial}{\partial \theta_{(u,x_1)}} i\gamma_5 \bar{\delta}_{(d,x_1)} D^{-1} \delta_{(d,x_2)} \cdot i\gamma_5 \bar{\delta}_{(u,x_2)} D^{-1} \theta$$

$$= -\text{Tr} \left[i\gamma_5 D_{(d,x_1),(d,x_2)}^{-1} i\gamma_5 D_{(u,x_2),(u,x_1)}^{-1} \right]$$

K^0 2pt func: $u \rightarrow s$
simplest example

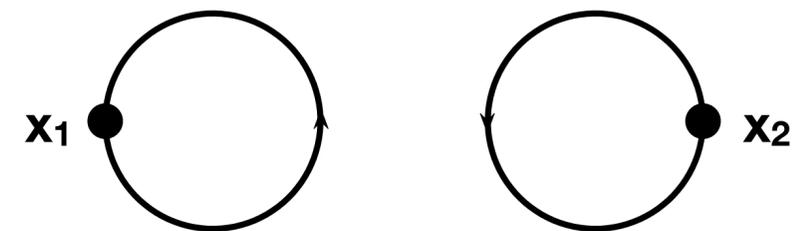
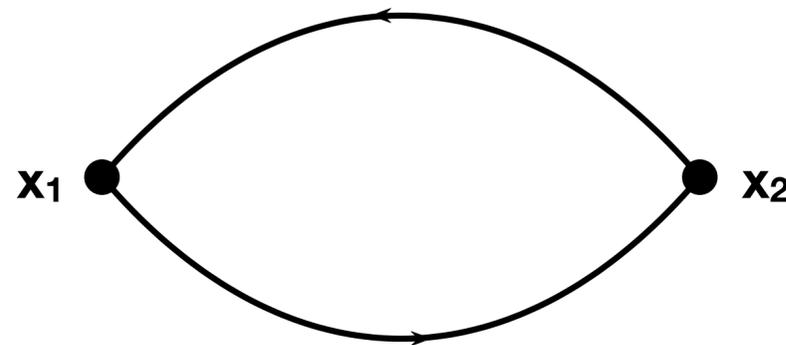
example 2: $\eta_{\text{SU}(2)}$

- source & sink operators

$$O_1(x_1) = \frac{\bar{q}(x_1)i\gamma_5 q(x_1)}{\sqrt{2}} \left(= \frac{\bar{u}(x_1)i\gamma_5 u(x_1) + \bar{d}(x_1)i\gamma_5 d(x_1)}{\sqrt{2}} \right), \quad O_2(x_2) = O_1(x_2)^\dagger = \frac{\bar{q}(x_2)i\gamma_5 q(x_2)}{\sqrt{2}}$$

- contraction:

$$\text{Tr} \left[\gamma_5 D_{x_1, x_2}^{-1} \gamma_5 D_{x_2, x_1}^{-1} \right] - \text{Tr} \left[\gamma_5 D_{x_1, x_1}^{-1} \right] \text{Tr} \left[\gamma_5 D_{x_2, x_2}^{-1} \right]$$



$\text{Tr} \left[\gamma_5 D_{x_1, x_2}^{-1} \gamma_5 D_{x_2, x_1}^{-1} \right]$: connected diagram

$\text{Tr} \left[\gamma_5 D_{x_1, x_1}^{-1} \right] \text{Tr} \left[\gamma_5 D_{x_2, x_2}^{-1} \right]$: disconnected diagram

**Automated Wick contractor for
more complicated correlators**

How should we obtain the contractions for $\pi\pi$ 2pt functions & $K \rightarrow \pi\pi$ 3pt functions and compute them?

$$\langle O^{\pi\pi}(x_1) O^{\pi\pi}(x_2)^\dagger \rangle$$

$$\langle O^{\pi\pi}(x_1) Q_i(x_2) O_K(x_3)^\dagger \rangle$$

$$\langle O^{\pi\pi}(x_1) O_\sigma(x_2)^\dagger \rangle$$

$$\langle O_\sigma(x_1) Q_i(x_2) O_K(x_3)^\dagger \rangle$$

$$O^{\pi\pi} = \begin{cases} \frac{\pi^+\pi^- + 2\pi^0\pi^0 + \pi^-\pi^+}{\sqrt{6}} & (I = 2, I_z = 0) \\ \frac{\pi^+\pi^- - \pi^0\pi^0 + \pi^-\pi^+}{\sqrt{3}} & (I = 0) \end{cases}$$

$$Q_{1,2} = \bar{s}_\alpha \gamma_\mu (1 - \gamma_5) u_{\beta/\alpha} \bar{u}_\beta \gamma_\mu (1 - \gamma_5) d_{\alpha/\beta}$$

$$Q_{3,4,5,6} = \bar{s}_\alpha \gamma_\mu (1 - \gamma_5) d_{\alpha/\beta} \sum_q \bar{q}_\beta \gamma_\mu (1 \pm \gamma_5) q_{\beta/\alpha}$$

$$Q_{7,8,9,10} = \bar{s}_\alpha \gamma_\mu (1 - \gamma_5) d_{\alpha/\beta} \sum_q e_q \bar{q}_\beta \gamma_\mu (1 \pm \gamma_5) q_{\beta/\alpha}$$

done in earlier works but ...

PRD84,114503(2011)

$$A_{0,1}(t_\pi, t_{\text{op}}, t_K) = i \frac{1}{\sqrt{3}} \{-\textcircled{1} - 2 \cdot \textcircled{5} + 3 \cdot \textcircled{9} + 3 \cdot \textcircled{17} - 3 \cdot \textcircled{33}\}$$

$$A_{0,2}(t_\pi, t_{\text{op}}, t_K) = i \frac{1}{\sqrt{3}} \{-\textcircled{2} - 2 \cdot \textcircled{6} + 3 \cdot \textcircled{10} + 3 \cdot \textcircled{18} - 3 \cdot \textcircled{34}\}$$

$$A_{0,3}(t_\pi, t_{\text{op}}, t_K) = i\sqrt{3} \{-\textcircled{5} + 2 \cdot \textcircled{9} - \textcircled{13} + 2 \cdot \textcircled{17} + \textcircled{21} - \textcircled{25} - \textcircled{29} - 2 \cdot \textcircled{33} - \textcircled{37} + \textcircled{41} + \textcircled{45}\}$$

$$A_{0,4}(t_\pi, t_{\text{op}}, t_K) = i\sqrt{3} \{-\textcircled{6} + 2 \cdot \textcircled{10} - \textcircled{14} + 2 \cdot \textcircled{18} + \textcircled{22} - \textcircled{26} - \textcircled{30} - 2 \cdot \textcircled{34} - \textcircled{38} + \textcircled{42} + \textcircled{46}\}$$

$$A_{0,5}(t_\pi, t_{\text{op}}, t_K) = i\sqrt{3} \{-\textcircled{7} + 2 \cdot \textcircled{11} - \textcircled{15} + 2 \cdot \textcircled{19} + \textcircled{23} - \textcircled{27} - \textcircled{31} - 2 \cdot \textcircled{35} - \textcircled{39} + \textcircled{43} + \textcircled{47}\}$$

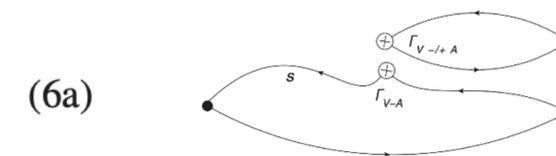
$$A_{0,6}(t_\pi, t_{\text{op}}, t_K) = i\sqrt{3} \{-\textcircled{8} + 2 \cdot \textcircled{12} - \textcircled{16} + 2 \cdot \textcircled{20} + \textcircled{24} - \textcircled{28} - \textcircled{32} - 2 \cdot \textcircled{32} - \textcircled{40} + \textcircled{44} + \textcircled{48}\}$$

$$A_{0,7}(t_\pi, t_{\text{op}}, t_K) = i \frac{\sqrt{3}}{2} \{-\textcircled{3} - \textcircled{7} + \textcircled{11} + \textcircled{15} + \textcircled{19} - \textcircled{23} + \textcircled{27} + \textcircled{31} - \textcircled{35} + \textcircled{39} - \textcircled{43} - \textcircled{47}\}$$

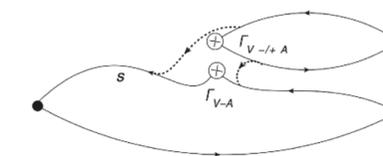
$$A_{0,8}(t_\pi, t_{\text{op}}, t_K) = i \frac{\sqrt{3}}{2} \{-\textcircled{4} - \textcircled{8} + \textcircled{12} + \textcircled{16} + \textcircled{20} - \textcircled{24} + \textcircled{28} + \textcircled{38} - \textcircled{32} + \textcircled{40} - \textcircled{44} - \textcircled{48}\}$$

$$A_{0,9}(t_\pi, t_{\text{op}}, t_K) = i \frac{\sqrt{3}}{2} \{-\textcircled{1} - \textcircled{5} + \textcircled{9} + \textcircled{13} + -\textcircled{21} + \textcircled{25} + \textcircled{29} - \textcircled{33} + \textcircled{37} - \textcircled{41} - \textcircled{45}\}$$

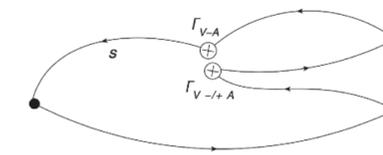
$$A_{0,10}(t_\pi, t_{\text{op}}, t_K) = i \frac{\sqrt{3}}{2} \{-\textcircled{2} - \textcircled{6} + \textcircled{10} + \textcircled{14} + \textcircled{18} - \textcircled{22} + \textcircled{26} + \textcircled{30} - \textcircled{34} + \textcircled{38} - \textcircled{42} - \textcircled{46}\},$$



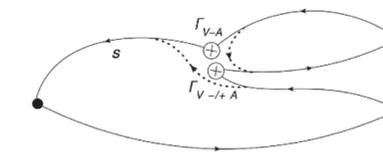
(6a)



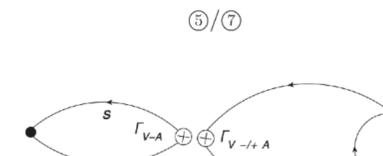
(6b)



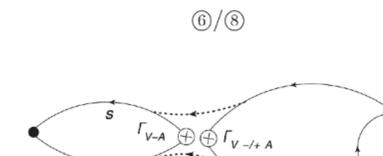
(6c)



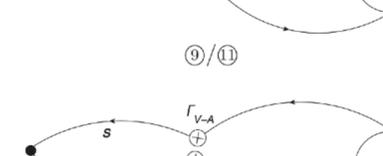
(6d)



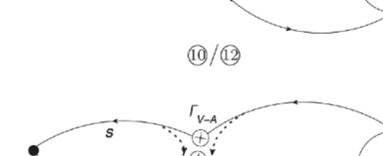
(6e)



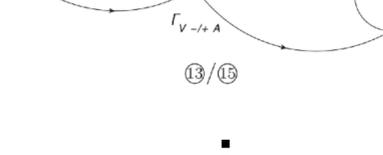
(6f)



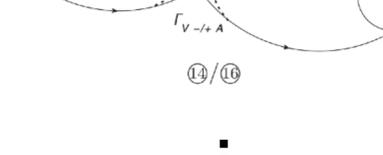
(6g)



(6h)



(6i)



(6j)

⋮

⋮

48 contractions

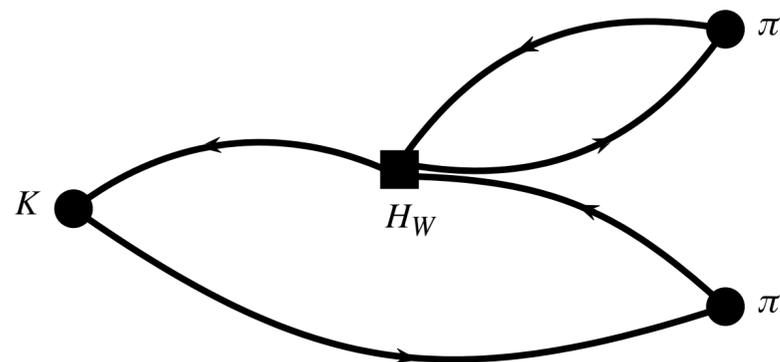
- easy to make typos in hand coding (just as the PRD proofreader did)
- another headache to ensure about normalization
- $K \rightarrow \sigma$ contraction only in GPBC work (where contractions slightly differ)

Automated Wick contractor

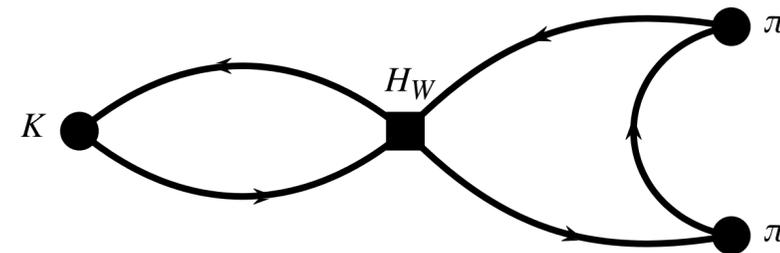
- Input: a set of operators
- Output: Wick contractions for the correlation function of the given operators

Automated Wick contractor

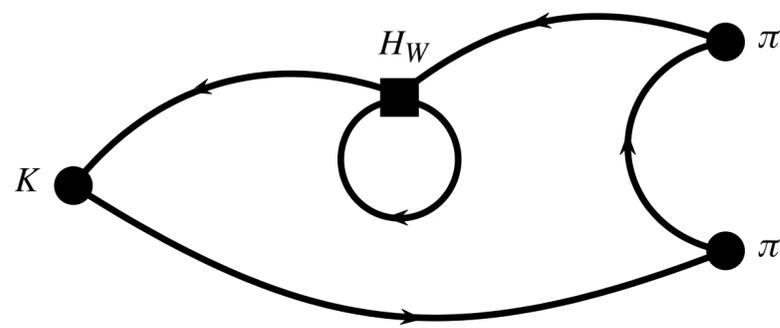
- Input: a set of operators
- Output: Wick contractions for the correlation function of the given operators



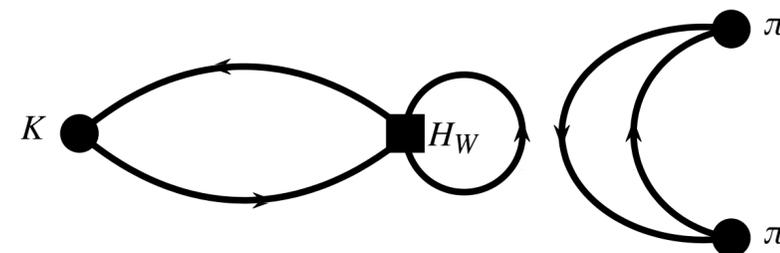
type 1



type 2



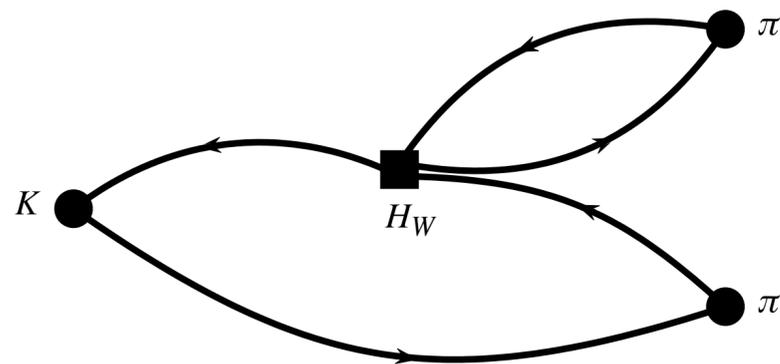
type 3



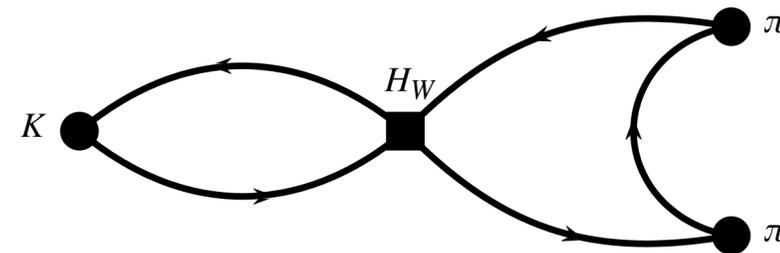
type 4

Automated Wick contractor

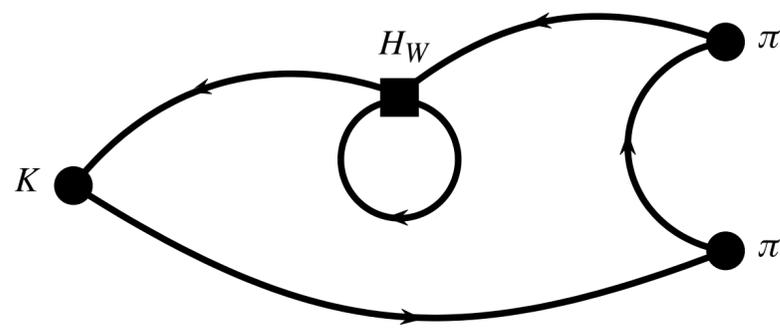
- Input: a set of operators
- Output: Wick contractions for the correlation function of the given operators



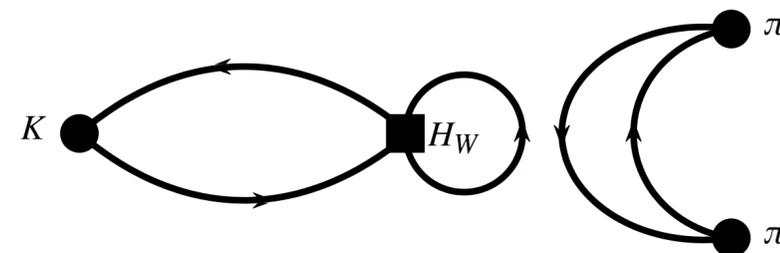
type 1



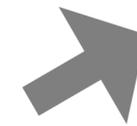
type 2



type 3



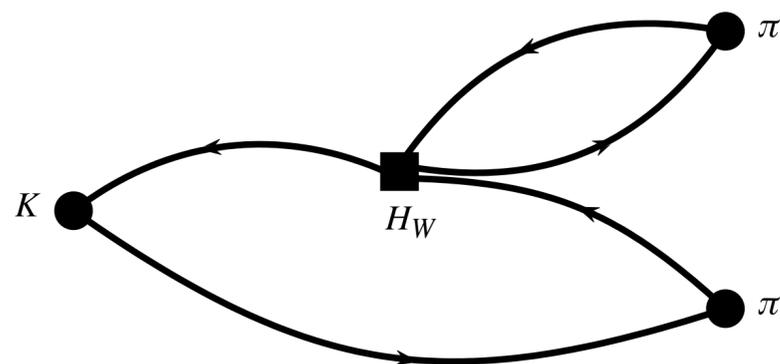
type 4



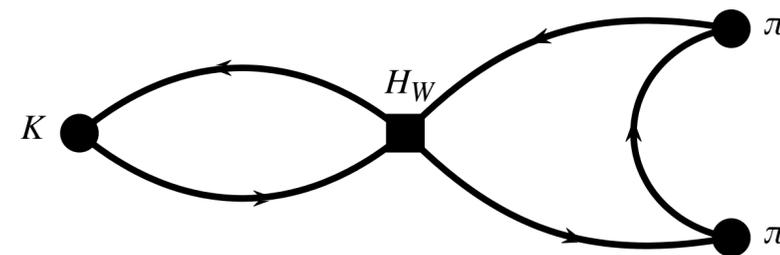
Let the script recognize these diagrams and rename contractions

Automated Wick contractor

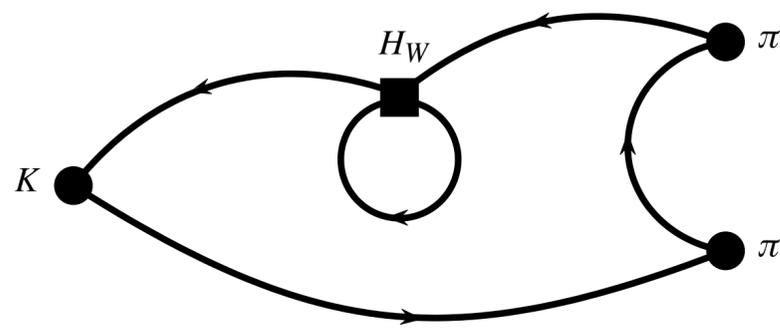
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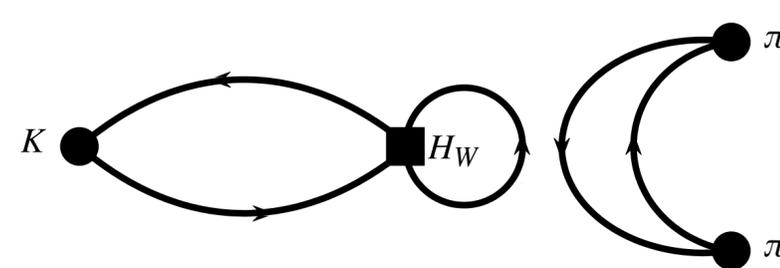
type 1



type 2



type 3



type 4

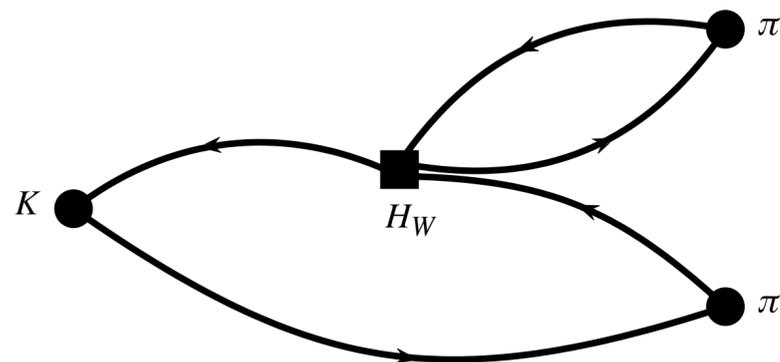
Let the script recognize these diagrams and rename contractions

```
-3/2 type1_singleTr_cmix_LR
+3 type2_multiTr_cmix_LR
-3/2 type2_singleTr_cmix_LR
+3 type3_lloop_multiTr_cmix_LR
-3/2 type3_lloop_singleTr_cmix_LR
+3/2 type3_sloop_multiTr_cmix_LR
-3/2 type3_sloop_singleTr_cmix_RL
-6 type4_lloop_multiTr_cmix_LR
+3 type4_lloop_singleTr_cmix_LR
-3 type4_sloop_multiTr_cmix_LR
+3 type4_sloop_singleTr_cmix_RL
```

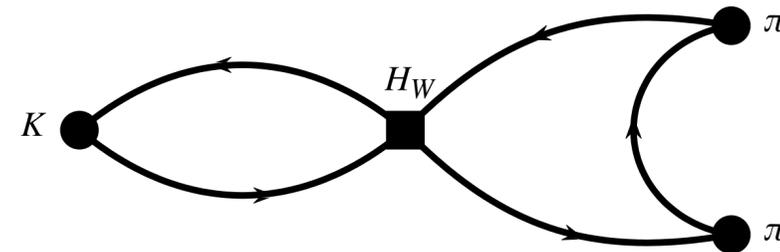
example: $\langle O^{\pi\pi, l=0}(x_1) Q_6(x_2) O_K(x_3)^\dagger \rangle$

Automated Wick contractor

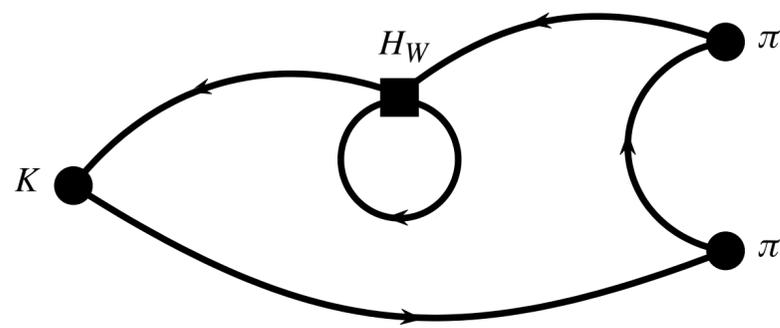
- Input: a set of operators
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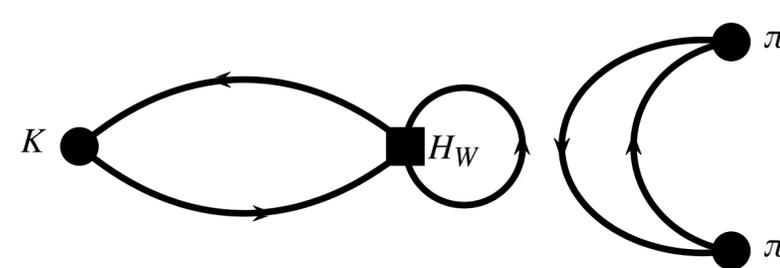
type 1



type 2



type 3



type 4

Let the script recognize these diagrams and rename contractions

```
-3/2 type1_singleTr_cmix_LR
+3 type2_multiTr_cmix_LR
-3/2 type2_singleTr_cmix_LR
+3 type3_lloop_multiTr_cmix_LR
-3/2 type3_lloop_singleTr_cmix_LR
+3/2 type3_sloop_multiTr_cmix_LR
-3/2 type3_sloop_singleTr_cmix_RL
-6 type4_lloop_multiTr_cmix_LR
+3 type4_lloop_singleTr_cmix_LR
-3 type4_sloop_multiTr_cmix_LR
+3 type4_sloop_singleTr_cmix_RL
```

example: $\langle O^{\pi\pi, l=0}(x_1) Q_6(x_2) O_K(x_3)^\dagger \rangle$

compute each contraction, and let analysis code do the linear combination

Summary so far and what's next

- We now know how to combine each contraction to calculate correlation functions
- Need to figure out
 - spatial momentum projection
 - how to precisely compute these momentum-projected contractions

Detailed strategy for $K \rightarrow \pi\pi$

Momentum projection

- Kaon operator: zero spatial momentum (rest frame)

$$O_K(t)^\dagger = \sum_{\vec{x}} \bar{d}(\vec{x}, t) i\gamma_5 s(\vec{x}, t) e^{i\vec{0}\cdot\vec{x}}$$

- $\pi\pi$ operators made with back-to-back momenta

$$O_{\vec{p}}^{\pi\pi, l}(t)^\dagger = \sum_{a,b} c_{ab}^l \sum_{\vec{p}' \in \hat{T}[\vec{p}]} \sum_{\vec{x}} e^{i\vec{p}'\cdot\vec{x}} \pi^a(\vec{x}, t) \sum_{\vec{y}} e^{-i\vec{p}'\cdot\vec{y}} \pi^b(\vec{y}, t + \Delta)$$

Sum over 3D cubic rotation: s-wave projection

Isospin projection taken into account by auto contractor

Momentum projection

- Kaon operator: zero spatial momentum (rest frame)

$$O_K(t)^\dagger = \sum_{\vec{x}} \bar{d}(\vec{x}, t) i\gamma_5 s(\vec{x}, t) e^{i\vec{0}\cdot\vec{x}}$$

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Sum over 3D cubic rotation: s-wave projection

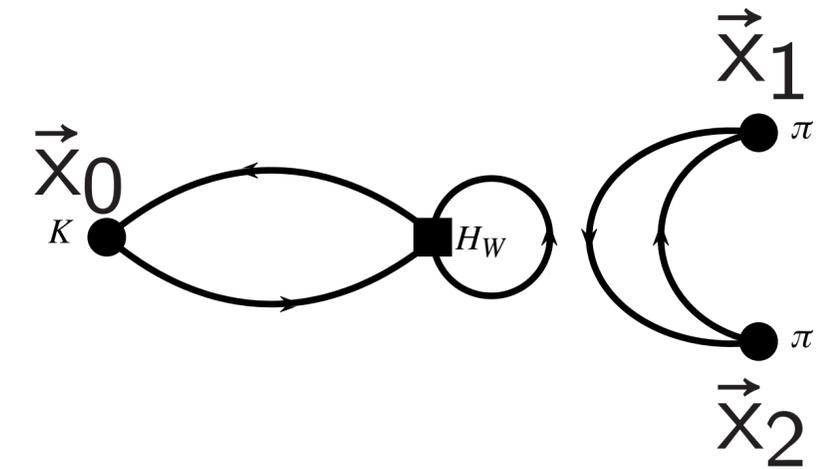
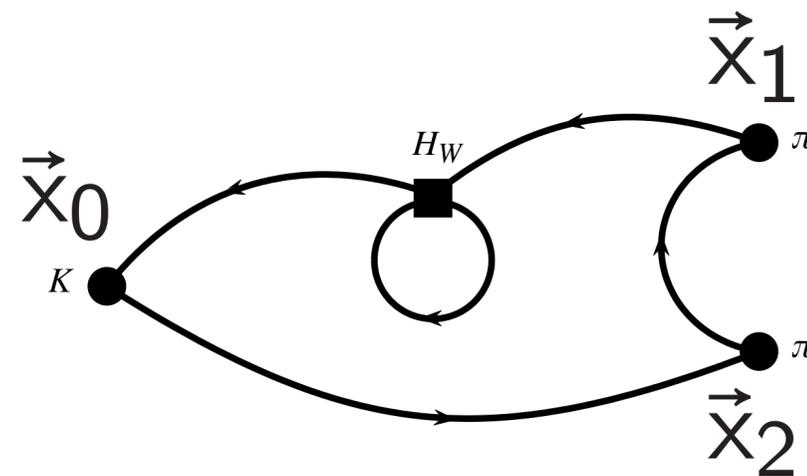
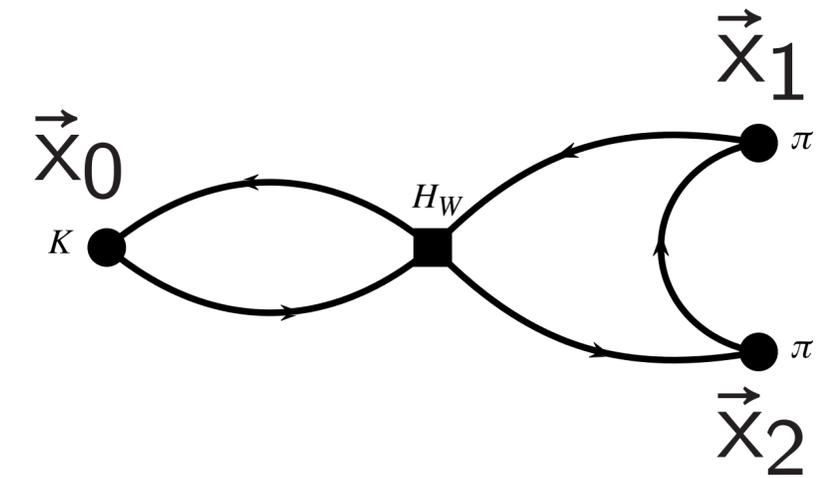
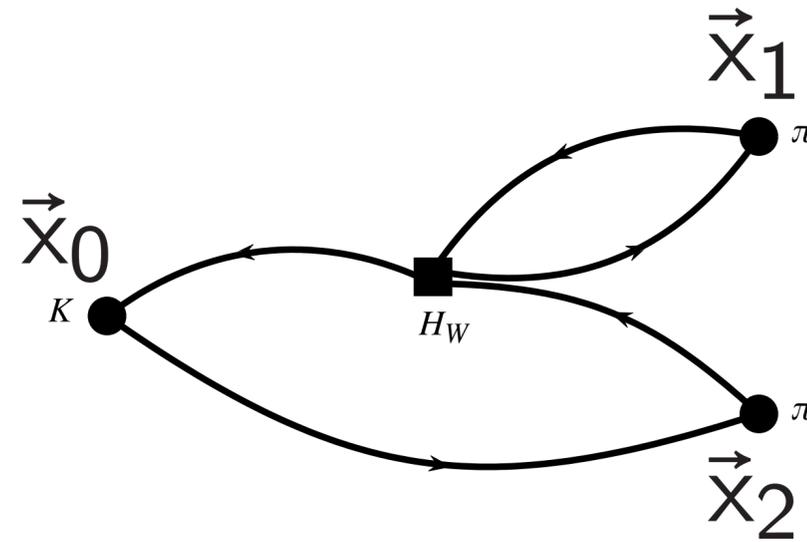
Isospin projection taken into account by auto contractor

presence of spatial sums

How contractions look

$$\sum_{\vec{x}_0} \sum_{\vec{x}_1} e^{i\vec{p}' \cdot \vec{x}_1} \sum_{\vec{x}_2} e^{-i\vec{p}' \cdot \vec{x}_2}$$

- minimal positional sums presumed
- adding other sums wrt translational invariance may help statistics



Disconnected diagram noisiest

$$S/N \left[\begin{array}{c} \text{Diagram} \end{array} \right] \sim e^{-E_n^{\pi\pi} t_2} / 1$$

$$S/N \text{ [other diagrams]} \sim e^{-E_n^{\pi\pi} t_2} / e^{-2m_\pi t_2}$$

- Natural thing to consider: maximize effective sampling
- In this work
 - averaging over all spacetime translations of H_W for disconnected diagram
 - don't need to sample other diagrams as many if it's expensive

Calculation of quark propagators

Lattice calculation of quark propagators

- Not possible to get the exact inverse of Dirac operator in large volumes
- What we can do: solve linear equations of Dirac operator

- ▶ point-source propagator

$$\sum_y D(x, y) X(y) = \delta_{x, x_0} \rightarrow X(x) = D^{-1}(x, x_0)$$

spin, color (and flavor)
indices suppressed

- ▶ momentum-source propagator

$$\sum_y D(x, y) X(y) = e^{i\mathbf{p}\cdot\mathbf{x}} \rightarrow X(x) = \sum_y e^{i\mathbf{p}\cdot\mathbf{y}} D^{-1}(x, y)$$

4D momentum

$$\sum_y D(x, y) X(y) = e^{i\vec{\mathbf{p}}\cdot\vec{\mathbf{x}}} \delta_{x_4, t_0} \rightarrow X(x) = \sum_{\vec{y}} e^{i\vec{\mathbf{p}}\cdot\vec{y}} D^{-1}(x, (\vec{y}, t_0))$$

3D momentum

Lattice calculation of quark propagators

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- What we can do: solve linear equations of Dirac operator

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$$\sum_y D(x, y) X(y) = \delta_{x, x_0} \rightarrow X(x) = D^{-1}(x, x_0)$$

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$$\sum_y D(x, y) X(y) = e^{i\mathbf{p}\cdot\mathbf{x}} \rightarrow X(x) = \sum_y e^{i\mathbf{p}\cdot\mathbf{y}} D^{-1}(x, y)$$

4D momentum

$$\sum_y D(x, y) X(y) = e^{i\vec{\mathbf{p}}\cdot\vec{\mathbf{x}}} \delta_{x_4, t_0} \rightarrow X(x) = \sum_{\vec{y}} e^{i\vec{\mathbf{p}}\cdot\vec{y}} D^{-1}(x, (\vec{y}, t_0))$$

3D momentum

These were considered unrealistic for the disconnected diagram

all-to-all (A2A) propagator method

- method to calculate quark propagator connecting all sources to all sinks
- useful particularly (but not only) when a quark loop present in contraction diagrams
- Low-mode decomposition

▶ Dirac operator $\gamma_5 D(x, y) = \sum_i v_i(x) \lambda_i v_i(y)^\dagger$
spin, color (and flavor) indices suppressed

▶ Quark propagator $S_F(x, y) = D^{-1}(x, y) = \sum_i v_i(x) \frac{1}{\lambda_i} v_i(y)^\dagger \gamma_5$

↑ truncated at $i = N_\ell \ll V$
 good approximation for light quarks

- Noise method for strange-quark propagator & light-quark high modes (next slide)

Noise method

if we find vectors $\xi_i(x)$ that satisfy

$$\sum_{i=1}^{N_h} \xi_i(x) \xi_i(y)^\dagger \approx \delta_{x,y}$$

solve

$$\sum_y D(x,y) X_i(y) = \xi_i(x) \rightarrow X_i(x) = \sum_y D^{-1}(x,y) \xi_i(y)$$

$$\rightarrow \sum_i X_i(x) \xi_i(y)^\dagger \approx D^{-1}(x,y)$$

Pure noise method used for strange-quark propagator

Noise method

if we find vectors $\xi_i(x)$ that satisfy

$$\sum_{i=1}^{N_h} \xi_i(x) \xi_i(y)^\dagger \approx \delta_{x,y}$$

$\xi_i(x)$: Random values in $U(1) / \sqrt{N_h}$ or its subgroup

$O(1/\sqrt{N_h})$ error taken into account as statistical error

solve

$$\sum_y D(x,y) X_i(y) = \xi_i(x) \rightarrow X_i(x) = \sum_y D^{-1}(x,y) \xi_i(y)$$

$$\rightarrow \sum_i X_i(x) \xi_i(y)^\dagger \approx D^{-1}(x,y)$$

Pure noise method used for strange-quark propagator

Combining low-mode approximation & noise method

$$D^{-1}(x, y) \approx \sum_{i=1}^{N_\ell} v_i(x) \frac{1}{\lambda_i} v_i(y)^\dagger \gamma_5 + \sum_{j=1}^{N_h} \left(X_j(x) - \sum_{i=1}^{N_\ell} \sum_z v_i(x) \frac{1}{\lambda_i} v_i(z)^\dagger \gamma_5 \xi_j(z) \right) \xi_j(y)^\dagger$$

low- & high-mode decomposition

$$D^{-1}(x, y) \approx \sum_{i=1}^{N_\ell + N_h} V_i(x) W_i(y)^\dagger$$

$O(10^9 \times 10^9)$ matrix \rightarrow $O(10^3)$ vectors of size $O(10^8)$
lost information is not important for long-distance physics

Combining low-mode approximation & noise method

$$D^{-1}(x, y) \approx \sum_{i=1}^{N_\ell} v_i(x) \frac{1}{\lambda_i} v_i(y)^\dagger \gamma_5 + \sum_{j=1}^{N_h} \left(X_j(x) - \sum_{i=1}^{N_\ell} \sum_z v_i(x) \frac{1}{\lambda_i} v_i(z)^\dagger \gamma_5 \xi_j(z) \right) \xi_j(y)^\dagger$$

low- & high-mode decomposition

$$D^{-1}(x, y) \approx \sum_{i=1}^{N_\ell + N_h} V_i(x) W_i(y)^\dagger$$

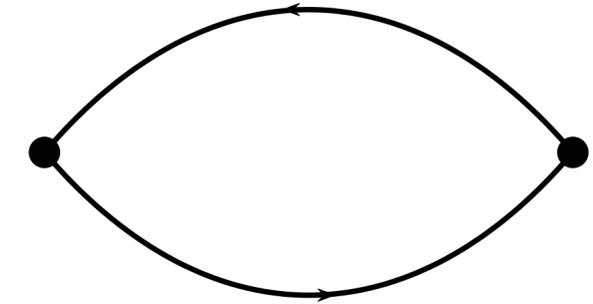
10^{11} complex numbers \rightarrow $O(1)$ TB
good to consider for serious
calculations

$O(10^9 \times 10^9)$ matrix \rightarrow $O(10^3)$ vectors of size $O(10^8)$
lost information is not important for long-distance physics

A2A propagators for simplest contraction

- cannot do a huge “for loop” over V^2
- disentangle and find a way for the contraction

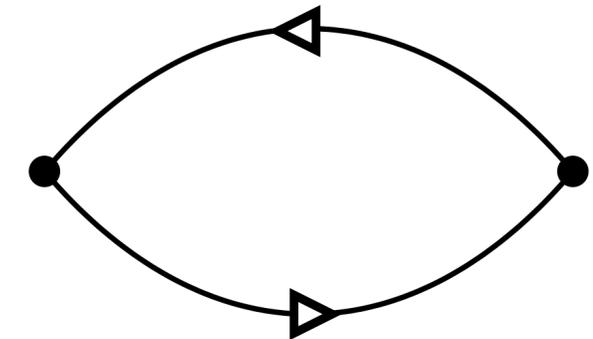
$$\begin{aligned}
 & \sum_{\vec{x}, \vec{y}} \text{Tr}[\gamma_5 D^{-1}((\vec{x}, x_4), (\vec{y}, y_4)) \gamma_5 D^{-1}((\vec{y}, y_4), (\vec{x}, x_4))] \\
 &= \sum_{\vec{x}, \vec{y}} \sum_{i,j} \text{Tr}[\gamma_5 V_i(\vec{x}, x_4) W_i(\vec{y}, y_4)^\dagger \gamma_5 V_j(\vec{y}, y_4) W_j(\vec{x}, x_4)^\dagger] \\
 &= \sum_{i,j} \underbrace{\sum_{\vec{x}} W_j(\vec{x}, x_4)^\dagger \gamma_5 V_i(\vec{x}, x_4)}_{\Pi_{ij}^{\gamma_5}(x_4)} \cdot \underbrace{\sum_{\vec{y}} W_i(\vec{y}, y_4)^\dagger \gamma_5 V_j(\vec{y}, y_4)}_{\Pi_{ji}^{\gamma_5}(y_4)} \\
 &= \sum_{i,j} \Pi_{ij}^{\gamma_5}(x_4) \Pi_{ji}^{\gamma_5}(y_4)
 \end{aligned}$$



A2A propagators for simplest contraction

- cannot do a huge “for loop” over V^2
- disentangle and find a way for the contraction

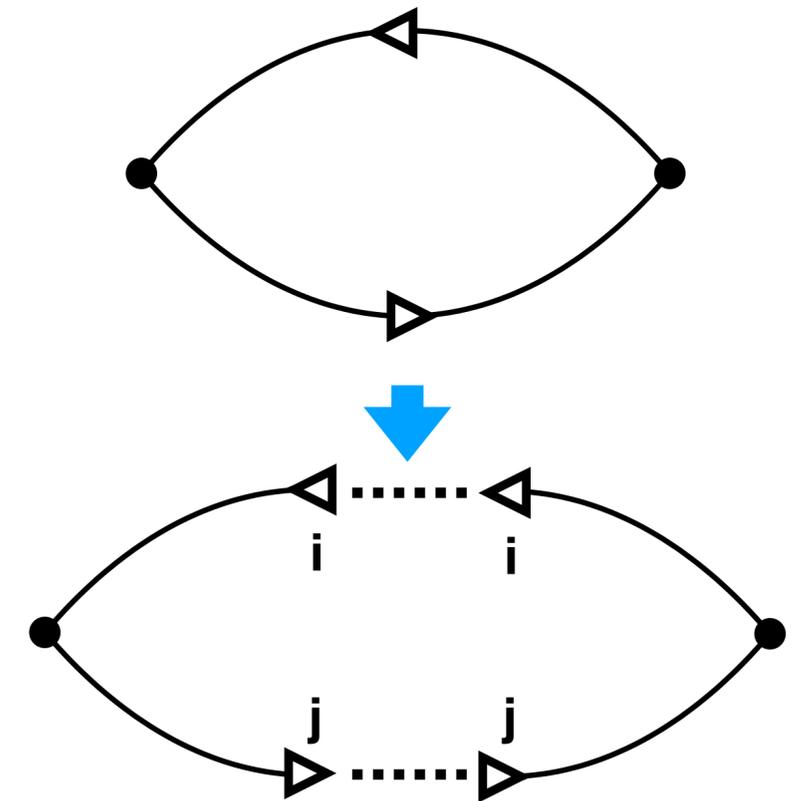
$$\begin{aligned}
 & \sum_{\vec{x}, \vec{y}} \text{Tr}[\gamma_5 D^{-1}((\vec{x}, x_4), (\vec{y}, y_4)) \gamma_5 D^{-1}((\vec{y}, y_4), (\vec{x}, x_4))] \\
 &= \sum_{\vec{x}, \vec{y}} \sum_{i,j} \text{Tr}[\gamma_5 V_i(\vec{x}, x_4) W_i(\vec{y}, y_4)^\dagger \gamma_5 V_j(\vec{y}, y_4) W_j(\vec{x}, x_4)^\dagger] \\
 &= \sum_{i,j} \underbrace{\sum_{\vec{x}} W_j(\vec{x}, x_4)^\dagger \gamma_5 V_i(\vec{x}, x_4)}_{\Pi_{ij}^{\gamma_5}(x_4)} \cdot \underbrace{\sum_{\vec{y}} W_i(\vec{y}, y_4)^\dagger \gamma_5 V_j(\vec{y}, y_4)}_{\Pi_{ji}^{\gamma_5}(y_4)} \\
 &= \sum_{i,j} \Pi_{ij}^{\gamma_5}(x_4) \Pi_{ji}^{\gamma_5}(y_4)
 \end{aligned}$$



A2A propagators for simplest contraction

- cannot do a huge “for loop” over V^2
- disentangle and find a way for the contraction

$$\begin{aligned}
 & \sum_{\vec{x}, \vec{y}} \text{Tr}[\gamma_5 D^{-1}((\vec{x}, x_4), (\vec{y}, y_4)) \gamma_5 D^{-1}((\vec{y}, y_4), (\vec{x}, x_4))] \\
 &= \sum_{\vec{x}, \vec{y}} \sum_{i,j} \text{Tr}[\gamma_5 V_i(\vec{x}, x_4) W_i(\vec{y}, y_4)^\dagger \gamma_5 V_j(\vec{y}, y_4) W_j(\vec{x}, x_4)^\dagger] \\
 &= \underbrace{\sum_{i,j} \sum_{\vec{x}} W_j(\vec{x}, x_4)^\dagger \gamma_5 V_i(\vec{x}, x_4)}_{\Pi_{ij}^{\gamma_5}(x_4)} \cdot \underbrace{\sum_{\vec{y}} W_i(\vec{y}, y_4)^\dagger \gamma_5 V_j(\vec{y}, y_4)}_{\Pi_{ji}^{\gamma_5}(y_4)} \\
 &= \sum_{i,j} \Pi_{ij}^{\gamma_5}(x_4) \Pi_{ji}^{\gamma_5}(y_4)
 \end{aligned}$$



A2A propagators for simplest contraction

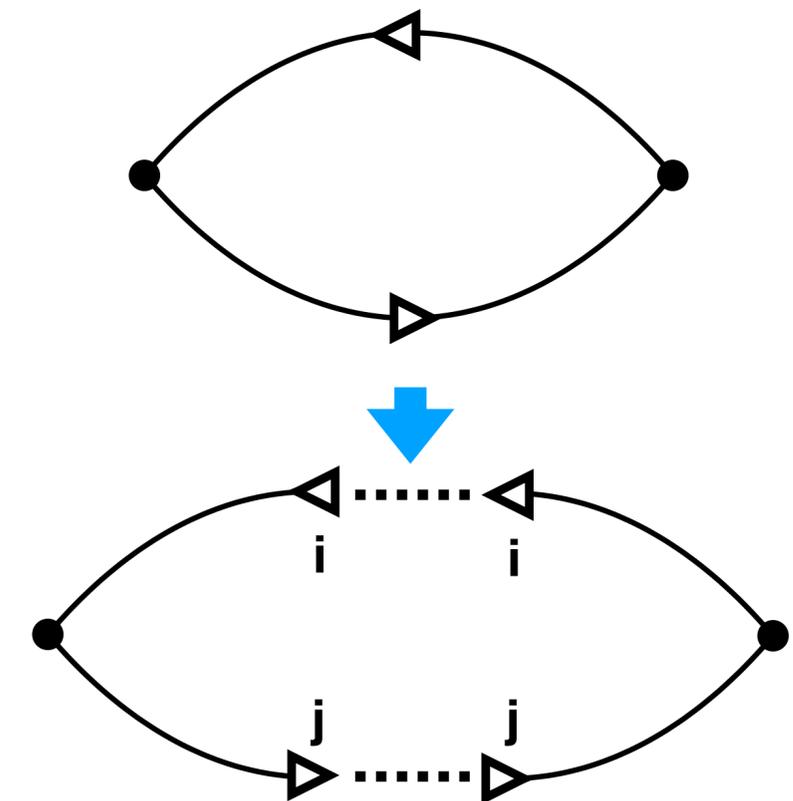
- cannot do a huge “for loop” over V^2
- disentangle and find a way for the contraction

$$\begin{aligned} & \sum_{\vec{x}, \vec{y}} \text{Tr}[\gamma_5 D^{-1}((\vec{x}, x_4), (\vec{y}, y_4)) \gamma_5 D^{-1}((\vec{y}, y_4), (\vec{x}, x_4))] \\ &= \sum_{\vec{x}, \vec{y}} \sum_{i,j} \text{Tr}[\gamma_5 V_i(\vec{x}, x_4) W_i(\vec{y}, y_4)^\dagger \gamma_5 V_j(\vec{y}, y_4) W_j(\vec{x}, x_4)^\dagger] \\ &= \underbrace{\sum_{i,j} \sum_{\vec{x}} W_j(\vec{x}, x_4)^\dagger \gamma_5 V_i(\vec{x}, x_4)}_{\Pi_{ij}^{\gamma_5}(x_4)} \cdot \underbrace{\sum_{\vec{y}} W_i(\vec{y}, y_4)^\dagger \gamma_5 V_j(\vec{y}, y_4)}_{\Pi_{ji}^{\gamma_5}(y_4)} \end{aligned}$$

$$= \sum_{i,j} \Pi_{ij}^{\gamma_5}(x_4) \Pi_{ji}^{\gamma_5}(y_4)$$



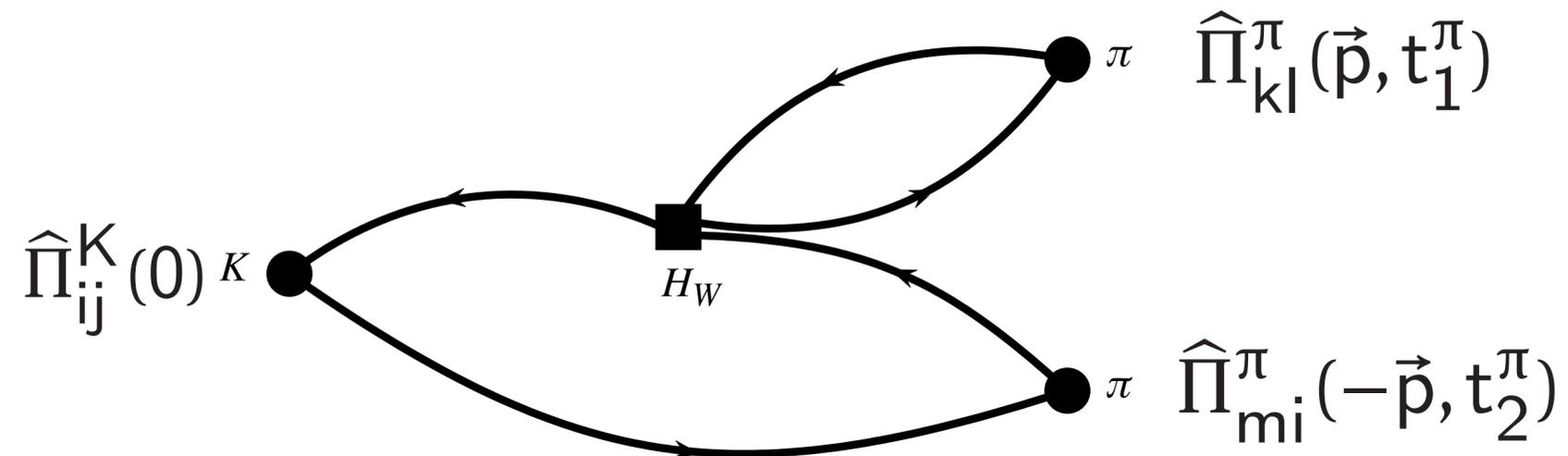
- A2A Meson field
- $O(10^3 \times 10^3 \times 10^2)$ complex numbers $\rightarrow O(1)$ GB
- should be saved for other projects



Meson fields for $K \rightarrow \pi\pi$

$$\hat{\Pi}_{ij}^K(t) = \sum_{\vec{x}} W_i^\ell(\vec{x}, t) W_j^S(\vec{x}, t)$$

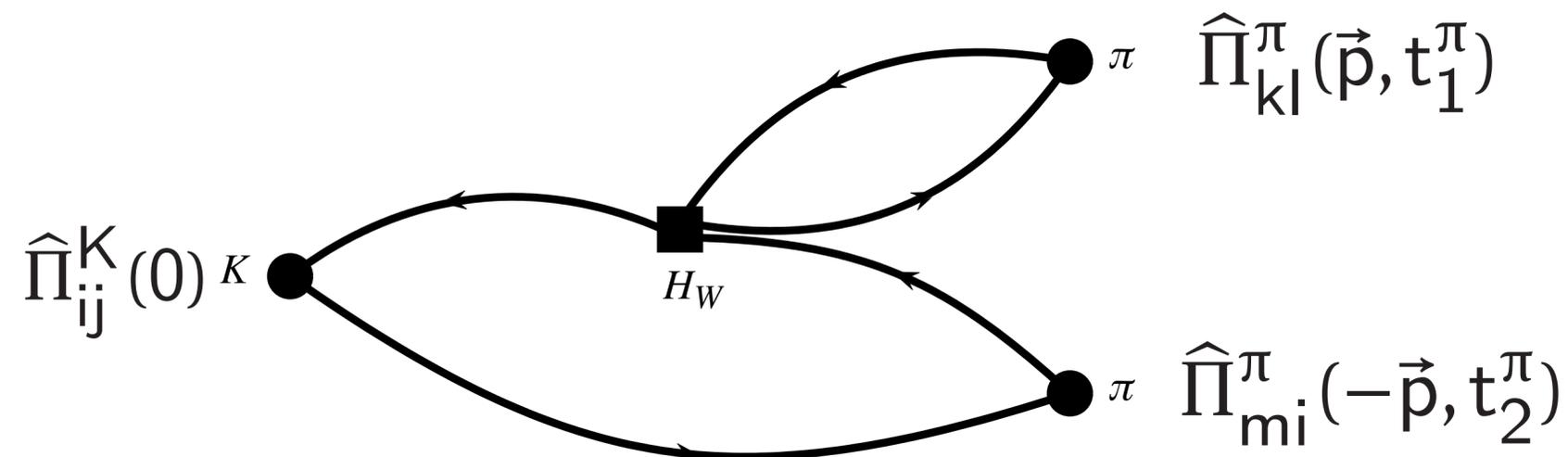
$$\hat{\Pi}_{ij}^\pi(\vec{p}, t) = \sum_{\vec{x}} e^{i\vec{p}\cdot\vec{x}} W_i^\ell(\vec{x}, t) \gamma_5 V_j^\ell(\vec{x}, t)$$



Meson fields for $K \rightarrow \pi\pi$

$$\hat{\Pi}_{ij}^K(t) = \sum_{\vec{x}} W_i^\ell(\vec{x}, t) W_j^S(\vec{x}, t)$$

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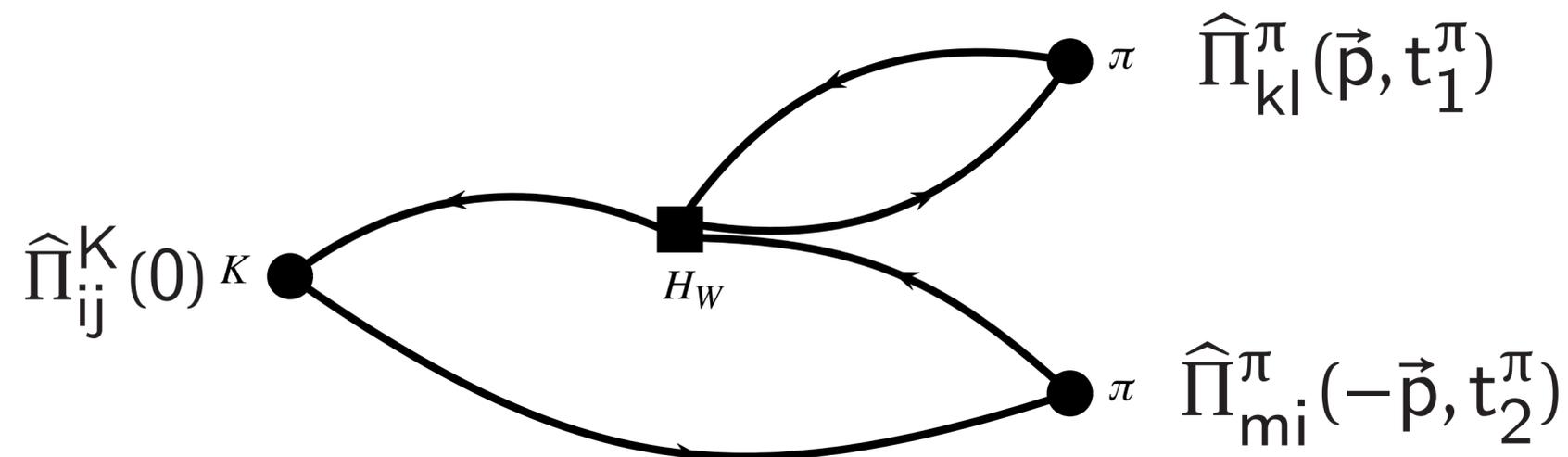


Only 4-quark operator remain with spin, color (& position) indices uncontracted

Meson fields for $K \rightarrow \pi\pi$

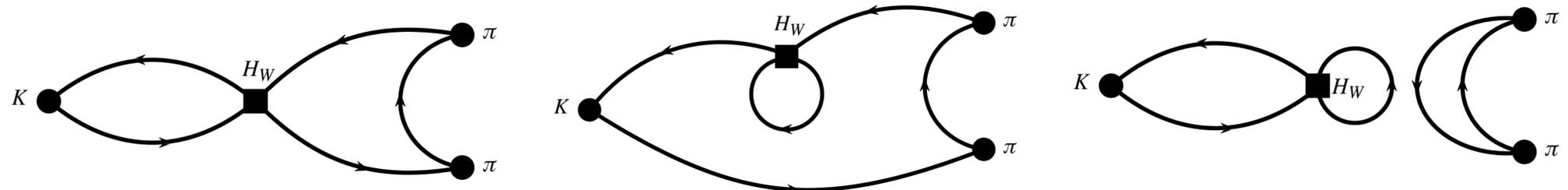
$$\hat{\Pi}_{ij}^K(t) = \sum_{\vec{x}} W_i^\ell(\vec{x}, t) W_j^S(\vec{x}, t)$$

$$\hat{\Pi}_{ij}^\pi(\vec{p}, t) = \sum_{\vec{x}} e^{i\vec{p}\cdot\vec{x}} W_i^\ell(\vec{x}, t) \gamma_5 V_j^\ell(\vec{x}, t)$$



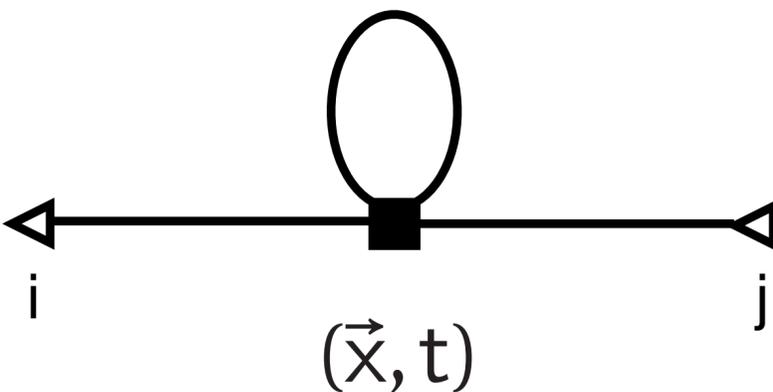
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Same for other diagrams:

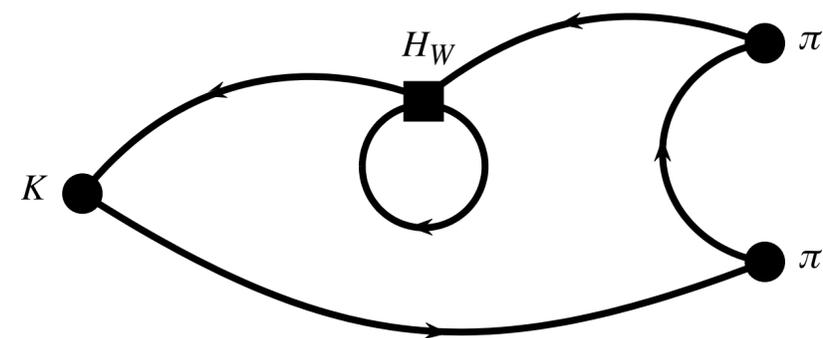


Contraction for eye diagrams

- Calculate meson field-like object

$$\Pi_{ij}^{4q}(t) = \sum_{\vec{X}} \text{Diagram}$$


**Doing GPU optimization for
64³x128 lattice calculation**

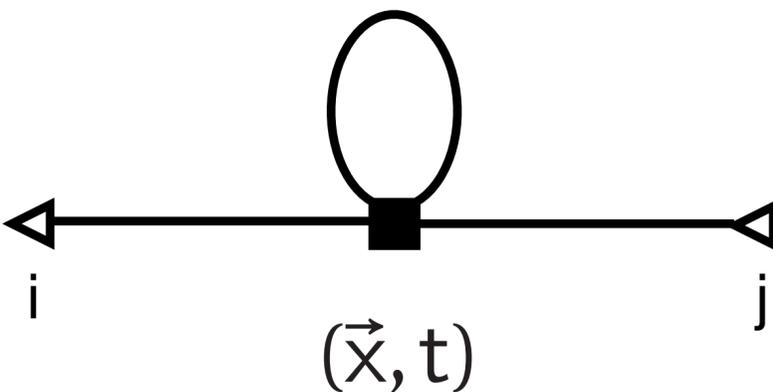


$$= \sum_{i,j,k,l} \Pi_{ij}^K(t_K) \Pi_{jk}^{4q}(t_{4q}) \Pi_{kl}^\pi(\vec{p}, t_1^\pi) \Pi_{li}^\pi(-\vec{p}, t_2^\pi)$$

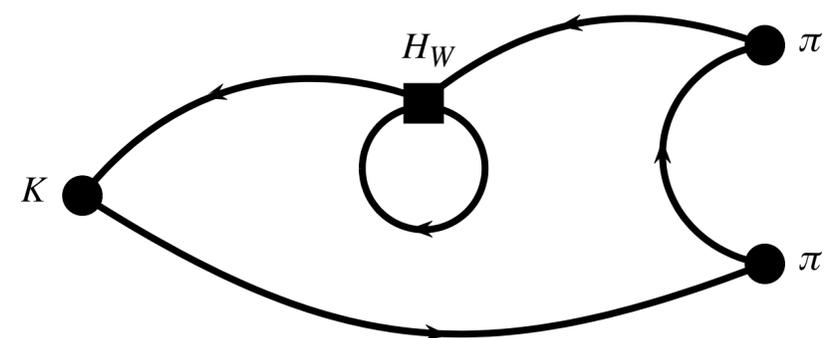
$$= \sum_{i,j} \Pi_{ij}^K(t_K) \Pi_{ji}^{4q}(t_{4q}) \cdot \sum_{k,l} \Pi_{kl}^\pi(\vec{p}, t_1^\pi) \Pi_{lk}^\pi(-\vec{p}, t_2^\pi)$$

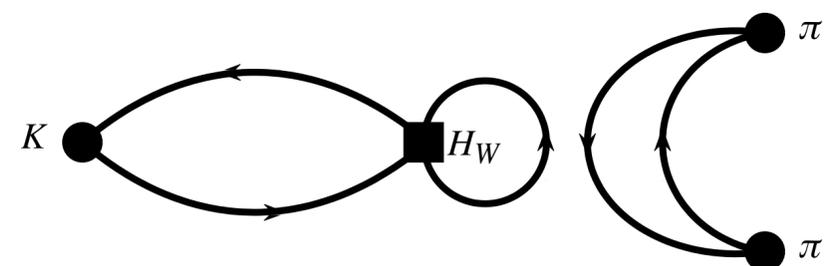
Contraction for eye diagrams

- Calculate meson field-like object

$$\Pi_{ij}^{4q}(t) = \sum_{\vec{X}} \text{Diagram}$$


Doing GPU optimization for $64^3 \times 128$ lattice calculation

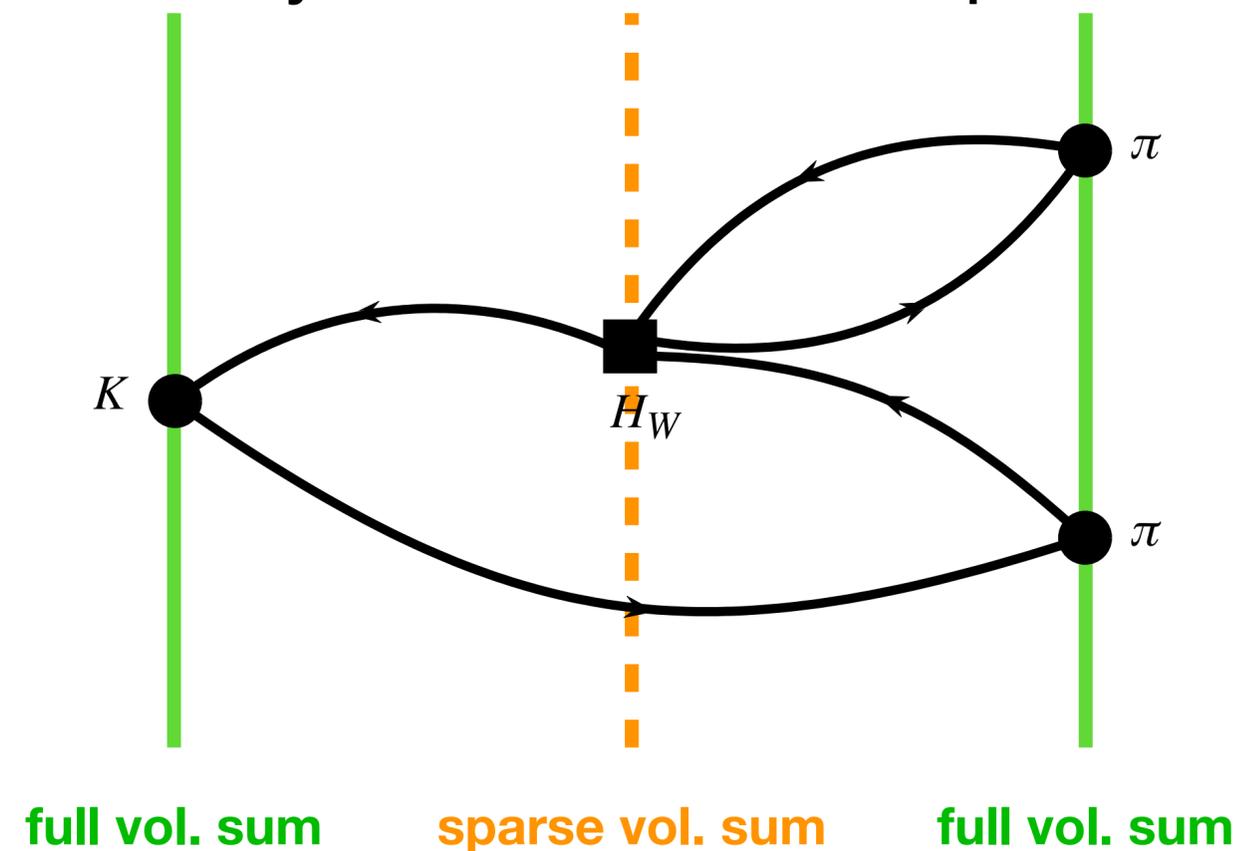


$$= \sum_{i,j,k,l} \Pi_{ij}^K(t_K) \Pi_{jk}^{4q}(t_{4q}) \Pi_{kl}^\pi(\vec{p}, t_1^\pi) \Pi_{li}^\pi(-\vec{p}, t_2^\pi)$$


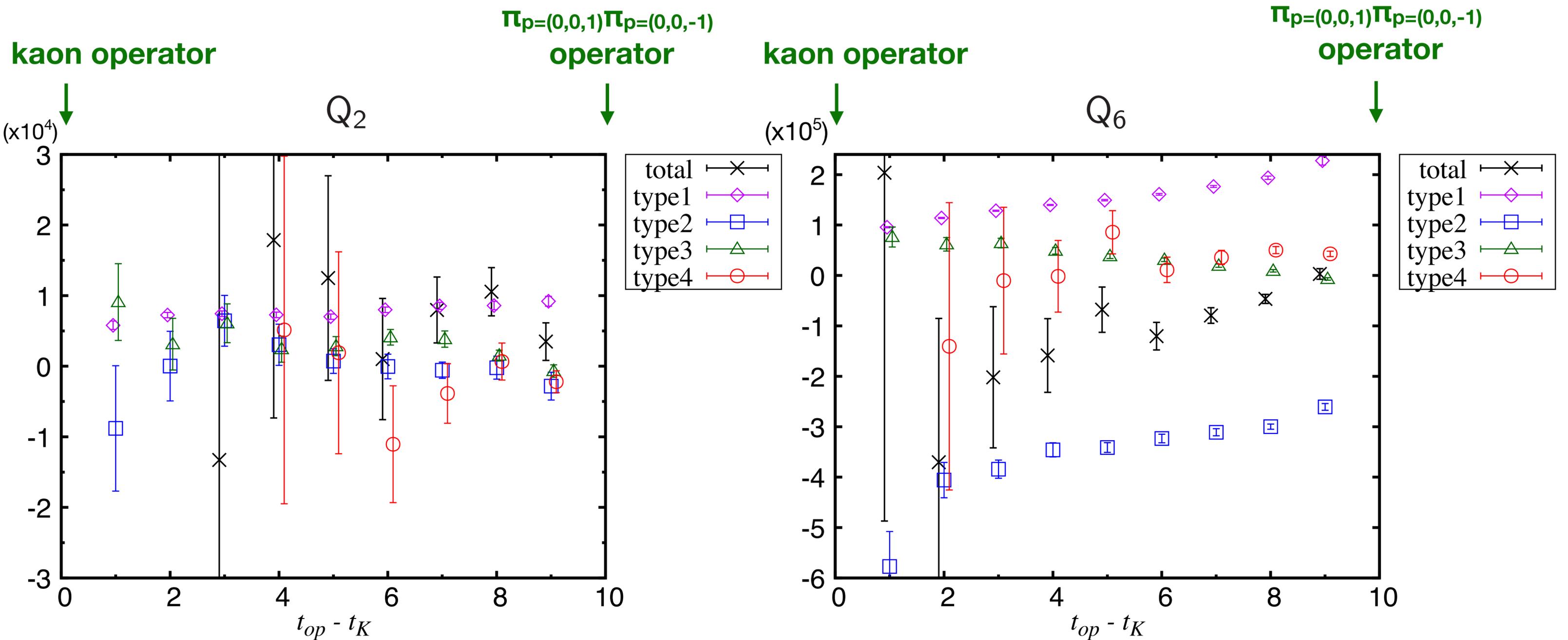
$$= \sum_{i,j} \Pi_{ij}^K(t_K) \Pi_{ji}^{4q}(t_{4q}) \cdot \sum_{k,l} \Pi_{kl}^\pi(\vec{p}, t_1^\pi) \Pi_{lk}^\pi(-\vec{p}, t_2^\pi)$$

Contraction for connected diagrams

- Connected diagrams more expensive
 - Cost proportional to volume of Q_i
 - but statistically much more precise
- reduce average volume by factor of 64 for spatial volume and 8 for time translation



$I = 0$ correlation functions



- Sparsen H_W for types1,2 (connected) – still more precise than type4 (disconnected)

Summary

- Contractions becomes increasingly complicated as increasing number of quark propagators
- Wick contraction automated for such cases
- For $K \rightarrow \pi\pi$, not fully automated to further consider cost reductions
- Fully automated version also used for nonperturbative 3/4-flavor matching & photon structure, but the efficiency hasn't been seriously considered

Summary

- Contractions becomes increasingly complicated as increasing number of quark propagators
- Wick contraction automated for such cases
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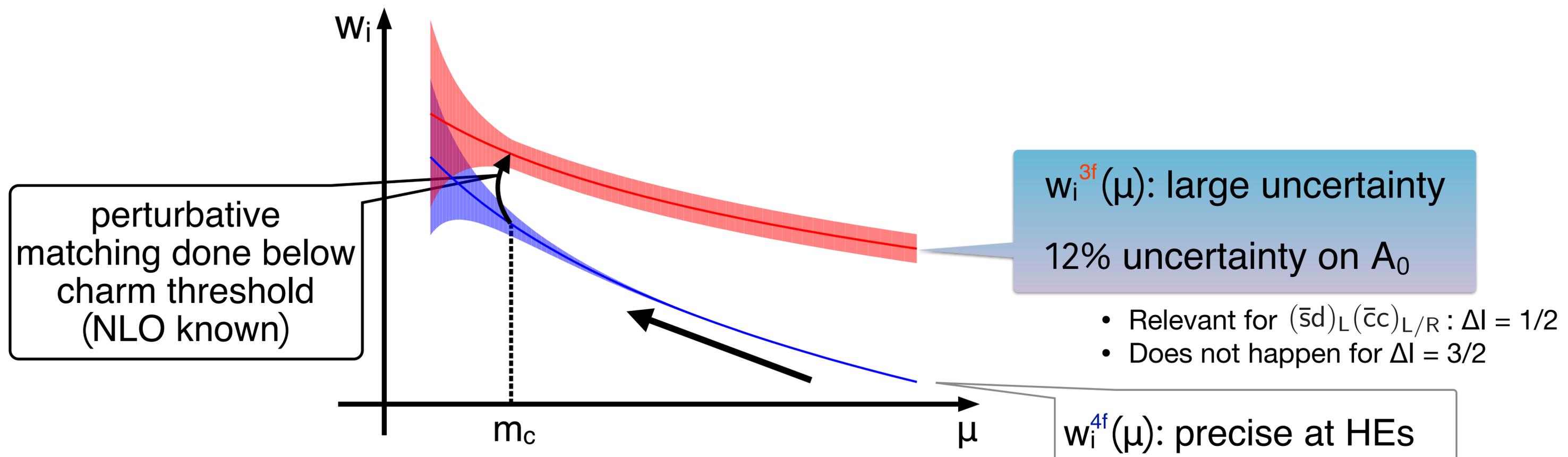
One of my dreams:

To create a fully automated measurement platform that identifies and suggests the maximally efficient approach considering various situations such as what data we already have

**Nonperturbative matching of $\Delta S=1$
operators b/w 3 & 4-flavor theories**

Wilson coefs

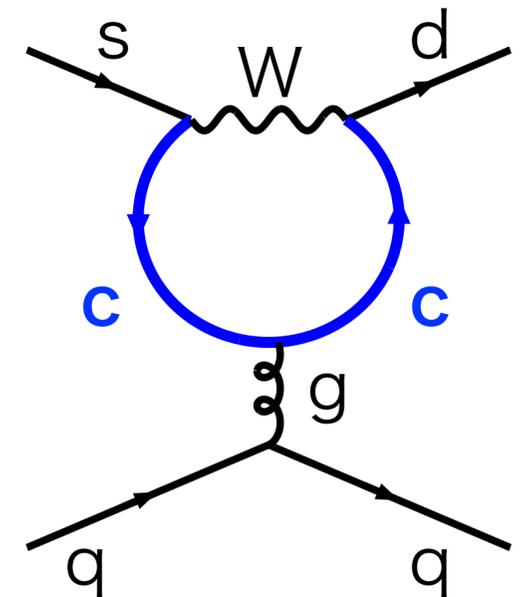
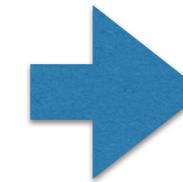
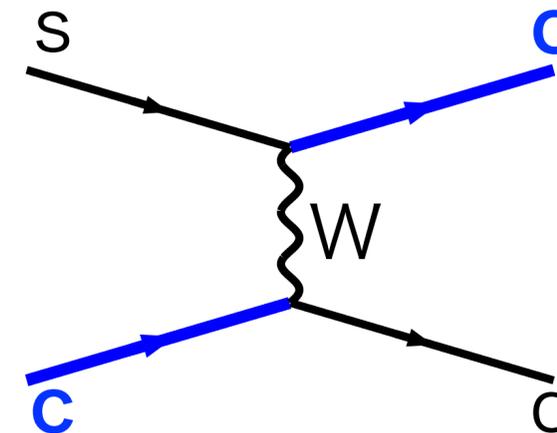
$$\langle f | H_W | i \rangle = \sum_i \underbrace{w_i^{3f}(\mu)}_{\text{pQCD}} \underbrace{\langle f | O_i^{3f}(\mu) | i \rangle}_{\text{LQCD}}$$



- Possible resolutions
 - NNLO perturbative matching [Cerdeira-Sevilla et al. *Acta Phys.Polon.B* 4 (2018) 1087-1096]
 - Matching nonperturbatively [MT, LATTICE2019]

How much $w_i^{3f} \neq w_i^{4f}$?

- Sea charm quark $\rightarrow O(\alpha_s^2)$
- If O_i^{4f} involves charm quark...
 - WCs of charm operators will be a part of 3f WCs
 - Difference can be $O(\alpha_s)$



- w_i^{3f} necessary if MEs are calculated w O_i^{3f}
 - our fine lattice: $a^{-1} \approx 1.38$ GeV used for MEs
 - not appropriate to introduce charm on this lattice
 - $80^3 \times 160$ may be needed to have fine enough lattice maintaining m_π^{phys}

NP matching of 4-quark operators

- Basic idea

$$O_i^{4f} \rightarrow \sum_j M_{ij} O_j^{3f}$$

i.e. $\langle E_{\text{out}} | O_i^{4f} | E_{\text{in}} \rangle = \sum_j M_{ij} \langle E_{\text{out}} | O_j^{3f} | E_{\text{in}} \rangle$ for small E_{out} & E_{in} compared to m_c

- Strategy

- ▶ Consider many 3pt functions on fine lattice

$$C_{i,ab}^{3f/4f}(t_{\text{out}}, t, t_{\text{in}}) = \langle \mathcal{O}_a(t_{\text{out}}) O_i^{3f/4f}(t) \mathcal{O}_b(t_{\text{in}}) \rangle$$

- ▶ Perform fit with many pairs of O_a & O_b at large $t_{\text{out}} - t$ & $t - t_{\text{in}}$
- ▶ Trying with ~ 200 relevant pairs of O_a & O_b
- ▶ Automatic Wick contractor in use

$$C_{i,ab}^{4f} = M_{ij} C_{j,ab}^{3f}$$

Operator basis for $\Delta S=1$

(n_L, n_R) : Representation of $SU(3)_L \times SU(3)_R$

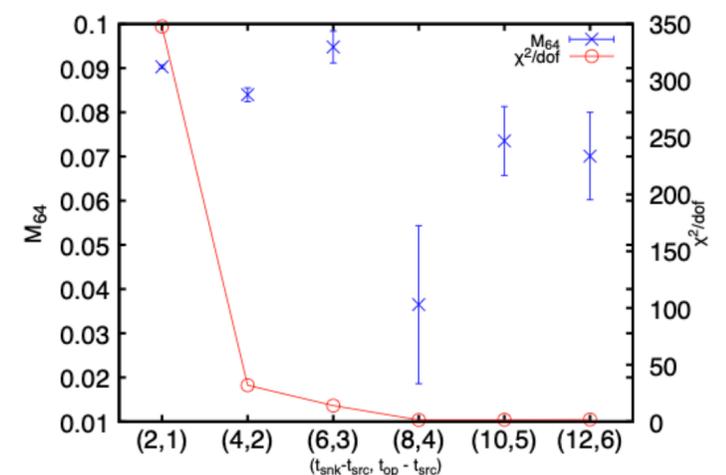
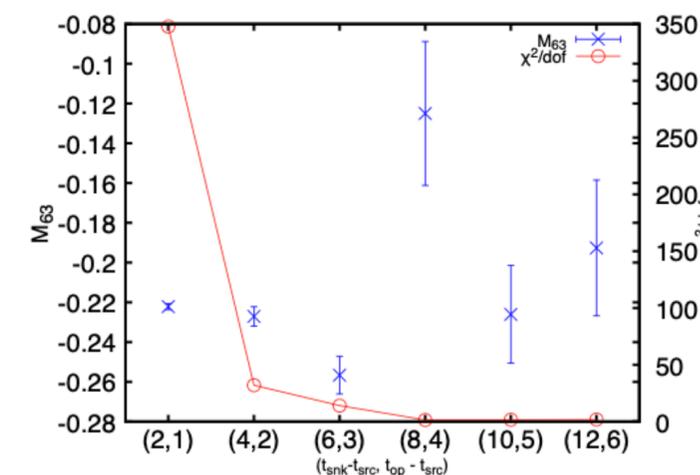
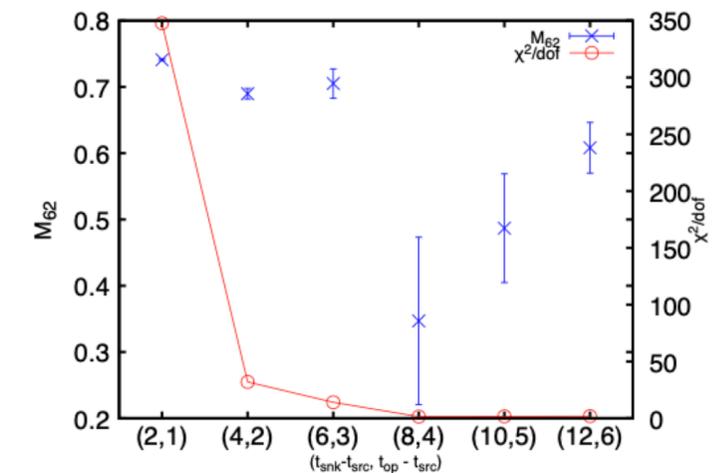
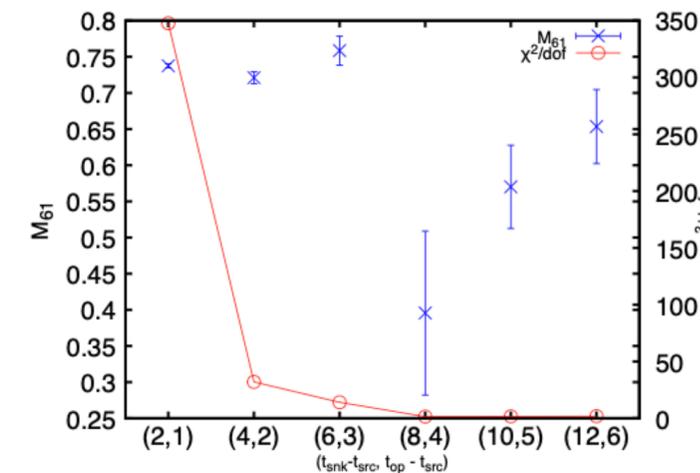
- Classification of 7 independent $n_f = 3$ operators
 - 1 in $(27,1)$; 4 in $(8,1)$; 2 in $(8,8)$
- 4 charm operators $(\bar{s}_\alpha d_{\alpha/\beta})_L (\bar{c}_\alpha c_{\beta/\alpha})_{L/R}$ all in $(8,1)$ with $SU(3)_L \times SU(3)_R$
- Only operators in $(8,1)$ matter
 - $O_j^{3f} = (Q'_1, Q'_2, Q'_3, Q'_4)$
 - $O_i^{4f} = (Q'_1, Q'_2, Q'_3, Q'_4, P_1, P_2, P_3, P_4)$

$$\Rightarrow M_{ij} = \begin{pmatrix} \mathbf{1}_{4 \times 4} \\ \dots\dots\dots \\ \bullet & \bullet & \bullet & \bullet \end{pmatrix}$$

16 nontrivial elements

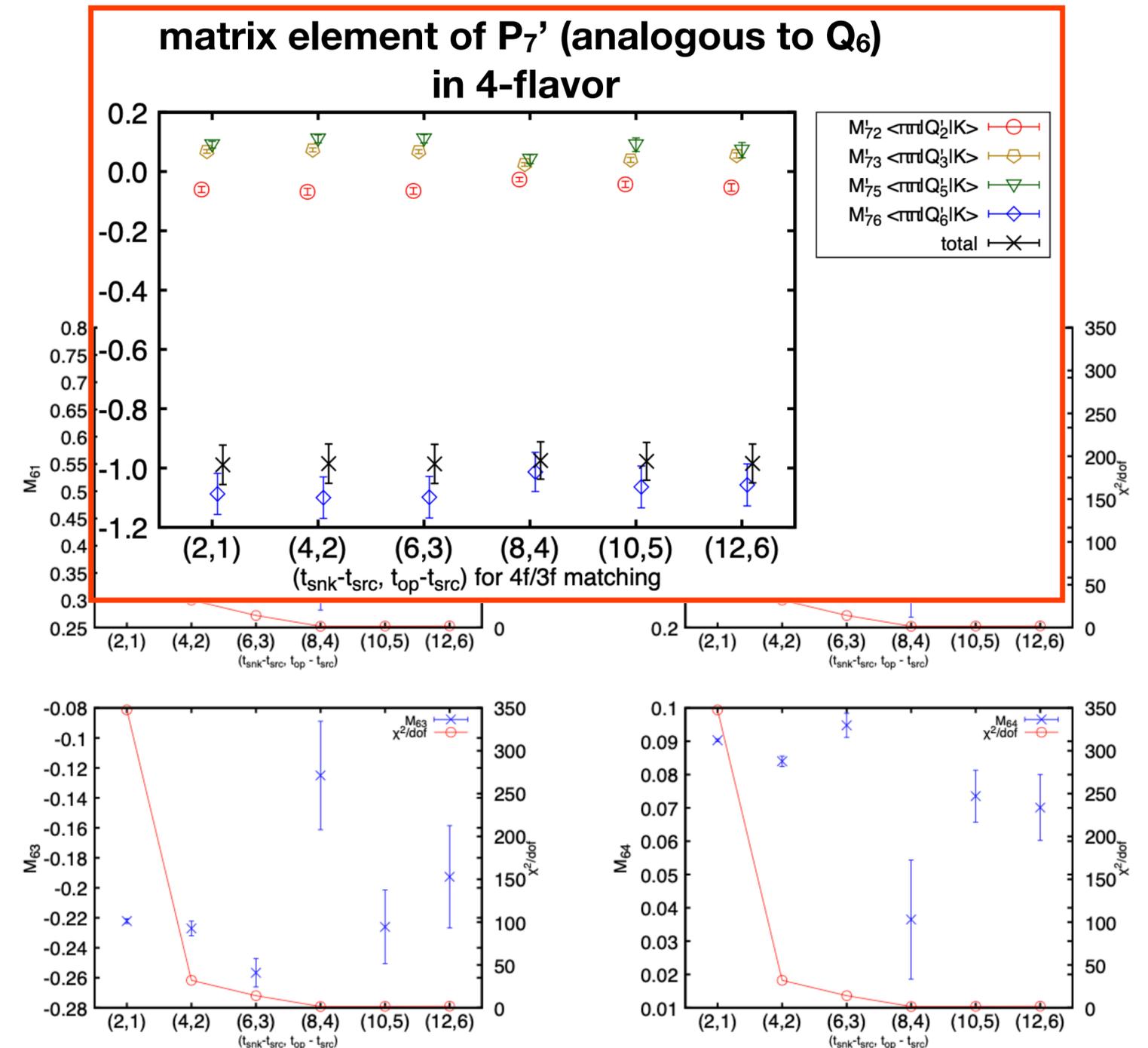
$SU(3)_L \times SU(3)_R$ to $SU(4)_L \times SU(4)_R$ chiral bases

- 7-operator basis w $n_f = 3$
 - $(27,1) \times 1, (8,1) \times 4, (8,8) \times 2$
- 9-operator basis w $n_f = 4$
 - $(84,1) \times 2, (20,1) \times 1, (15,1) \times 4, (15,15) \times 2$
- 9x7 matching matrix can be determined once the 16 elements of M_{ij} are obtained
- Instability of M_{ij} doesn't propagate to 4-flavor matrix elements
 - Instability still concerning and trying to better understand



$SU(3)_L \times SU(3)_R$ to $SU(4)_L \times SU(4)_R$ chiral bases

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Example results on finer lattice

		value [GeV]	significant statistical errors	significant systematic errors
ReA ₀	perturbative	$2.89(23)_{\text{stat}}(35)_{\text{sys}} \times 10^{-7}$	matrix elements 8.0%	Wilson coefficients 12%
	nonperturbative	$2.97(22)_{\text{stat}}(1)_{\text{sys}} \times 10^{-7}$	<ul style="list-style-type: none"> matrix elements 6.5% 3/4-flavor matching 2.3% 	
ImA ₀	perturbative	$-7.11(54)_{\text{stat}}(94)_{\text{sys}} \times 10^{-11}$	matrix elements 7.6%	<ul style="list-style-type: none"> Wilson coefficients 12% High-energy parameters 5.6%
	nonperturbative	$-6.82(94)_{\text{stat}}(37)_{\text{sys}} \times 10^{-11}$	<ul style="list-style-type: none"> matrix elements 11% 3/4-flavor matching 6.3% 	High-energy parameters 5.4%

****outdated results**

****Discretization effects (12% overall) and finite volume effects (7% overall) not included above**

Summary

- So many issues to address for precise SM prediction of $K \rightarrow \pi\pi$
 - ▶ better continuum limit \rightarrow calculation at $a^{-1} \approx 1.7$ GeV underway, 2.3 GeV planned
 - ▶ continuum limit of step scaling
 - ▶ dependence on intermediate scheme/scale on the high-energy side (μ_h)
 - ▶ NNLO perturbative matching would be very helpful
 - ▶ Nonperturbative 3/4-flavor matching mostly done, but maybe a bit more to understand before writing up a paper
 - ▶ NNLO Wilson coefficients should significantly reduce the systematic error

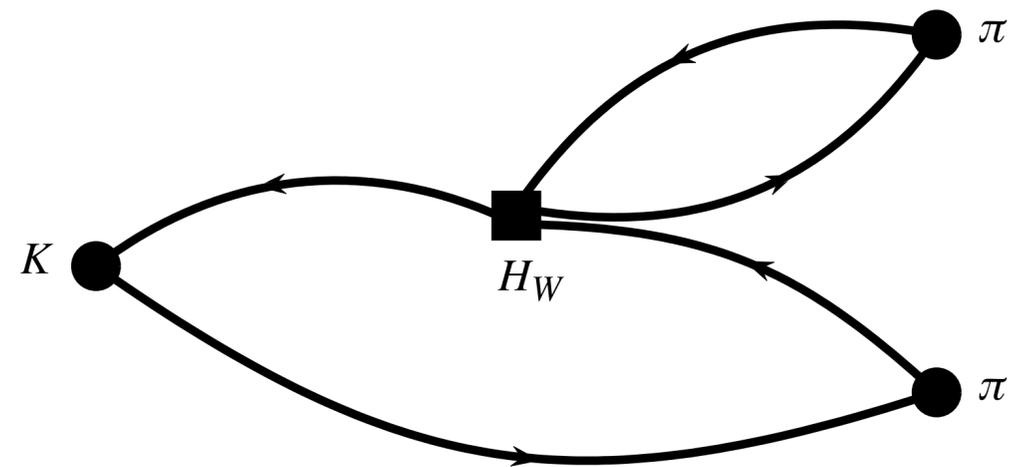
Why periodic BC?

- Already have lattice ensembles with physical pion mass
 - $a^{-1} = 1 \text{ GeV}$, $24^3 \times 64$ & $a^{-1} = 1.4 \text{ GeV}$, $32^3 \times 64$ & ...
 - Continuum limit easier
- Hope to introduce QED/IB effects near future
 - G-parity BC violate charge conservation
 - PBC appear necessary
- Presence of $E_{\pi\pi} = 2m_{\pi}$ state challenging
 - S/N ratio of $E_{\pi\pi} = m_{\kappa}$ state should be the same as in G-parity BC: $\sim e^{-(m_{\kappa} - 2m_{\pi})t}$
 - interesting to see feasibility of extracting signal of excited states

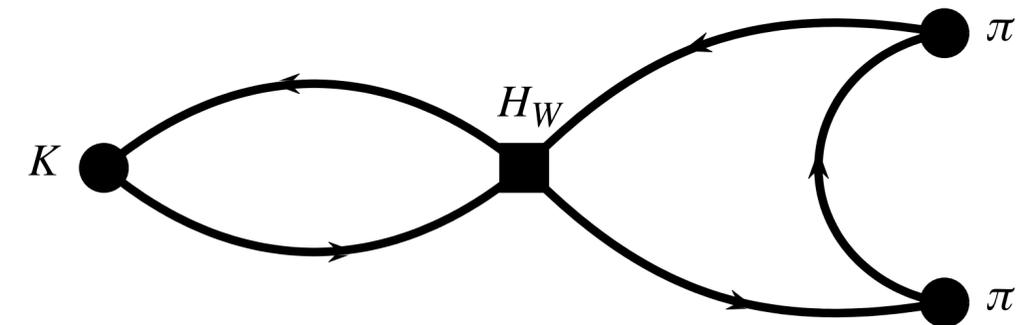
Lattice setup

- RBC/UKQCD's 2+1-flavor MDWF ensembles at physical pion & kaon masses
 - $24^3 \times 64$, $a^{-1} = 1.0$ GeV, 258 confs
 - $32^3 \times 64$, $a^{-1} = 1.4$ GeV, 107 confs
- Chiral symmetry of DWF → strong constraints on operator mixings
 - with lower-dimensional operators
 - among different representations w.r.t. chiral symmetry (8,1), (8,8) & (27,1)
- All-to-all quark propagators
 - 2,000 low modes for light quarks (no low mode for strange)
 - high-mode part: spin, color and time dilutions => 768 inversions

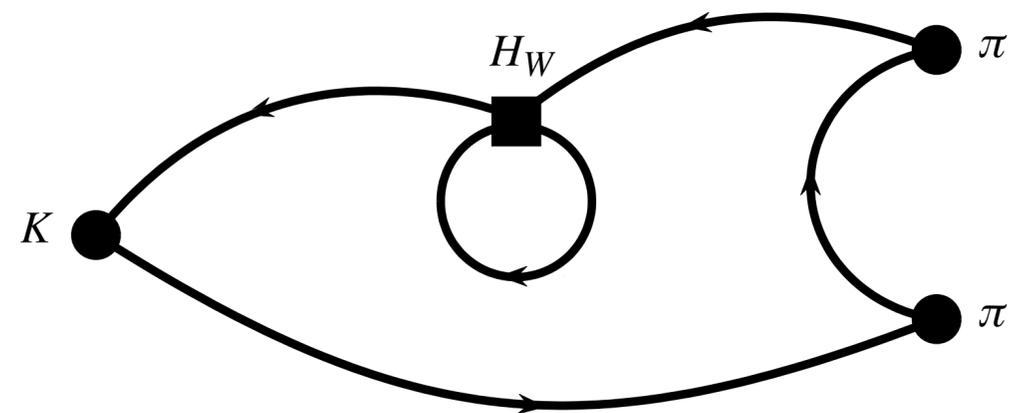
Diagrams for $K \rightarrow \pi\pi$ 3pt functions



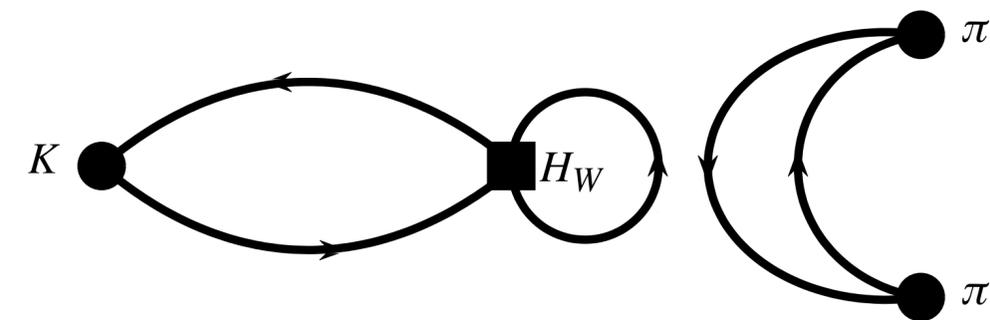
type 1



type 2



type 3



type 4

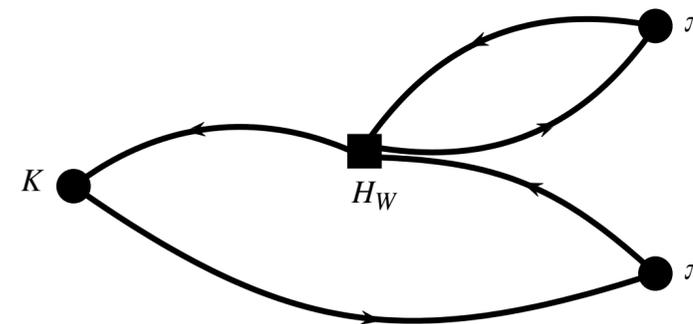
type 4 dominates stat. error

- Previous G-parity calculation

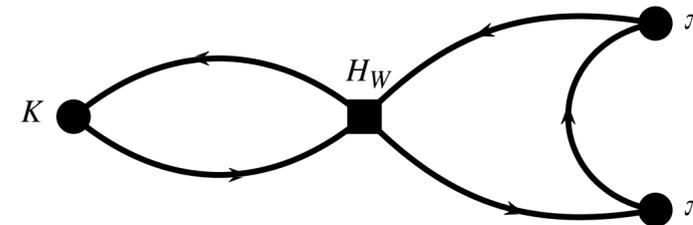
- types 1,2: averaged over every 8 time translations
- types 3,4: averaged over every time translation

- types 1,2 still expensive but no need of such precision

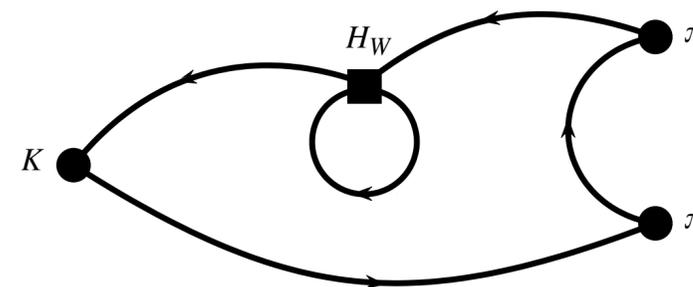
→ cost reduction?



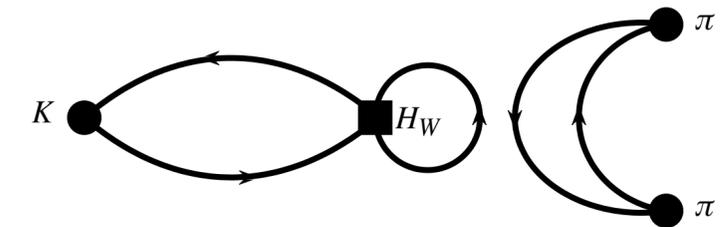
type 1



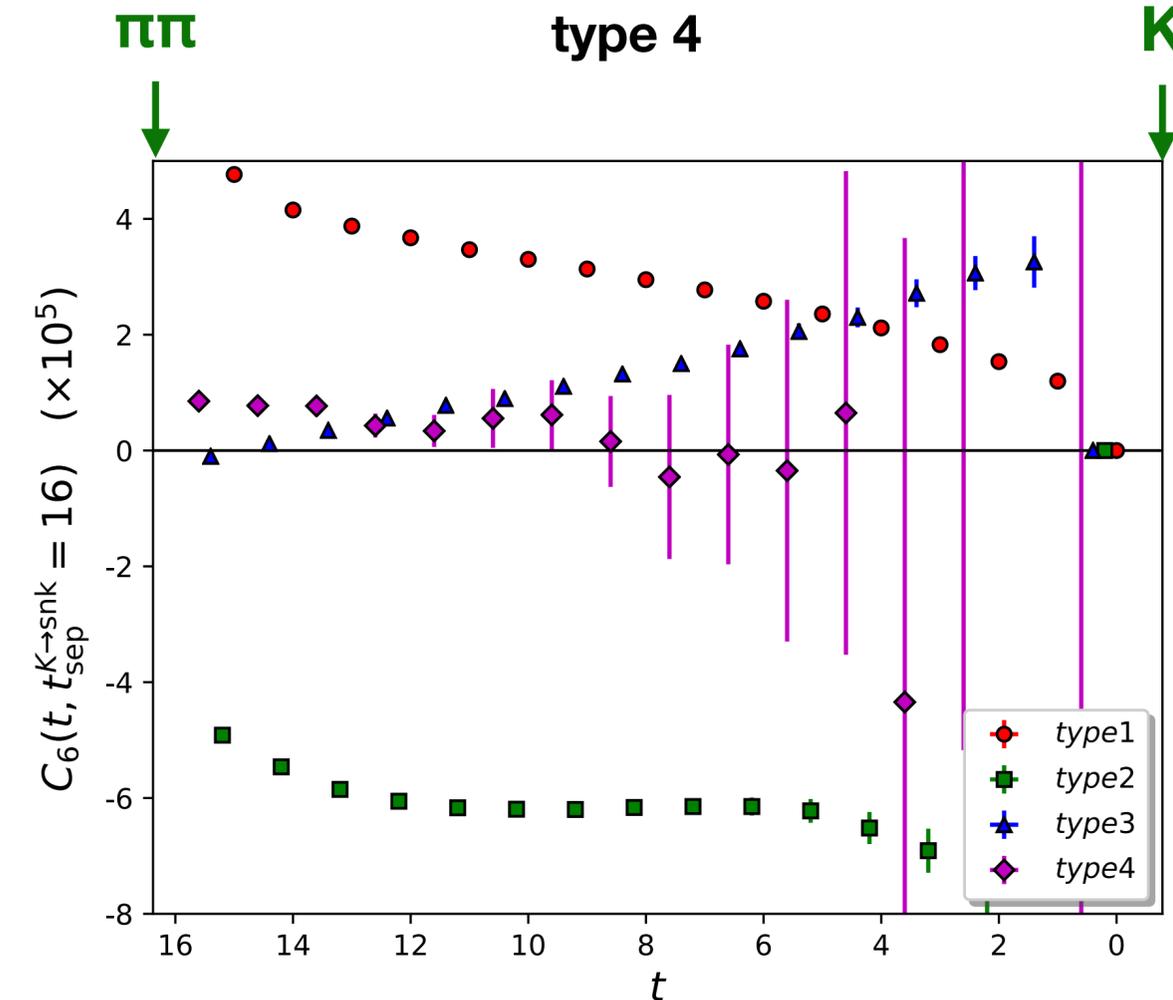
type 2



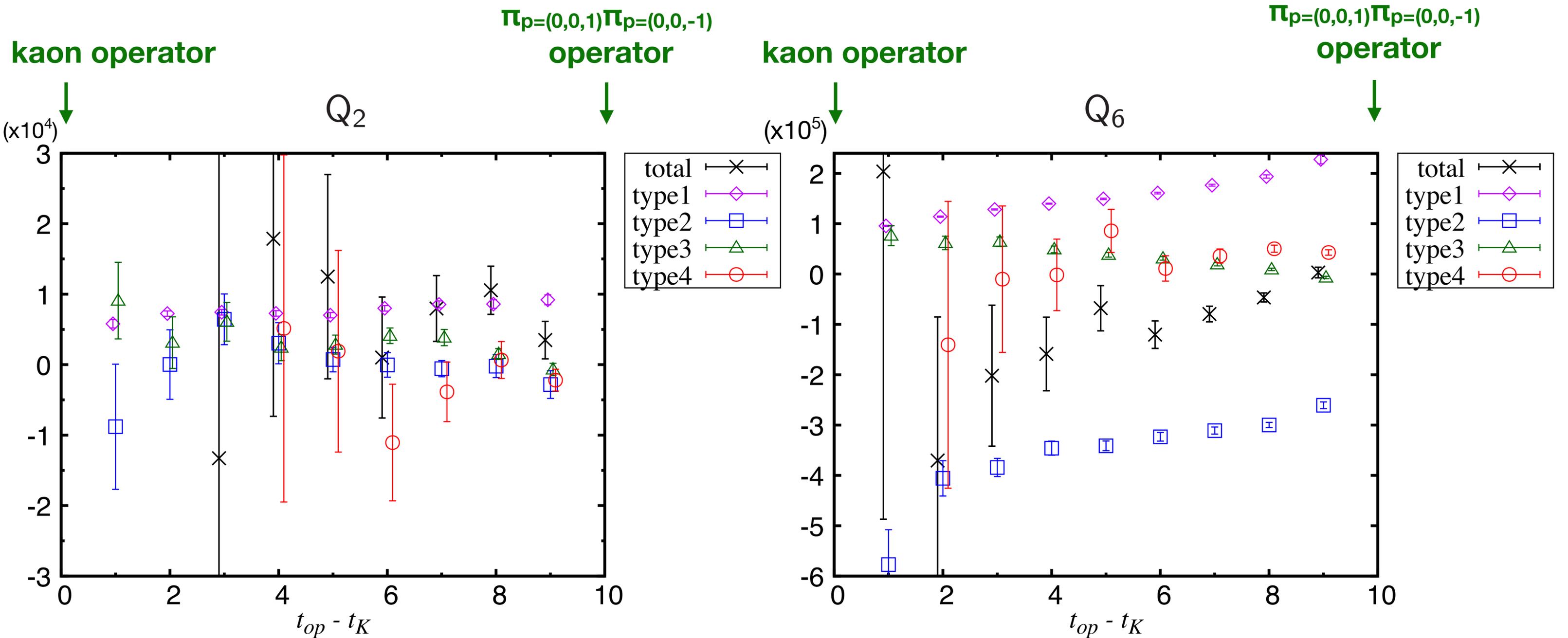
type 3



type 4



$I = 0$ correlation functions

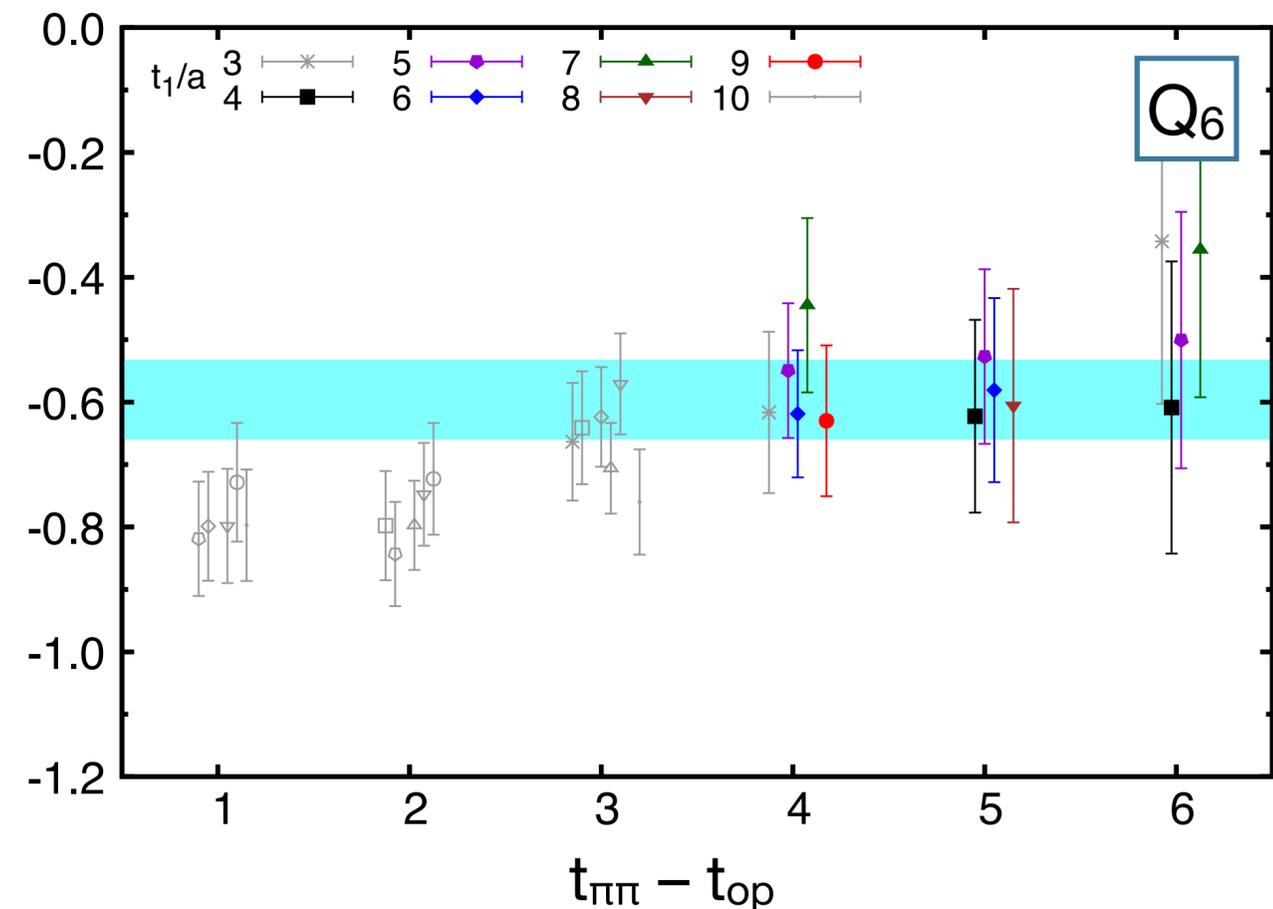
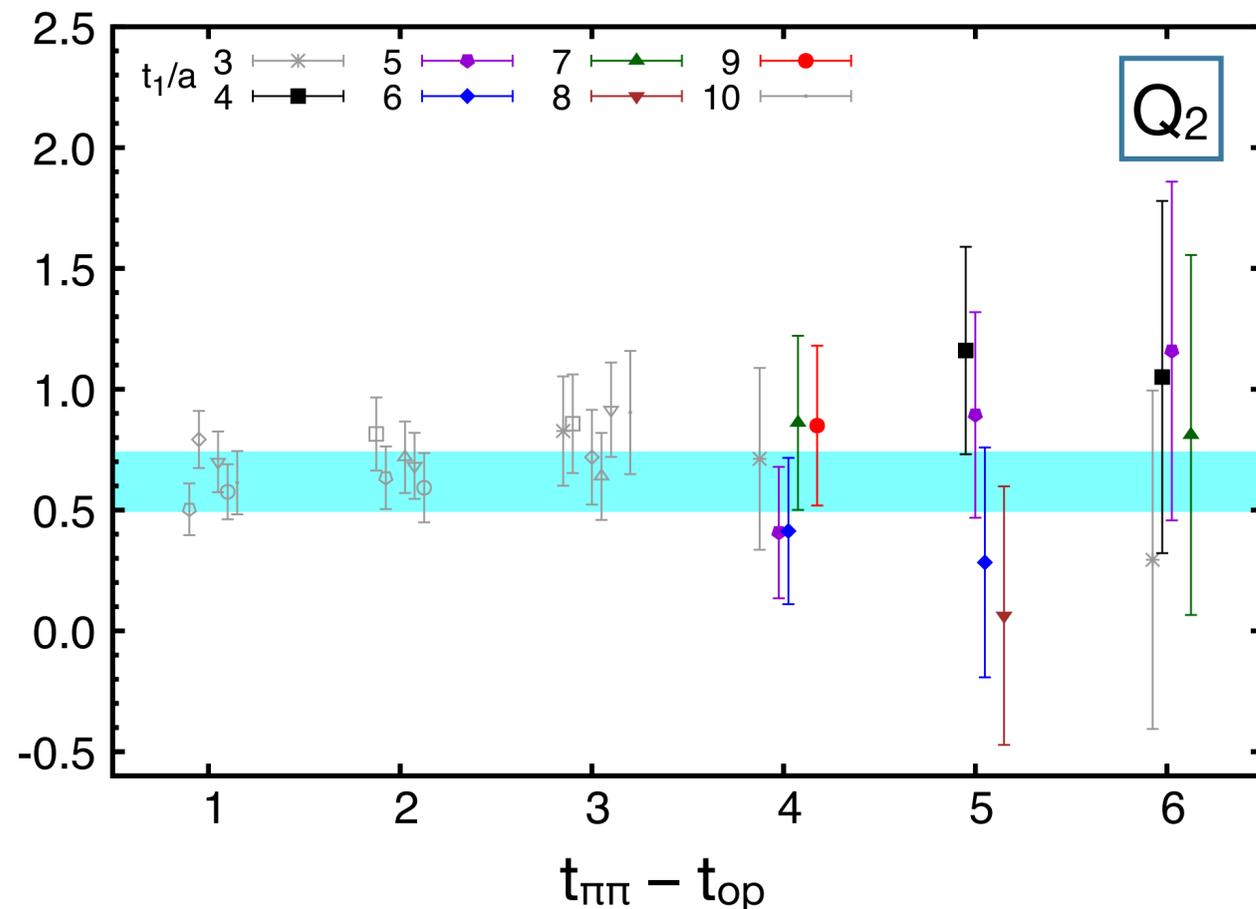


- Sparsen H_W for types1,2 – still more precise than type4
- Precision of type4 disconnected diagram

Effective matrix elements ($\Delta I = 1/2$)

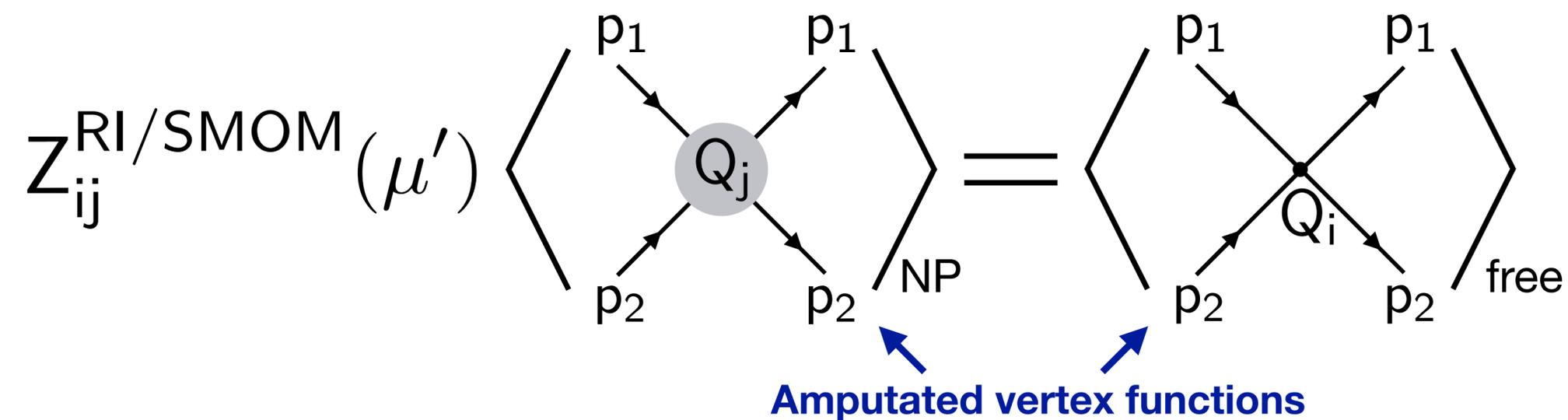
- $24^3 \times 64$
- Plateau appears
- : Correlated fit result with

$t_1 = t_{\text{op}} - t_K \geq 4$ && $t_2 = t_{\pi\pi} - t_{\text{op}} \geq 4$ (colored filled data points)



Translating to more physical ME

- Renormalization (RI/SMOM scheme)

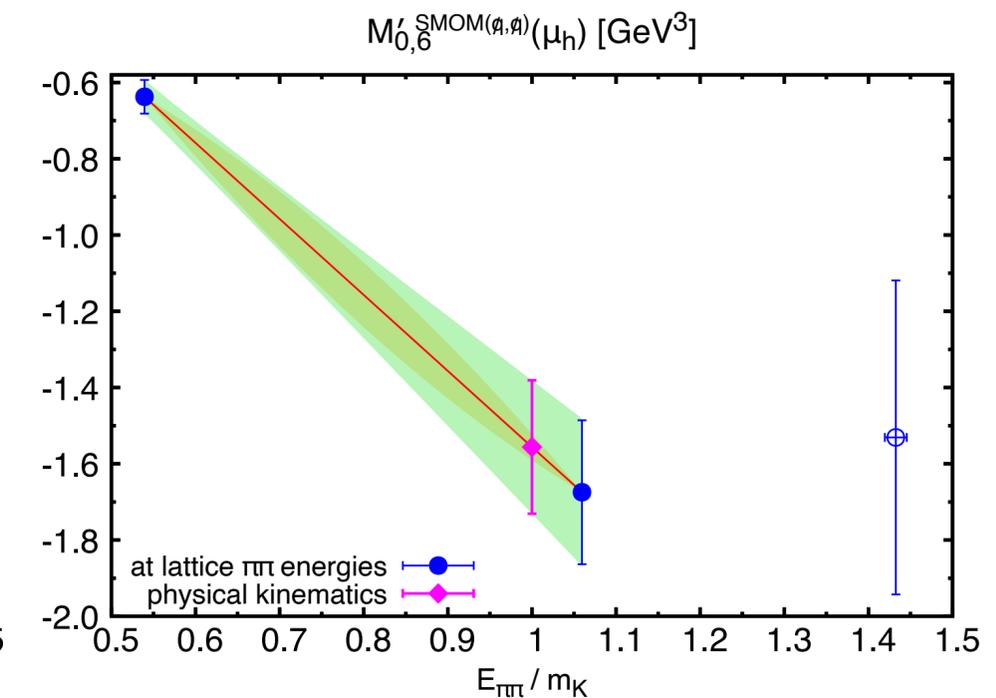
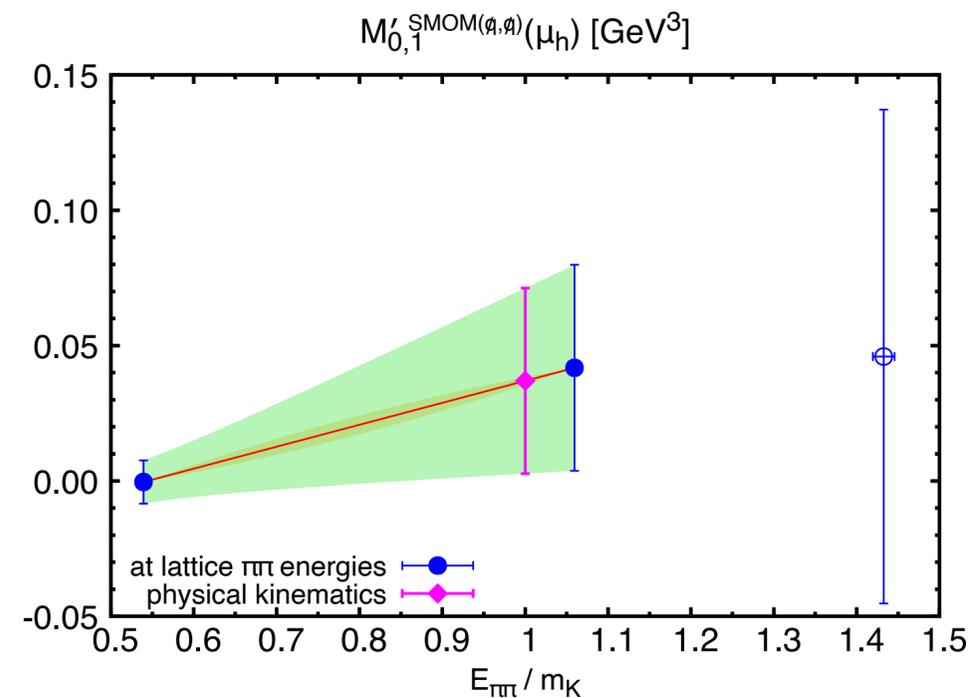


$$\mu'^2 = p_1^2 = p_2^2 = (p_1 - p_2)^2$$

- Interpolation

Examples of interpolation of renormalized ME

- Linear & quadratic in $E_{\pi\pi}/m_K$
- Systematic error estimated as lin vs quad is small as 1st excited st. close to on-shell



Precision performance

	32 ³ G-parity BC (previous work)	24 ³ Periodic BC	32 ³ Periodic BC
# of configurations	741	258 → 440	107 → 470
$\Delta I = 1/2$ ME via Q_2^{lat}	10%	14% → (11%)	14% → (6.7%)
$\Delta I = 1/2$ ME via Q_6^{lat}	6.5%	8.9% → (6.8%)	11% → (5.3%)
Re A_0	11%	13% → (10%)	14% → (6.7%)

Error % (statistical)

expectations of upcoming analysis in ()

- Good precision performance of PBC (ME with excited-state $\pi\pi$) compared to G-parity BC calculation (ME with ground-state $\pi\pi$)

Summary & Outlook

- Main sources of systematic errors at the moment
 - ▶ Finite lattice spacing - *Easier to take continuum limit with PBC as we already have lattice ensembles*
 - ▶ Wilson coefficients - *Independent study on-going*
 - ▶ QED/IB effects - *Theoretical approach being developed [Christ et al, PRD106, 014508 (2021)] with PBC*
- We are successful in
 - ▶ Extracting excited-state signals of the challenging $\Delta I = 1/2$ process
 - ▶ Good precision performance of PBC approach
- Precision will reach that of experiment in the near future
 - ▶ Could attract a lot of attention