# *Progress Towards the First Measurement of Direct CP-Violation in $K \to \pi\pi$ Decays From First Principles*

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# $K \to \pi\pi$ *Decays*

- Direct CP-violation first observed in $K \to \pi\pi$ decays.
- Two types of decay (Bose statistics forbids I=1):

$$\Delta I = 3/2 \;:\; K^+ \to (\pi^+\pi^0)_{I=2} \quad \text{with amplitude } A_2$$

$$\Delta I = 1/2 \;:\; K^0 \to (\pi^+\pi^-)_{I=0}, \quad K^0 \to (\pi^0\pi^0)_{I=0} \quad \text{with amplitude } A_0$$

- Direct CP-violation:

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

  where

  $\omega = \mathrm{Re}A_2/\mathrm{Re}A_0$ and $\delta_I$ are strong scattering phase shifts.

- $\epsilon'$ is highly sensitive to BSM sources of CPV.
- Strong interactions very important – origin ([arXiv:1212.1474]) of the so-called $\Delta I = 1/2$ rule: preference to decay to $I=0$ final state.
- Lattice QCD is the only known technique for accurately studying strong dynamics in the hadronic regime.

# *Brief Interlude: Lattice Methods*

- Discretize QCD Lagrangian in Euclidean space on finite volume.
- Integrate fermions out of path integral:
$$Z = \int \mathrm{d}U \ \det(D[U]) \exp\left(-S_g[U]\right)$$
- U are gauge links: $U_\mu = e^{iaA_\mu^a T^a} \in \mathrm{SU}(3)$
- Sample configurations of links from probability distribution Z using Monte Carlo methods.

# *Lattice Measurements*

- Measure amplitudes on each link configuration and average.

$$\int \mathrm{d}^3\vec{x}\ \langle 0|\bar{d}(x)\gamma^5 u(x)\bar{u}(0)\gamma^5 d(0)|0\rangle$$
$$= \frac{1}{N}\sum_{i=1}^{N}\int \mathrm{d}^3\vec{x}\ \mathrm{tr}\left(\gamma^5 D_d^{-1}(0,x)[U_i]\gamma^5 D_u^{-1}(x,0)[U_i]\right)$$
$$= a_0 e^{-m_\pi x_4} + a_1 e^{-E_1 x_4} + \ldots$$

- Ground state of system extracted in limit of large time separation.
- Excited state with energy $E_i\ (i > 0)$ requires multi-exponential fits to time dependence – typically very noisy and should be avoided if possible!

# *Lattice Techniques for* $K \to \pi\pi$ *Calculation*

- $M_W \ll$ hadronic scale ($1\ \mathrm{GeV}$): use Weak effective theory
- $\Delta S = 1$ effective operator:

$$\mathrm{CPV} : \tau = -V_{ts}^* V_{td}/(V_{ud} V_{us}^*)$$

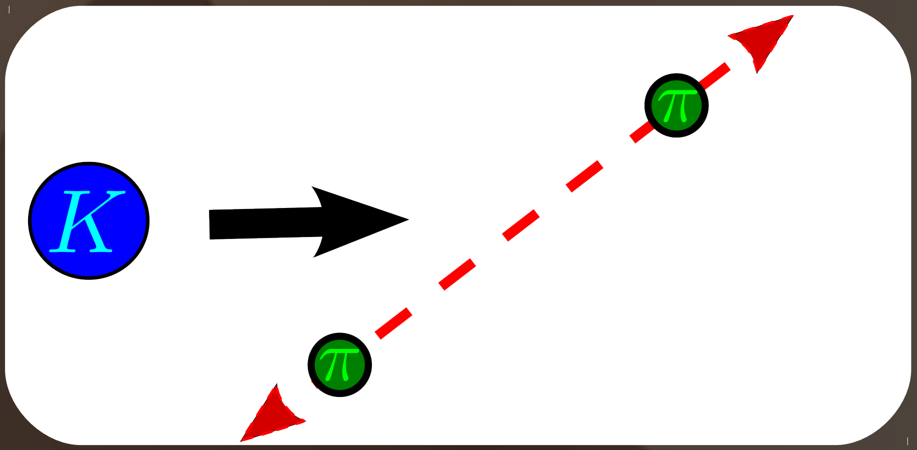
$$H_W^{\mathrm{eff}} = \frac{G_F}{\sqrt{2}} V_{us}^* V_{ud} \sum_{i=1}^{10} \left[ z_i(\mu) + \tau y_i(\mu) \right] Q_i(\mu)$$

  Wilson coefficients $y_i$ and $z_i$ calculated in perturbative regime.

- On lattice use low-energy operator: $\langle \pi\pi | Q_i | K \rangle$
- Non-perturbatively renormalize at high energy scale $\mu$

# *Finite-Volume Effects*

- Lattice has finite size $\sim (3\ \mathrm{fm})^3$ : finite-volume effects play large role: allowed energy states discretized. State normalization differs. Continuous pion FSI.
- Finite-volume lattice decay amplitudes are related to those in the infinite-volume by the "Lellouch-Luscher" formula.
- This requires physical kinematics - $E_{\pi\pi} = m_K$
- $m_\pi = 135\ \mathrm{MeV}$ and $m_K = 500\ \mathrm{MeV}$ : need moving pions




- However ground state (easiest and cleanest state to isolate on lattice) comprises stationary pions. How can we solve this?

# *Workaround for* $\Delta I = 3/2$ *calculation*

- On the lattice we have the freedom to choose boundary conditions imposed when calculating quark propagators.
- Typically use periodic BCs: $\psi(x+L) = \psi(x) \;\Rightarrow\; p = 2\pi n/L$
- Applying antiperiodic BCs on just d-quark prop:

$$d(x+L) = -d(x) \;\Rightarrow\; p_d = (2n+1)\pi/L$$

- Charged pion $(u\bar{d})(x+L) = -(u\bar{d})(x)$ : ground state $p_{\pi^\pm} = \pm\pi/L$
- Problem: we need $\pi^+\pi^0$ but $(d\bar{d})(x+L) = +(d\bar{d})(x)$ i.e. periodic BCs with minimum momentum 0. However...
- Wigner-Eckart theorem (in SU(2) isospin):

$$\langle(\pi^+\pi^0)_{I=2}|Q^{\Delta I_z=1/2}|K^+\rangle = \frac{\sqrt{3}}{2}\langle(\pi^+\pi^+)_{I=2}|Q^{\Delta I_z=3/2}|K^+\rangle$$

- APBCs on d-quark break isospin symmetry allowing mixing between isospin states: however $\pi^+\pi^+$ is the only charge-2 state hence it cannot mix.

# Results

- RBC & UKQCD recently published (arXiv:1111.1699) calculation of $\Delta I = 3/2$ decay using:
  - 2+1f domain wall fermions on a $32^3 \times 64 \times 32$ lattice with $a^{-1} = 1.37(1)$ GeV.
  - Near physical pions: $m_\pi^{PQ} \sim 140$ MeV$, m_\pi^{\rm uni} \sim 170$ MeV
  - (Nearly) energy conserving decays: $p = \sqrt{2}\pi/L$ gave $E_{\pi\pi} = 486$ MeV vs. $m_K = 506$ MeV
- Determined

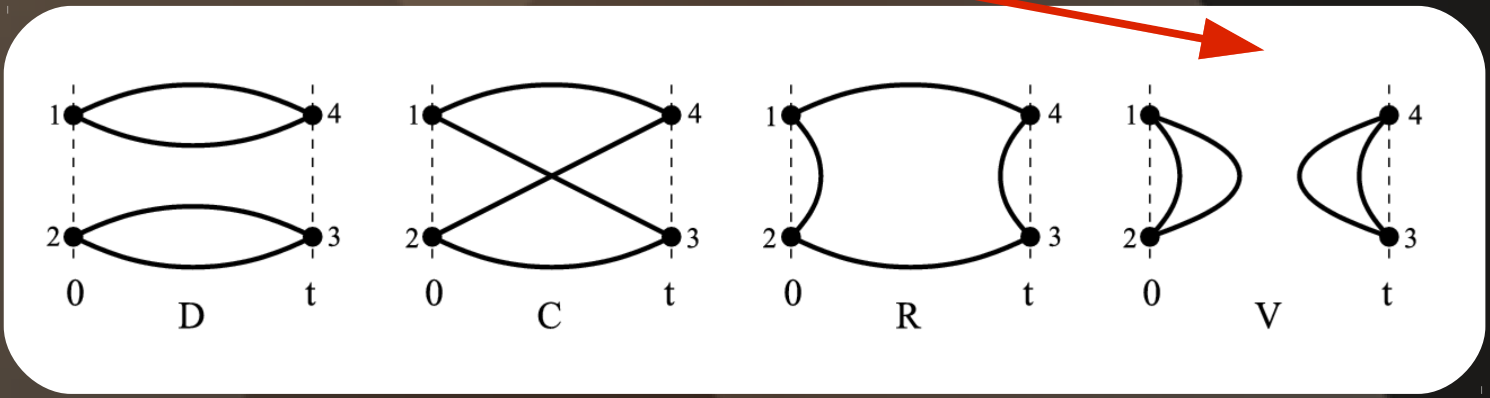
$$\mathrm{Re}A_2 = [1.436(62)_{\rm stat}(258)_{\rm sys}] \times 10^{-8}\ \mathrm{GeV}$$

$$\mathrm{Im}A_2 = -[6.83(51)_{\rm stat}(1.30)_{\rm sys}] \times 10^{-8}\ \mathrm{GeV}$$

- Large systematic error: 15% discretization error: continuum limit needed. 7% FV corrections, 6% renormalization and 8% from PT truncation of Wilson coeffs.
- New ensembles have since been generated which will substantially reduce systematics.

# *Computational challenges of* $\Delta I = 1/2$ *calculation*

- Measuring $A_0$ is considerably more challenging.
- Measure both $K^0 \to \pi^+\pi^-$ and $K^0 \to \pi^0\pi^0$ .
- $\pi\pi$ state has vacuum quantum numbers, hence there are disconnected diagrams:




- Need large statistics and many source positions but with modern hardware (e.g. IBM BlueGene/Q machines codeveloped with members of RBC/UKQCD) we can now perform such calculations with large enough physical volumes.

# *Obtaining physical kinematics in the $\Delta I = 1/2$ calculation*

- Must measure $K^0 \to \pi^+\pi^-$ and $K^0 \to \pi^0\pi^0$
- Wigner-Eckart trick cannot be used for $I = 0$ final state
- If we stay with APBC on d-quarks, isospin-breaking would allow mixing between $I = 0$ and $I = 2$ final states.
- Require moving $\pi^0$, but momentum cancels in $d\bar{d}$
- Need to apply BCs that commute with isospin and produce moving $\pi^0$ as well as $\pi^+$ and $\pi^-$.
- G-parity boundary conditions satisfy these criteria.

# *G-Parity Boundary Conditions*

- G-parity is a charge conjugation followed by a 180 degree isospin rotation about the y-axis:

$$\hat{G} = \hat{C}e^{i\pi \hat{I}_y} \quad : \quad \begin{aligned} \hat{G}|\pi^{\pm}\rangle &= -|\pi^{\pm}\rangle \\ \hat{G}|\pi^{0}\rangle &= -|\pi^{0}\rangle \end{aligned}$$

- Pions are all eigenstates with e-val -1, hence G-parity BCs make pion wavefunctions antiperiodic, with minimum momentum $\pi/L$ .
- G-parity commutes with isospin.

Kim, arXiv:hep-lat/0311003 (2003)

Wiese, Nucl.Phys.B375, (1992)

- At the quark level:

$$\hat{G}\begin{pmatrix} u \\ d \end{pmatrix} = \begin{pmatrix} -C\bar{d}^T \\ C\bar{u}^T \end{pmatrix}$$

where $C = \gamma^2\gamma^4$ . in our conventions

- Requires extensive code modifications to treat two flavours that mix at the boundary.

# *Gauge Field Boundary Conditions*

- Dirac operator for $C\bar{u}^T$ field involves conjugate links $U^*$ .
- As this field transitions seamlessly to the $d$ -field at the boundary, the links must also transition from $U$ to $U^*$ , i.e. links obey complex conjugate BCs (equiv to charge conjugation BCs).
- Boundary link gauge transformation is unusual:

$$U_\mu(L-1) \to V^\dagger(L-1)U_\mu(L-1)V^*(0)$$

- Necessitates generation of new ensemble of gauge links satisfying these BCs.

(Note: for other choices of BC, e.g. APBC, new ensembles would still need to be generated, but due to presence of disconnected diagrams)

# *Unusual Contractions*

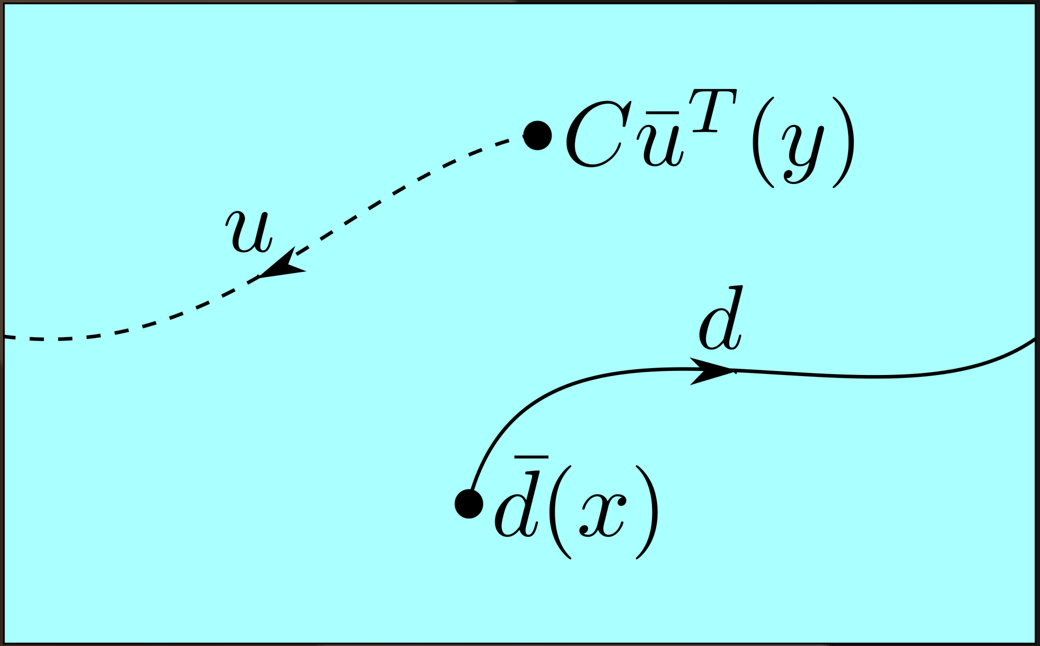
- Flavor mixing at boundary allows contraction of up and down fields:

$$\mathcal{G}^{(2,1)}_{y,x} = C\bar{u}^T_y \bar{d}_x \,,$$
$$\mathcal{G}^{(1,2)}_{x,y} = -d_x u^T_y C^T$$

- Interpret as boundary creating/destroying flavor (violating baryon number)
- More Wick contractions to evaluate.
- Some states mix at the boundary, e.g.

$$uud \leftrightarrow \bar{d}\bar{d}\bar{u}$$

hence the proton is not an eigenstate.



# *Kaons*

- $K \to \pi\pi$ calculation needs stationary $K^0$.
- Need an eigenstate with e-val +1 for periodic BCs and hence $p_{\min} = 0$ .
- $K^0 = \bar{s}d$ is not a G-parity eigenstate: $\bar{s}d \leftrightarrow \bar{s}\bar{u}$
- Introduce 'strange isospin' ($I'$): s-quark in doublet $\begin{pmatrix} s' \\ s \end{pmatrix}$
- Can now form an eigenstate:

$$K_0^g = \frac{1}{\sqrt{2}}(\bar{s}d + \bar{u}s') = \frac{1}{\sqrt{2}}(K_0 + K_0')$$

  with e-val +1.
- Unphysical partner $K_0'$ mixes with physical state $K_0$. For a physical operator, e.g. $A_\mu = \bar{s}\gamma^5\gamma^\mu d$ , $K_0'$ only contributes after propagating through the boundary: suppressed like $e^{-m_K L}$ , a sub-% effect.
- Up to these effects, only change is a normalization factor.

# *Locality*

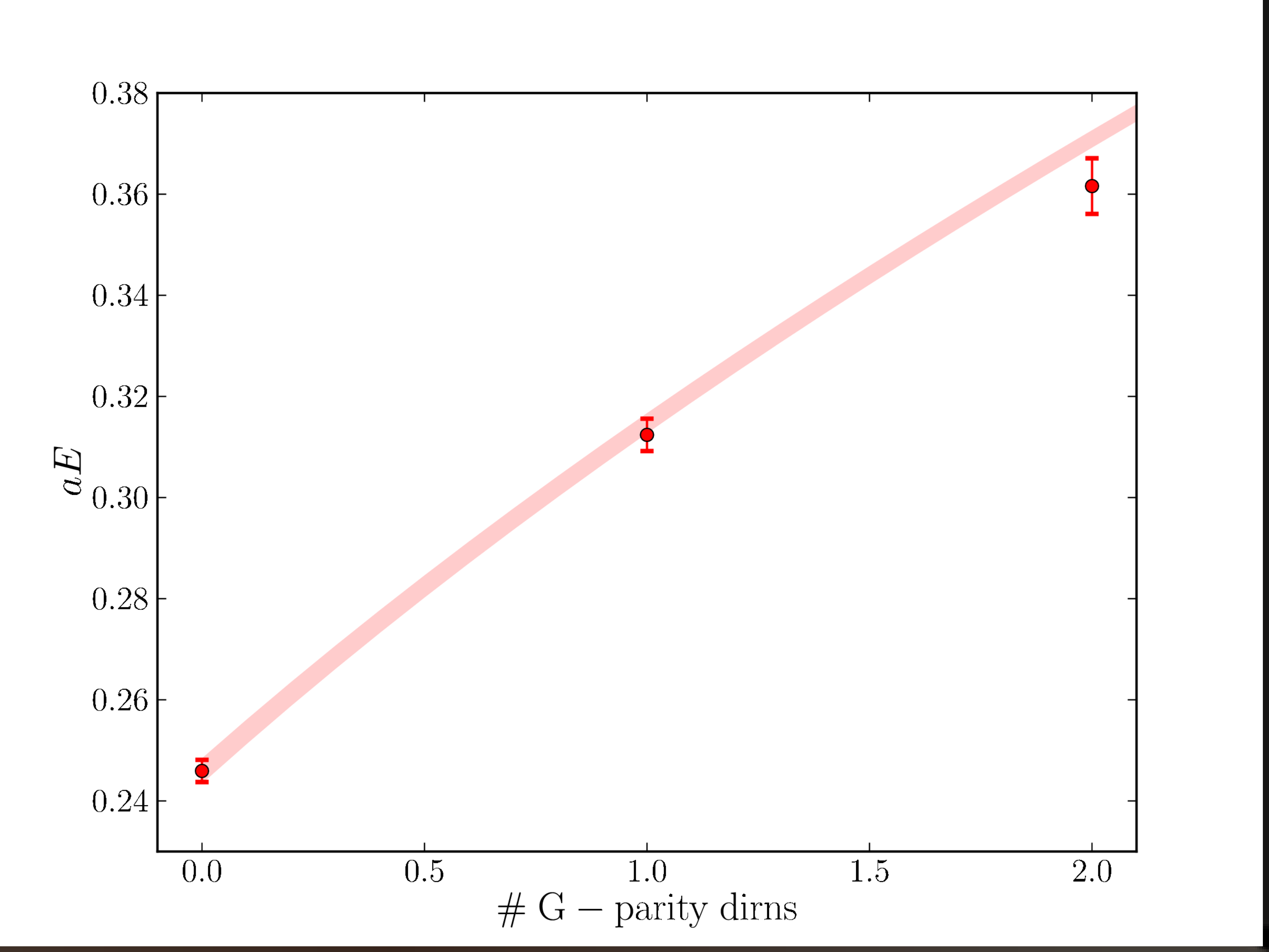
- Theory has one too many flavors. Must take square-root of $s'/s$ determinant in evolution to revert to 3 flavors.
- Determinant becomes non-local, violating a necessary condition for formal analytic continuation of Euclidean results to Minkowski (Osterwalder-Schrader theorem).
- Non-locality is however only a boundary effect that vanishes as $L \to \infty$ . With sufficiently large volumes the effect should be benign.
- Estimate size of effect : Staggered ChPT?

# Results: Pion Dispersion Relation

- Generated $16^3 \times 32$ fully dynamical test ensembles with G-parity BCs in 0,1,2 directions.

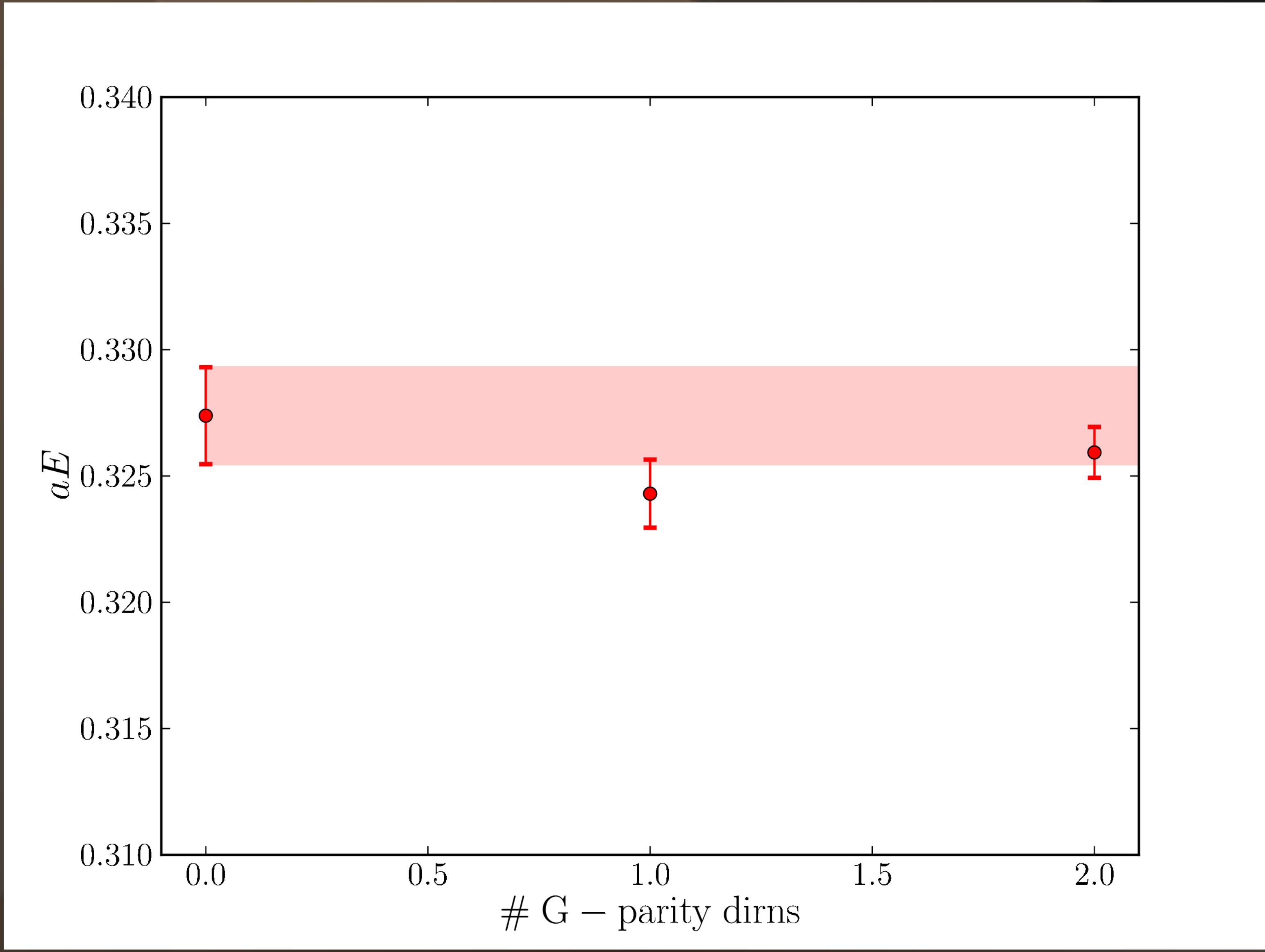
$a^{-1} = 1.73(3)$ GeV

$m_\pi \sim 420$ MeV



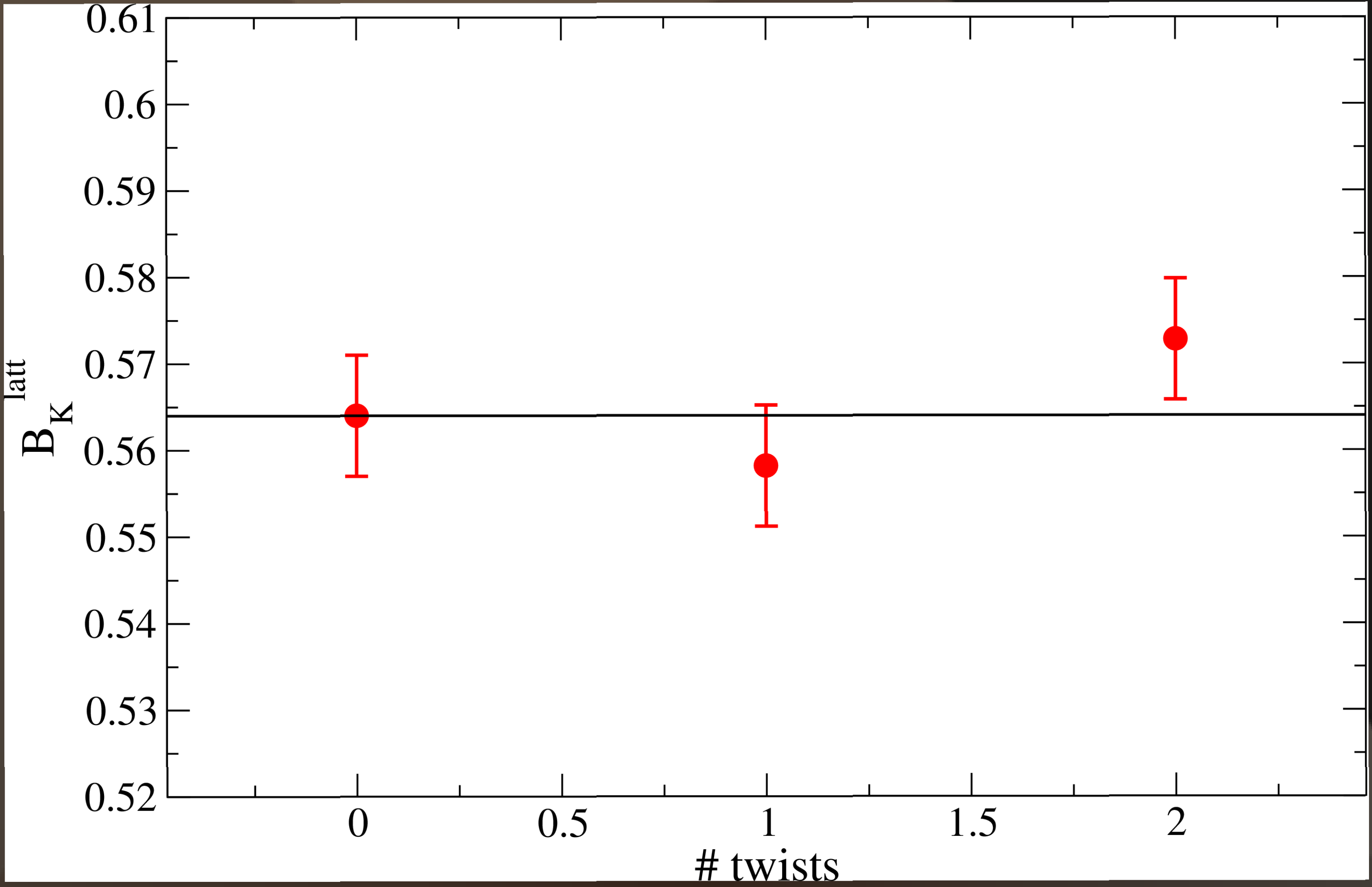
# Results: Kaon Dispersion Relation

- Stationary kaon states demonstrated:



# *Results:* $B_K$

- $\bar{K}^0 \leftrightarrow K^0$ mixing amplitude shown to be independent as expected. These 4-quark effective vertices are similar to those used in $K \to \pi\pi$ calculation, hence this is a valuable demonstration.



# *Ensemble for physical* $K \to (\pi\pi)_{I=0}$ *calculation*

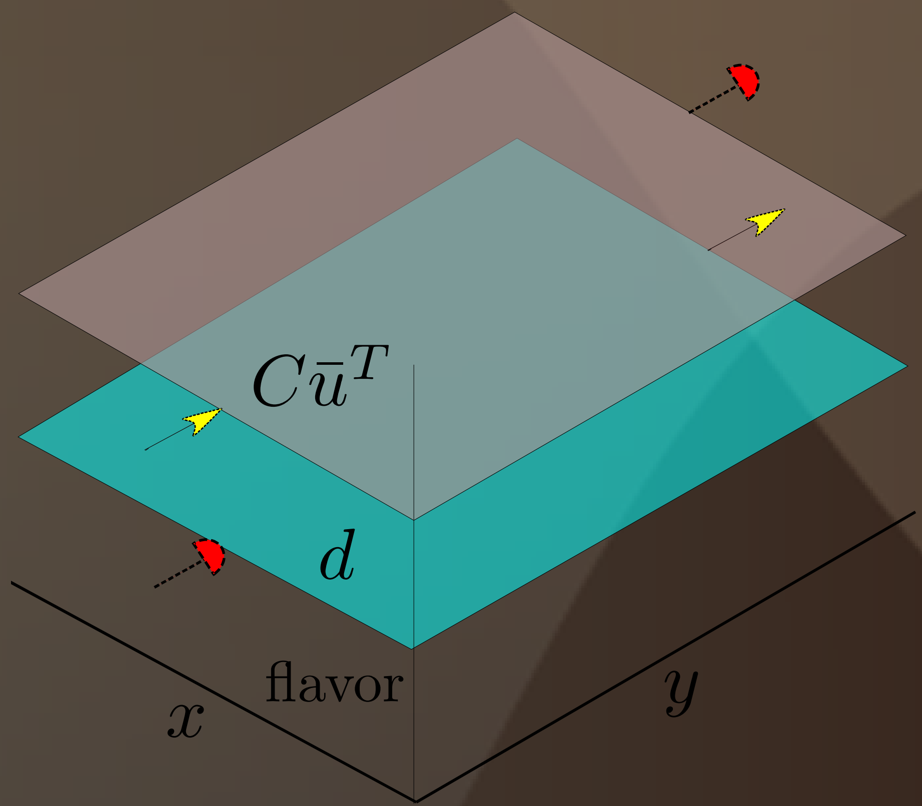
- Evolution code (CPS+BFM) for Mobius DW and Iwasaki+DSDR gauge action with G-parity BCs is now complete.
- Generation of $32^3 \times 64 \times 16$ configurations has been underway for over a month on the USQCD BGQ half-rack at BNL. Will soon have enough thermalized configurations to begin testing.
- Parameters are the same as the ensemble used for the $\Delta I = 3/2$ calculation: $\beta = 1.75$ $(a^{-1} = 1.37(1)\ \mathrm{GeV})$ and $m_\pi = 143(1)\ \mathrm{MeV}$ (PQ) , $171(1)\ \mathrm{MeV}$ (unitary)
- Mobius parameters tuned to match to regular DWF, allows factor of 2 reduction in Ls for same physics.
- Dirac matrix is intrinsically 2-flavor, hence $\det(M^\dagger M)$ contains 4 flavors: must use RHMC even for light quarks.
- RHMC cost overhead (no chronological inverter) makes using multiple Hasenbusch steps more expensive. Ensemble is more difficult to tune.

# Status and Outlook

- More precise measurements of $\Delta I = 3/2$ amplitude will soon be completed.
- Substantial progress has been made in the march towards calculating the $\Delta I = 1/2$ amplitude.
- Further investigation of systematic errors associated with G-parity technique is required. However all tests to date have not indicated any sicknesses with the approach.
- Work still to be done in deciding best technique for measuring disconnected diagrams in the more complex environment of the calculation with G-parity.
- G-parity techniques may be useful for controlling errors in other frontier calculations performed by RBC & UKQCD, e.g. $K_L - K_S$ mass difference.

# *Extra Slides*

# *Layout of the Problem*




- Two fermion fields on each site indexed by flavor index:

$$\psi^{(1)}(x) = d(x),\ \psi^{(2)}(x) = C\bar{u}^T(x)$$

- BCs are:

$$\psi^{(1)}(x + L\hat{y}) = \psi^{(2)}(x),$$
$$\psi^{(2)}(x + L\hat{y}) = -\psi^{(1)}(x),$$

- Periodic BCs in other dirs.
- Single U-field shared by both flavors, with complex conj BCs.
- Dirac op for $\psi^{(2)}$ uses $U_\mu^*$.

# *Exploiting the Gauge-Field Symmetry*

- Quark fields interact with the same gauge fields. Suggests propagators are related in some way.
- In fact, we find that:
$$\begin{aligned}\mathcal{G}^{(2,2)}_{x,z} &= -\gamma^5 C \left[\mathcal{G}^{(1,1)}_{x,z}\right]^* C\gamma^5 \\ \mathcal{G}^{(1,2)}_{x,z} &= +\gamma^5 C \left[\mathcal{G}^{(2,1)}_{x,z}\right]^* C\gamma^5\end{aligned}$$
- Relative sign due to – sign at boundary between u and d.
- Can be rewritten $\mathcal{G}_{x,z} = \gamma^5 C \sigma_1 \sigma_3 [\mathcal{G}_{x,z}]^* \sigma_3 \sigma_1 C^\dagger \gamma^5$ where $\mathcal{G}$ are 2x2 flavour (also spin/colour) matrices.
- Substantially simplifies contractions: form is often identical to standard form up to additional flavour matrices: e.g.

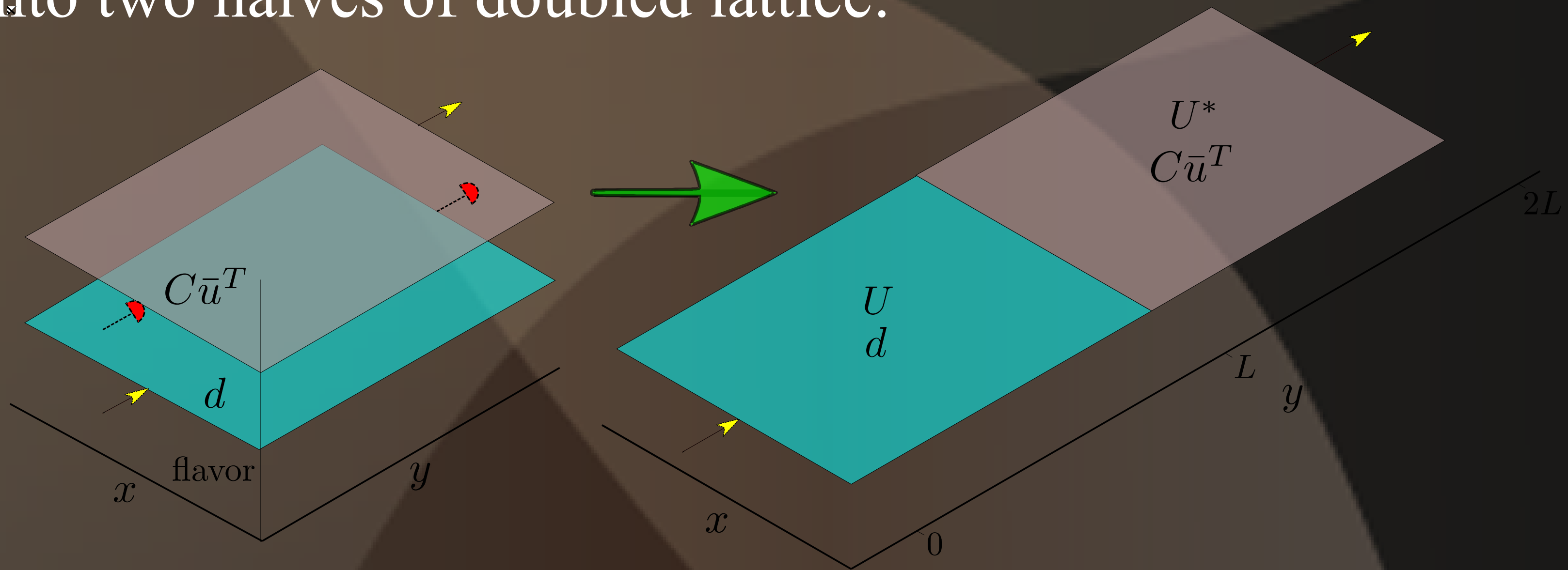
$$\langle \pi(x) | \pi(y) \rangle = \mathrm{tr}\ F_1 \mathcal{G}_{x,y} \sigma_3 \mathcal{G}^\dagger_{x,y}$$ (in large time limit)

$$F_1 = \frac{1}{2}(1-\sigma_3)$$

Usually $\mathrm{tr}\ \mathcal{G}_{x,y}\mathcal{G}^\dagger_{x,y}$

# *The One-Flavor Method*

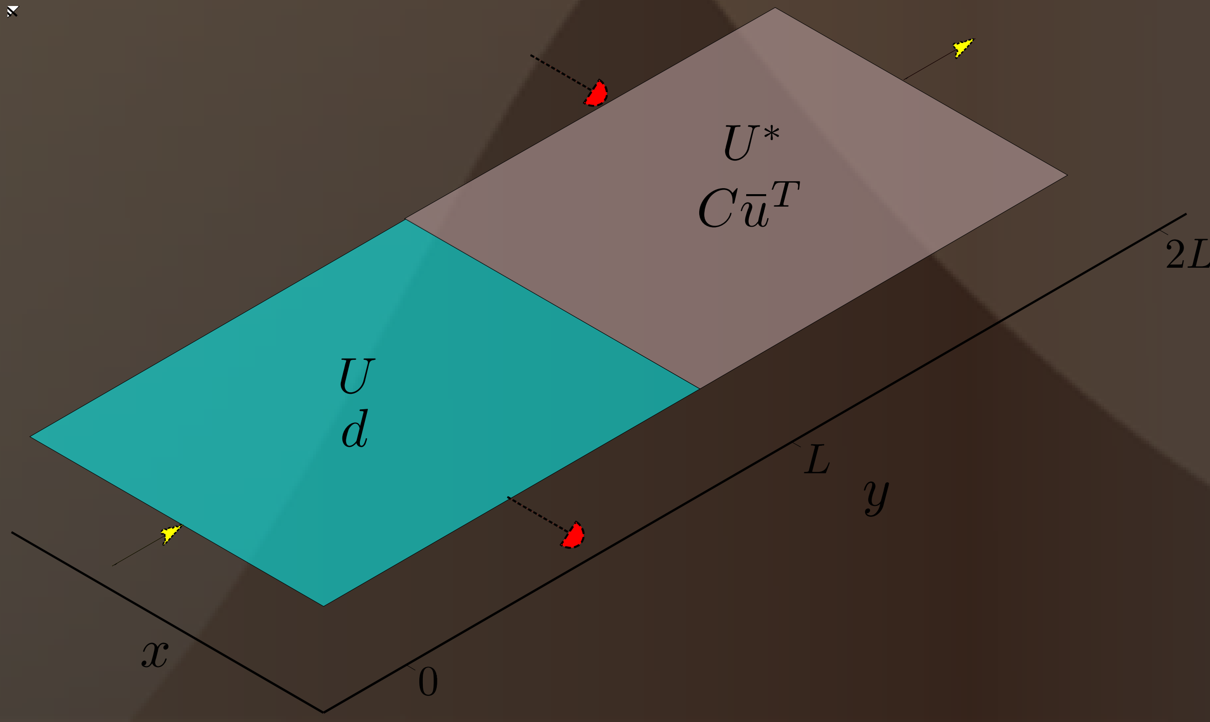
- Obtain equivalent formulation by unwrapping flavor indices onto two halves of doubled lattice:




- Antiperiodic boundary conditions in G-parity direction.
- $U$ -field on first half and $U^*$-field on second half.

# Choosing an Approach

- One flavor setup is much easier to implement.
- However recall that we needed APBC in 2 directions for physical kinematics in $\Delta I = 3/2$ calculation.
- G-parity in >1 dir using one-flavor method requires doubling the lattice again, which is highly inefficient.
- A second approach requires non-nearest neighbour communication:




- Also inefficient depending on machine architecture.
- Choose to implement two-flavor method.

# K $\rightarrow \pi\pi$ *Decays on the Lattice*

- Energies are discretized in finite-volume.
- For two non-interacting pions $E_{\pi\pi} = 2\sqrt{m_\pi^2 + k_\pi^2}$ , where components of $k_\pi$ discretized in units of $2\pi/L$ assuming periodic BCs.
- Interactions shift the allowed energies such that $k_\pi$ are not known a priori and must be measured.
- Allowed $k_\pi$ are quantized by Luscher condition $\delta(k_\pi) + \phi(k_\pi) = n\pi$ , hence we can determine the scattering phase shifts $\delta(k_\pi)$ once $k_\pi$ is measured.
- Switching on effective weak interaction $H_W$ , allowed energies are further modified:

$$k - k_\pi = \Delta k = \pm \frac{m_K}{4k_\pi}|M| + O(|M|^2)$$

- Note this uses degenerate PT, thus <u>requires $E_{\pi\pi} = m_K$</u>

# $\mathbf{K} \to \pi\pi$ *Decays on the Lattice*

- Switching on $H_W$ induces corresponding change in infinite-volume scattering lengths:

$$\Delta\delta_0 = \mp \frac{k_\pi |A|^2}{32\pi m_K^2 |M|} + O(H_W^2)$$

- Imposing Luscher factor allows us to combine equations for $\Delta\delta_0$ and $\Delta k$, giving the Lellouch-Luscher formula:

$$|A|^2 = 8\pi \left\{ q\frac{\partial\phi}{\partial q} + k\frac{\partial\delta_0}{\partial k} \right\}_{k=k_\pi} \left(\frac{m_K}{k_\pi}\right)^3 |M|^2$$

  where $q = kL/2\pi$

- As $\phi$ is analytic, only unknown is $\partial\delta_0/\partial k$. We measure this from the phenomenological curve at the measured $k_\pi$ .

# $\mathrm{K} \to \pi\pi$ *Decays on the Lattice*

- Infinite-volume S-matrix $\langle \pi\pi | \mathcal{L}_W | K \rangle = A e^{i\delta_0}$
  final state scattering induces dependence on s-wave scattering length $\delta_0$ .

- Finite-volume matrix element: $M = \langle \pi\pi | H_W | K \rangle$
  where $H_W$ is effective weak vertex.

- Using degenerate PT (<u>requires $E_{\pi\pi} = m_K$</u>) ,weak effective theory and Luscher's quantization condition

$$\delta(k_\pi) + \phi(k_\pi) = n\pi \qquad\qquad E_{\pi\pi} = 2\sqrt{m_\pi^2 + k_\pi^2}$$

  one obtains the Lellouch-Luscher formula relating them:

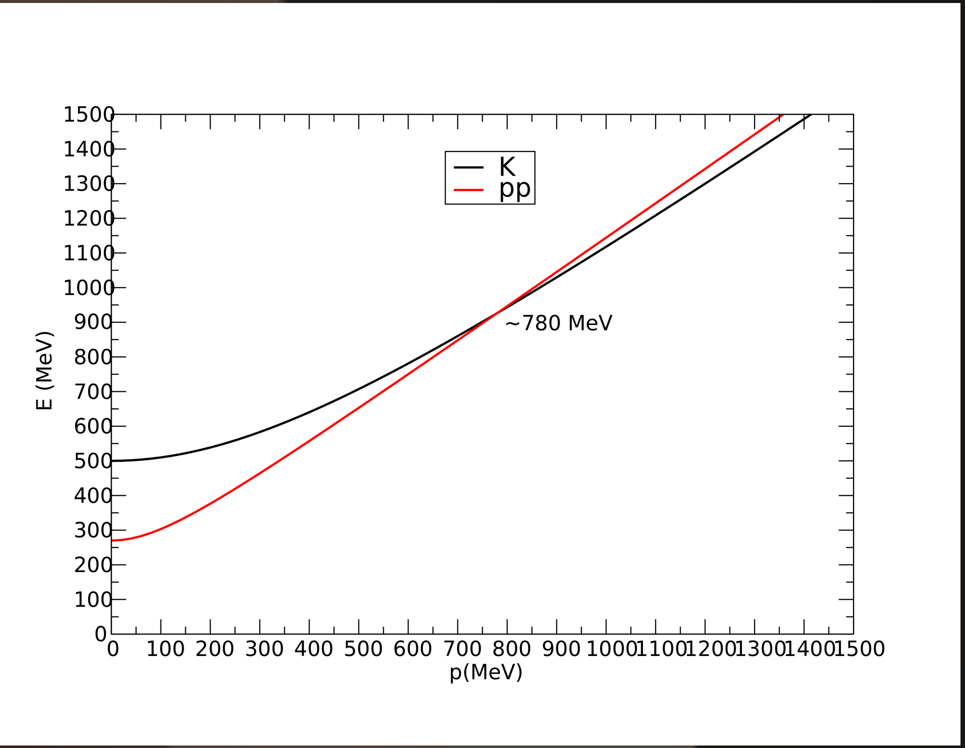
$$|A|^2 = 8\pi \left\{ q \frac{\partial \phi}{\partial q} + k \frac{\partial \delta_0}{\partial k} \right\}_{k=k_\pi} \left( \frac{m_K}{k_\pi} \right)^3 |M|^2$$

  where $q = kL/2\pi$

- As $\phi$ is analytic, only unknown is $\partial\delta_0/\partial k$. We measure this from the phenomenological curve at the measured $k_\pi$

# *Moving kaon?*

- One possibility is to consider a moving kaon $K(p_K)$ decaying to $\pi(p_\pi)\pi(0)$. Need $\sqrt{m_K^2 + p_K^2} \approx \sqrt{m_\pi^2 + p_\pi^2} + m_\pi$
- ~780 MeV energy required.
- SNR decreases exponentially in the energy difference between the state energy and the pion mass: this will be too noisy.



# *Physical kinematics and moving pions*

- Finite-volume lattice decay amplitudes are related to those in the infinite-volume by the "Lellouch-Luscher" formula.
- This requires physical kinematics - $E_{\pi\pi} = m_K$
- $m_\pi = 135\ \mathrm{MeV}$ and $m_K = 500\ \mathrm{MeV}$ : need moving pions
- However ground state comprises stationary pions.
- Could attempt to tune L such that first excited state energy matches kaon mass.
- This will be extremely noisy, and, especially when there are disconnected diagrams, it is highly unlikely that a decent signal could be extracted.

# *Force Histogram*

- Example force histogram produced during evolution tuning