Periodic Pion-Pion Scattering at the Physical Point: Update

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Lattice 2019

Outline

Motivation: $K \to \pi\pi$

- $\pi\pi$ scattering has not been studied using physical quark masses
- Direct comparison of low energy QCD - experiment vs. lattice
- $K \to \pi\pi$ - an important decay to understand CP violation
- Lattice calculation difficult, Gparity calculation already done, but needs a check
- See upcoming G-parity Pipi paper (work of T. Wang, C. Kelly, et. al)
- Continuum scattering phase shifts from lattice energies (main goal)

G-parity vs. Periodic Boundary Conditions

We compute using spatially periodic boundary conditions (antiperiodic in time)

- G-parity - charge conjugation + 180 degree isospin rotation
- G-parity eliminates (kinematically disallowed) stationary $\pi\pi$ state (afterwards no stationary pions exist on the lattice)
- G-parity and Periodic boundary conditions have different finite volume errors, useful check
- G-parity needs either double the lattice in each G-parity direction or double flavor (isospin couples to space; complicated!)
- Periodic lattices ready for use, evolution cost amortized
- Good exercise for $K \to \pi\pi$ (same physics is present, strong phase common to both)

Outline

Lüscher Method - Overview

Small interaction region (QCD is short range) $V(x) \neq 0, |x| < R$.
Interaction region is much smaller than lattice. Lüscher gives a quantization condition which maps lattice spectra onto infinite volume scattering phase shifts.
Lüscher's (Simplified) formula[1]:

$$E_{\pi\pi} = 2\sqrt{m_\pi^2 + p^2}$$

$$\delta(p) = -\phi(k) + \pi n, \;\; n \in \mathbb{Z}$$

$$\tan \;\phi(k) = \frac{\pi^{3/2}\kappa}{Z_{00}(1;\kappa^2)}$$

$$\kappa = \frac{pL}{2\pi}$$

(For lowest angular momentum states $J = 0, 1$; $J = 1$ in the center of mass frame)

Infinite Volume Scattering Phase Shifts

We can then compare to experiment via phenomenological data on phase shift vs. energy.

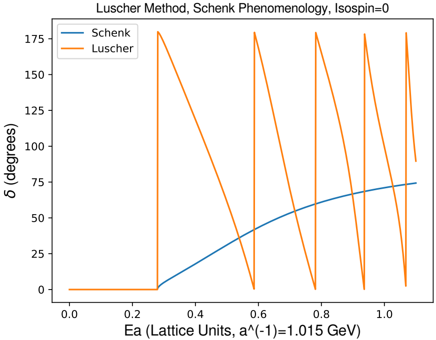


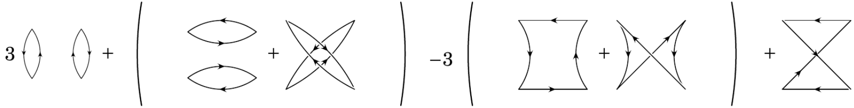
Figure: Phenomenology* v. Luscher, predictions for $I = 0$ on 24^3, $a^{-1} = 1.015$ GeV. The ultimate goal is to obtain enough phase shift points to fit to a Breit-Wigner form and extract the mass and resonance width.

(*=phenomology data is outdated, useful for illustrative purposes only)

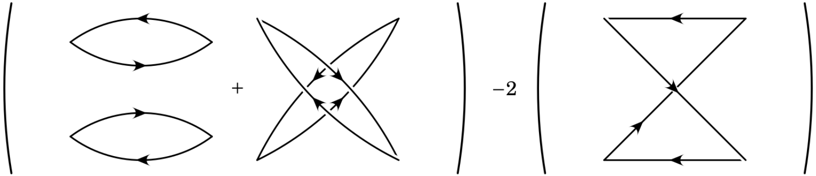
Operator Construction: Isospin Projection

On our lattices (2 + 1 flavors), isospin is a good symmetry. We want to know the spectra of the different isospin channels $I = 0, 1, 2$ Examples below. Note the disconnected diagram in $I = 0$ which is very noisy, but important (needs large statistics).

$\langle I = 0 | I = 0 \rangle$:



$\langle I = 2 | I = 2 \rangle$:



Operator Construction:Spin Irrep Projection

- We would like to project our operator set onto the lowest angular momentum in each isospin channel (K has $J = 0$).
- Continuum angular momentum states have known correspondence to irreps of the group of allowed lattice rotations O (we can project continuum representations to lattice irreps)
- Each irrep in general corresponds to a tower of angular momentum states
- We project onto irreps with the lowest spins $\rightarrow$ easier to resolve
- Pions (identical on the lattice) symmetric under exchange (Bose symmetry). $\Rightarrow I = 1$ needs p-wave irrep: T_1 ($J = 1, I = 1$ both antisymmetric)
- $I = 0, 2$ needs s-wave irrep: A_1

(group theory due to A. Meyer)

Outline

Extracting Spectra from Correlation Functions

We can define a generalized eigenvalue problem (GEVP) from an *NxN* matrix of correlation functions we compute on the lattice

$$C_{ij} \equiv \sum_m \left\langle m|\hat{O}_i(t)\hat{O}(0)_j^\dagger|m\right\rangle = \sum_{n=1}^{\infty} \left(e^{-E_n t}\psi_{ni}\psi_{nj}^* + e^{-E_n(L_t-(t-t_0))}\psi_{ni}^*\psi_{nj} \right)$$

$$\psi_{ni}^* = \left\langle 0|\hat{O}_i|n\right\rangle ; \psi_{ni}^*\psi_{nj} \in \mathbb{R}$$

$$\Rightarrow C(t)v_n(t,t_0) = \lambda_n(t,t_0)C(t_0)v_n(t,t_0)$$

$$\lambda_n(t,t_0) = e^{-E_n(t-t_0)} + e^{-E_n(L_t-(t-t_0))}$$

Important points:

- Systematic error[2] in nth energy state (if we take a t derivative of $\log(\lambda)$): $\epsilon_n \sim e^{-(E_{N+1}-E_n)t}$ if $t_0 \geq t/2$

Extracting Spectra (cont'd)

- Operator basis is composed of single meson operators $\overline{\psi}\psi(\sigma)$, $\overline{q}\gamma_i q(\rho)$ and $\pi\pi$ operator $2\overline{q}\gamma_5 q(\pi)$ with various momentum combinations and non-zero $\vec{p}_{CM}$ up to $\pm(1,1,1)$.
- Operators are projected onto A_1 irrep and definite isospin $(0,1,2)$.
- We fix $t - t_0$ to be either ≤ 4 or 1 (if later times aren't very noisy; extra exp fit ansatz gives better noise than t deriv.)
- GEVP also exists for matrix elements [3]. We plan to use this for $K \to \pi\pi$. (Recent theoretical improvements by the speaker improve the error rate $t_0 \to t$.)

Around the World (ATW) Systematic Error

$$(\cosh Et)^2 = \frac{1}{2}\cosh 2Et + const.$$

$$\pi \rightarrow \dots \qquad \dots \rightarrow \pi$$

$$\dots \leftarrow \pi \qquad \pi \leftarrow \dots$$

- A two particle QCD state in a finite box necessarily has an around the world contribution. This is a finite box size artifact.
- As size of box in time dimension increases, the artifact vanishes ($L_t \rightarrow \infty$).
- Very problematic for light particles that can travel the whole length of the box without decaying (physical mass pions).
- For every momentum difference between pions, we get a new ATW term (only one in center of mass frame).

Methods for ATW Removal: Matrix Subtraction

We subtract the re-weighted GEVP (correlation function) matrix at two different time separations.

- Matrix subtraction: $exp(\Delta E t)C(t) - exp(\Delta E(t-\delta_t))C(t-\delta_t)$. Shift the spectrum by a constant ΔE so the ATW term is constant between the t and $t-\delta_t$ term.
- $\Delta E = E_{\pi_1} - E_{\pi_2}$; Around the world terms are time dependent if and only if $\Delta E \neq 0$.
- In principle iterable, but we lose δ_t number of time slices every time we perform this operation.
- Most useful when $\Delta E = 0$ (the center of mass frame). All ATW terms are constant and all are then removed; We only use this method in the center of mass frame.

Methods for ATW Removal: Vacuum Saturation Subtraction

- We suppose: the largest part of ATW terms are the non-interacting piece (pions only have limited window in time to interact).
- Subtract the non-interacting ATW terms as follows:
  - Use two time slices to get the (config averaged) amplitude coefficients A_1, A_2 and effective energies E_1, E_2 of the single pion correlation functions ($A_i\left[exp(-E_i t) + exp(-E_i(L_t - t))\right]$).
  - Using the known form of the ATW terms, subtract two terms: $A_1 A_2 exp(-E_1 L_t) exp(-(E_2 - E_1)t), A_1 A_2 exp(-E_2 L_t) exp(-(E_1 - E_2)t)$
  - We can use the two GEVP time slices t, t_0 to get these terms (more correlated with $\pi\pi \to \pi\pi$ correlation functions leading to less noise)
- (Invented by the speaker to deal with large ATW errors in the 32^3.)

Aside: Pion Ratio Method (due to X. Feng/C. Lehner/D. Murphy)

$\langle \pi\pi | \pi\pi \rangle \approx \langle \pi | \pi \rangle^2$

1. $\langle \pi | \pi \rangle^2$ gives us a non-interacting energy E_{nonint}
2. Strong correlation exists between interacting and non-interacting correlation functions
3. Method add 0 (in large stat. limit): $E_{int,\text{ improved}} = E_{int} - E_{nonint} + E^2_{\pi,disp}$
4. $(E_{\pi,disp} = \sqrt{m^2 + p^2})$
5. factor of 10 (max) reduction in noise (better for lower energies)

Matrix Subtraction (2 iters for moving frames): Result

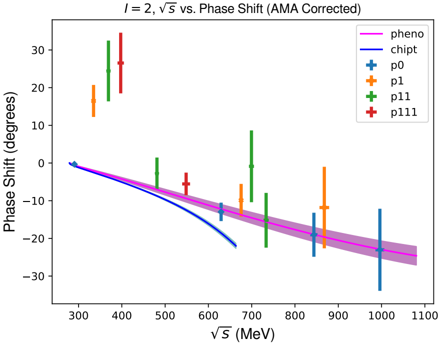


Figure: 32^3, $I = 2$, $65, 8$ (sloppy,exact) configs; with matrix subtraction

Vacuum Saturation Subtraction: Result

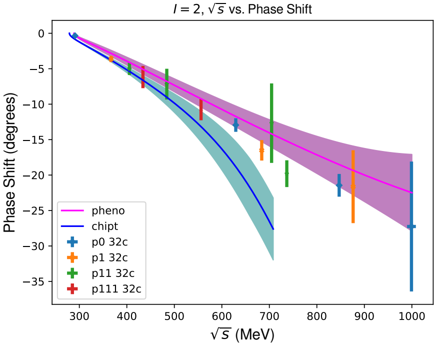
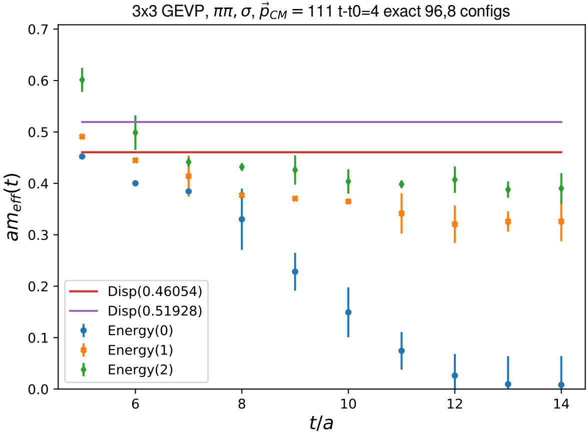


Figure: 32^3, $I = 2$, $99, 17$ (sloppy,exact) configs; with vacuum saturation subtraction

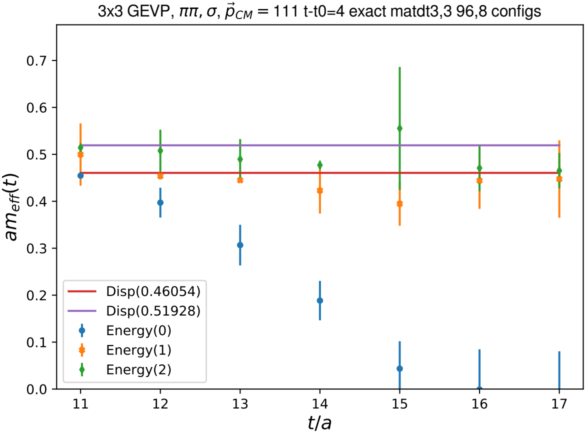
A Difficult Counter-example ($I = 0$, 32^3)

(Without subtraction, no GEVP derivative.)



A Difficult Counter-example (cont.d)

(With subtraction, no GEVP derivative.)



Outline

Lattice Details: 24^3

- $V = 24^3$ ID lattice, 1.015 GeV lattice spacing
- $L_t = 64$
- $2 + 1$ flavor Mobius Domain Wall Fermions (generated by RBC/UKQCD)
- ~ 6.5 fm box
- Physical quark mass, unquenched (no chiral extrapolation needed)

Lattice Details: 32^3

- $V = 32^3$ ID lattice, 1.3784 GeV lattice spacing
- $L_t = 64$ (N.B. smaller in physical units than 24^3)
- $2 + 1$ flavor Mobius Domain Wall Fermions (generated by RBC/UKQCD)
- ~ 6.5 fm box
- Also physical quark mass

Outline

Momentum Combinations

Compute pions with $p_{lat,max} = \pm(1,1,1)$ (also permutations) in units of $\frac{2\pi}{L}$.

- 27 possible individual pion momenta.
- Cube this if you want to get a rough estimate of the combinations allowed
- Using momenta for irreps we care about (e.g. A_1) we get 13890 separate $\pi\pi \to \pi\pi$ correlation functions.
- $\overline{q}q, \overline{q}\gamma^{\mu}q$ correlation functions are not included in this number.

Auxiliary Symmetry (aside)[1]

Can reduce this number by exactly a factor of 2 via labeling symmetry between source and sink. Swap these, we will get the exact same correlation function up to an overall phase. Stated again, we have

Rule of Thumb:

Two lattice correlation functions are bit-by-bit identical (up to time reordering, phase) if they are related via a swap of source and sink labels.

We refer to the diagram derived (at the analysis stage) via this auxiliary symmetry as the auxiliary diagram. In practice, our data set is not fully symmetric under auxiliary symmetry, so our (projected) gain is only 3/2. The G-parity calculation gains about a factor of 2.
We do not currently exploit this symmetry.

[1] (discovered by the speaker in 2017)

Outline

Fitting Methodology (Outline)

Steps to extract spectra:

- Solve the (subtracted) GEVP. Get eigenvalues.
- Take a log, force a fit ($dof = 0$) to two nearby time slices. We now have energies.
- Select a fit range (in an unbiased manner) and fit to constant. Optionally, fit to $E + exp(-(E_{N+1} - E_n)t)$.
- Optionally, do a p-value weighted average over fit ranges (all results displayed use this method)
- p-value: measures probability that model and data would disagree by chance if they agreed in the large statistics limit. Important, ongoing work from C. Kelly to understand uncertainty (see his talk).

Caveat Emptor

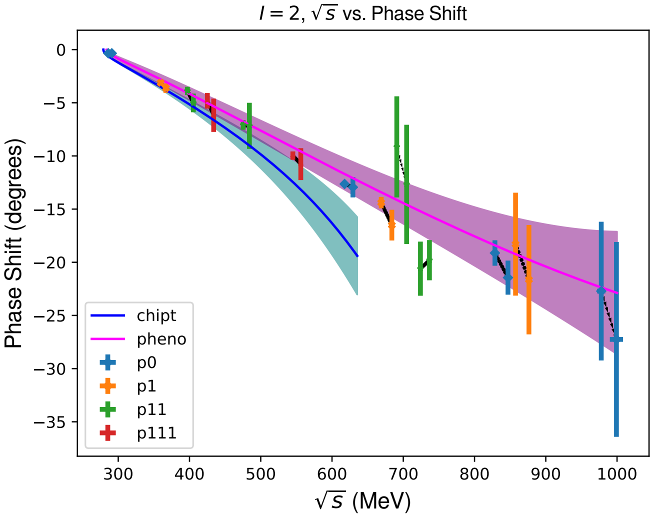
0) 4π threshold ignored (elastic scattering assumed)

Experimental amplitude is small, so we are probably safe to neglect until higher energies (Lüscher type formula does not exist for inelastic processes). Also, preliminary distillation data (A. Meyer) indicates the amplitude may actually be small enough to be neglected.

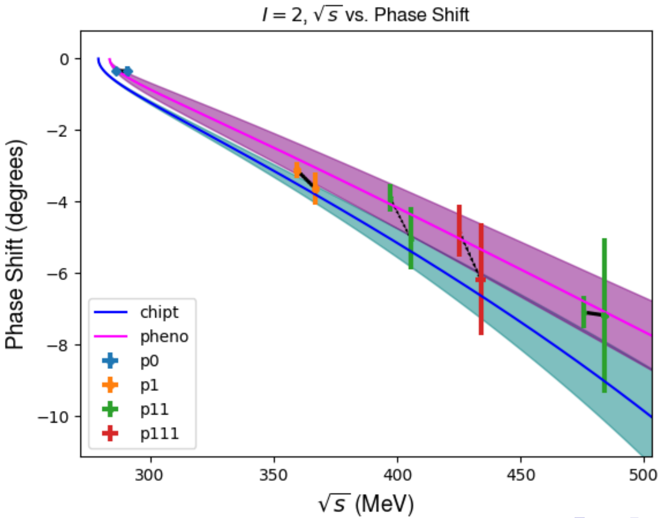
1) Interacting ATW Unestimated

Unsubtracted/Unestimated interacting ATW terms make the results questionable (especially when there is a visible defect!).

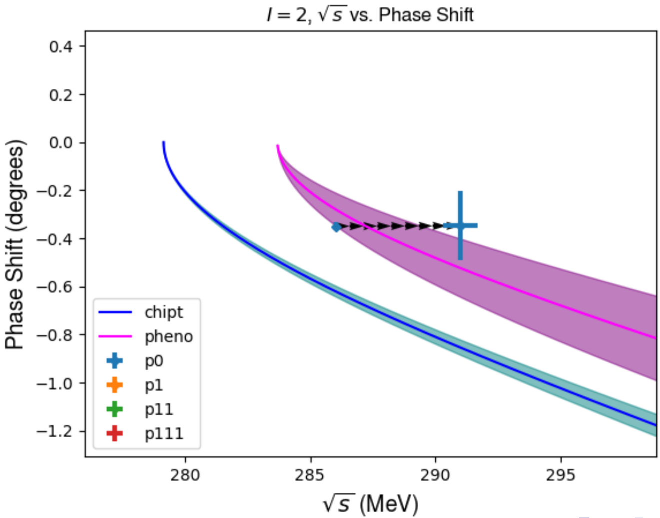
$I = 2$ phase shifts



$I = 2$ insets (1/3)

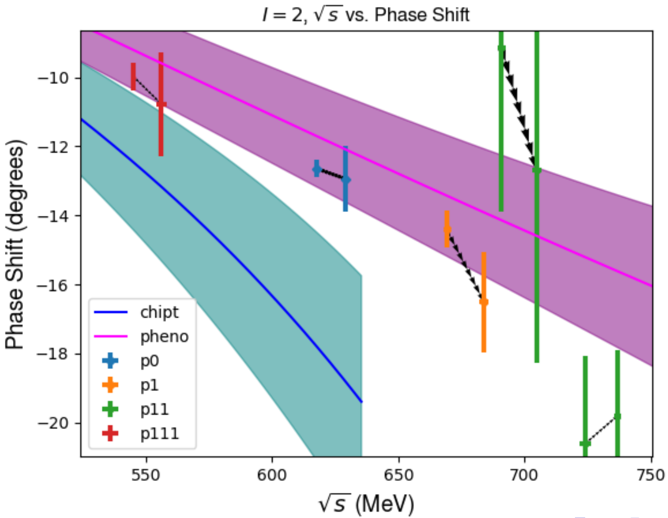

I = 2, √s vs. Phase Shift
Phase Shift (degrees)
0
−2
−4
−6
−8
−10
300
350
400
450
500
√s (MeV)
chipt
pheno
p0
p1
p11
p111

$I = 2$ insets (2/3)



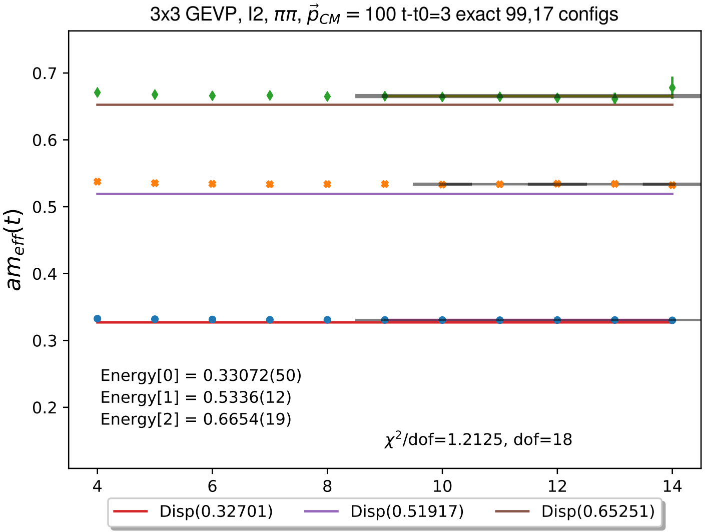
$I = 2$, $\sqrt{s}$ vs. Phase Shift
Phase Shift (degrees)
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−1.2
280
285
290
295
$\sqrt{s}$ (MeV)
chipt
pheno
p0
p1
p11
p111

$I = 2$ insets (3/3)

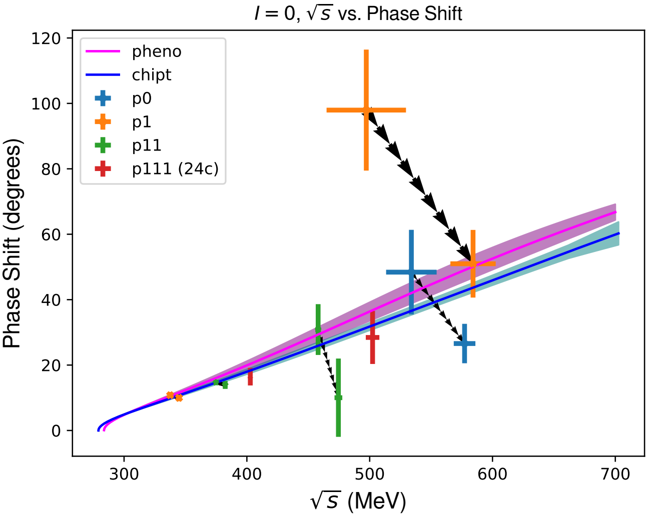


$I = 2$, $\sqrt{s}$ vs. Phase Shift
Phase Shift (degrees)
$\sqrt{s}$ (MeV)
−10
−12
−14
−16
−18
−20
550
600
650
700
750
chipt
pheno
p0
p1
p11
p111

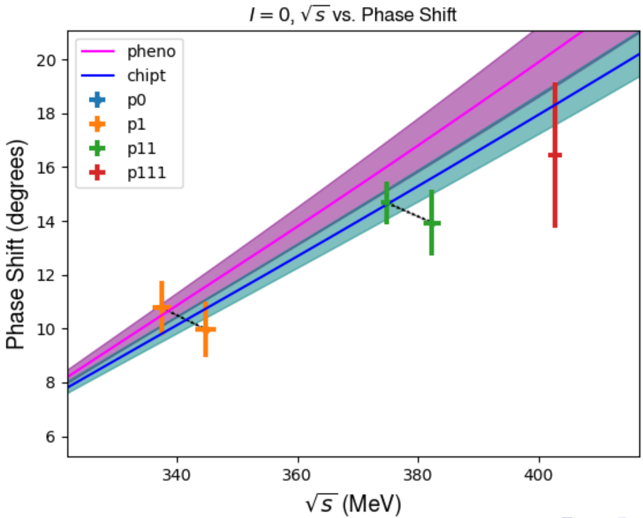
$I = 2$ Example Effective Mass Plot - 32^3 p1



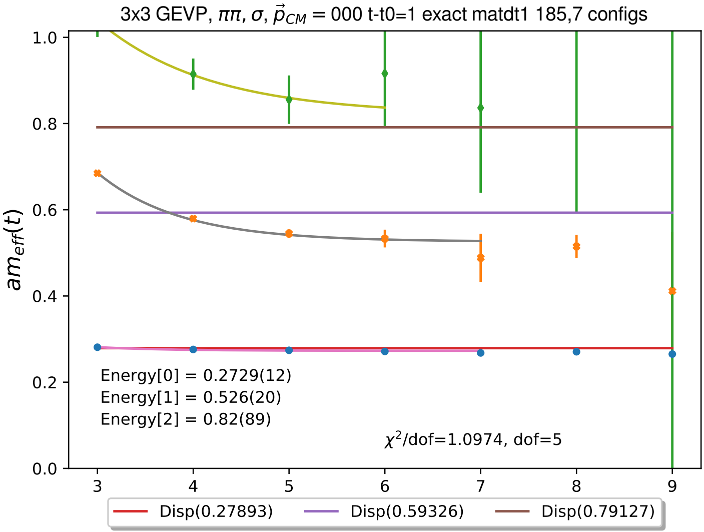
$I = 0$ phase shifts



$I = 0$ inset


$I = 0, \sqrt{s}$ vs. Phase Shift
pheno
chipt
p0
p1
p11
p111
Phase Shift (degrees)
20
18
16
14
12
10
8
6
340
360
380
400
$\sqrt{s}$ (MeV)

$I = 0$ Example Effective Mass Plot - 32^3 p0



Outline

Conclusions

We have run on $O(100)$ gauge configurations on coarse and fine ensembles and generated promising results. This is the first calculation of pipi scattering spectra from the lattice at physical pion mass.

- $K \to \pi\pi$ periodic code ready to be tested (statistically, free-field G-parity check).
- More statistics likely needed to resolve excited $I = 0$, (e.g., more A2A noise samples, assuming pion ratio correlations still work)
- Lots of analysis still to do (mainly $I = 1$ moving frames).
- Two other physical point $\pi\pi$ scattering studies (from RBC) are also soon to be completed (G-parity, distillation). See talks of C. Kelly, A. Meyer, T. Wang.
- $I = 1$ still being analyzed (moving frame analysis soon to start).

Pipi data is available on request in standard binary format hdf5. My analysis code is also publicly available on github: github.com/goracle/lattice-fitter

Thanks!

The RBC & UKQCD collaborations

BNL and BNL/RBRC

Yasumichi Aoki (KEK)
Taku Izubuchi
Yong-Chull Jang
Chulwoo Jung
Meifeng Lin
Aaron Meyer
Hiroshi Ohki
Shigemi Ohta (KEK)
Amarjit Soni

UC Boulder

Oliver Witzel

CERN

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Columbia University

Ryan Abbot
Norman Christ
Duo Guo
Christopher Kelly
Bob Mawhinney
Masaaki Tomii
Jiqun Tu
Bigeng Wang
Tianle Wang
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Luigi Del Debbio
Felix Erben
Vera Gülpers
Tadeusz Janowski
Julia Kettle
Michael Marshall
Fionn Ó hÓgáin
Antonin Portelli
Tobias Tsang
Andrew Yong
Azusa Yamaguchi

KEK

Julien Frison

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Nicolas Garron

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Peking University

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University of Regensburg

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University of Southampton

Nils Asmussen
Jonathan Flynn
Ryan Hill
Andreas Jüttner
James Richings
Chris Sachrajda

Stony Brook University

Jun-Sik Yoo
Sergey Syritsyn (RBRC)

Martin Luscher. "Two particle states on a torus and their relation to the scattering matrix". In: *Nucl. Phys.* B354 (1991), pp. 531–578. DOI: 10.1016/0550-3213(91)90366-6.

Benoit Blossier et al. "On the generalized eigenvalue method for energies and matrix elements in lattice field theory". In: *JHEP* 04 (2009), p. 094. DOI: 10.1088/1126-6708/2009/04/094. arXiv: 0902.1265 [hep-lat].

John Bulava, Michael Donnellan, and Rainer Sommer. "On the computation of hadron-to-hadron transition matrix elements in lattice QCD". In: *JHEP* 01 (2012), p. 140. DOI: 10.1007/JHEP01(2012)140. arXiv: 1108.3774 [hep-lat].

Justin Foley et al. "Practical all-to-all propagators for lattice QCD". In: *Comput. Phys. Commun.* 172 (2005), pp. 145–162. DOI: 10.1016/j.cpc.2005.06.008. arXiv: hep-lat/0505023 [hep-lat].

All-to-All Propagators

$$D_{A2A}^{-1} \equiv \sum_{l=0}^{N_l-1} |\phi_l\rangle \frac{1}{\lambda_l} \langle\phi_l| + \sum_{h=0}^{N_h-1} \underbrace{\left(D^{-1} - \sum_{l=0}^{N_l-1} |\phi_l\rangle \frac{1}{\lambda_l} \langle\phi_l| \right)}_{D_{Defl}^{-1}} |\eta_h\rangle \langle\eta_h|$$

$$\mathbb{I} = \lim_{N_h\to\infty} |\eta_h\rangle \langle\eta_h| , \quad \Rightarrow \lim_{N_h\to\infty} D_{A2A}^{-1} = D^{-1}$$

- Deflate with 2000 low modes of Dirac operator $|\phi_l\rangle$
- In practice, set $N_h = 1$ (more hits improve excited state noise. Gauge noise dominates lower energy states.)
- $12 * L_t * N_h$ high modes (spin, color, time diluted) $\rightarrow$ 768 high modes.
- We obtain the exact point-to-point propagator in this stochastic limit.[4]

Motivation: $K \to \pi\pi$

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

$$\eta_{00} = \frac{A(K_L \to \pi^0\pi^0)}{A(K_S \to \pi^0\pi^0)} \quad \eta_{\pm} = \frac{A(K_L \to \pi^+\pi^-)}{A(K_S \to \pi^+\pi^-)}$$

$$Re(\frac{\epsilon'}{\epsilon}) = \frac{1}{6}\left(1 - \left|\frac{\eta_{00}}{\eta_{\pm}}\right|^2\right) = 1.66(23) \ x \ 10^{-3}(\text{Experiment})$$

$K \to \pi\pi$ (cont'd.)

In terms of isospin states,

$\Delta I = 3/2$ decays to $I = 2$ final states, amplitude A_2
$\Delta I = 1/2$ decays to $I = 0$ final states, amplitude A_0

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

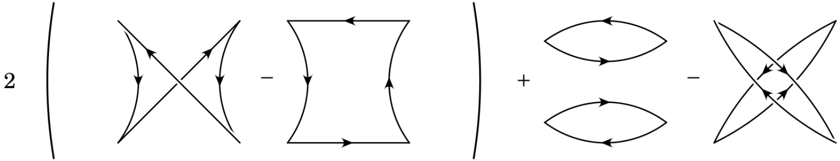
$$A(K^0 \to \pi^0\pi^0) = \sqrt{\frac{2}{3}} A_0 e^{i\delta_0} - 2\sqrt{\frac{1}{3}} A_2 e^{i\delta_2}$$

$$\Rightarrow \epsilon' = \frac{i\omega e^{i(\delta_2 - \delta_0)}}{\sqrt{2}} \left(\frac{Im\ A_2}{Re\ A_2} - \frac{Im\ A_0}{Re\ A_0} \right) \quad \boxed{\omega = \frac{ReA_2}{ReA_0}}$$

Small size of ϵ' makes it particularly sensitive to new direct-CPV introduced by most BSM models.

Isospin (cont'd)

$\langle I = 1 | I = 1 \rangle$:



Timing Summary: 24^3

For our 24^3 run, we compute on 32 KNL nodes (64 cores, 192 GB memory) for 20 hours (current wall time). Timing breakdown (of expensive steps)

- Lanczos - low mode eigenvectors (amortized, not in an individual config run) - 6 hours
- 400 iterations of Zmobius Split CG ($ls = 12$) 1.3 hours (split-MADWF= 6 hours)
- π meson field computation (all-to-all propagators[4]) 1 hour
- $\pi\pi \to \pi\pi$ contractions 10 hours
- σ meson field 1 hour
- ρ meson field 3 hours (3 polarizations, projected)
- σ (scalar) contractions 1 hour
- ρ (vector) contractions 2 hours

Our time is dominated not by inversions, but contractions. We are still improving (changing) this number. Communications are $10 - 20\%$ of the total time (ongoing comms work on KNL).

Timing Summary: 32^3

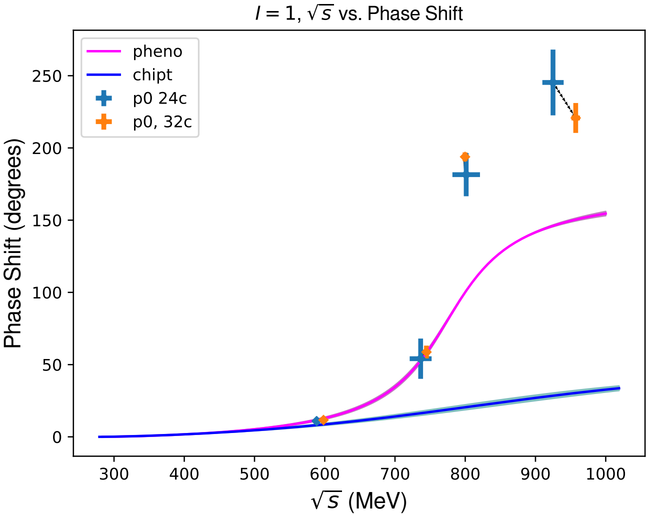
For our 32^3 run, we also compute on 32 KNL nodes (64 cores, 192 GB memory) for 36 hours (current wall time). Timing breakdown (of expensive steps)

- Lanczos - low mode eigenvectors (amortized, not in an individual config run) - 10.5 hours on 16 (KNL) nodes
- 330 iterations of Sloppy Mobius Split CG ($ls = 12$) $2 - 3$ hours (exact$= 8^*$ hours)
- π meson field computation (all-to-all propagators[4]) 2.5 hours
- $\pi\pi \to \pi\pi$ contractions 12 hours
- σ meson field 3 hours
- ρ meson field 10 hours (3 polarizations, projected)
- σ (scalar) contractions 1.3 hours
- ρ (vector) contractions 4 hours

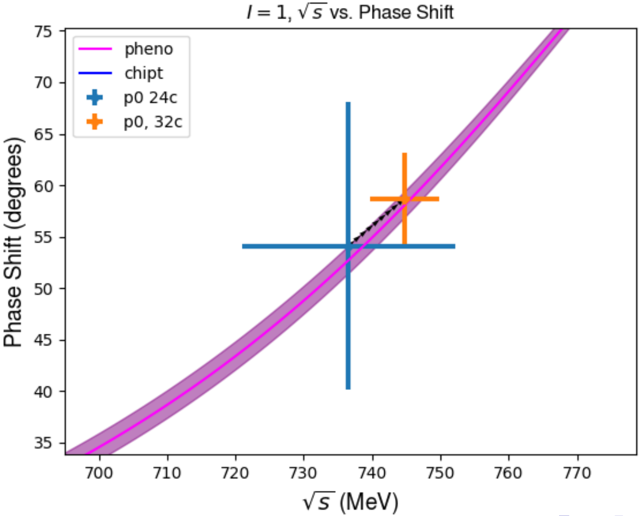
Methods for ATW Removal: Alternative Strategies

- Measure the ATW terms directly (distillation study, ongoing). For our all-to-all propagators, this could be quite expensive (but perhaps viable).
- Measure matrix element: $\langle\pi|\pi\pi|\pi\rangle$
- Fit (somehow?) to the terms using more fit parameters
- Fitting not really viable for moving frames (hard to estimate remaining systematic errors).

$I = 1$ phase shifts

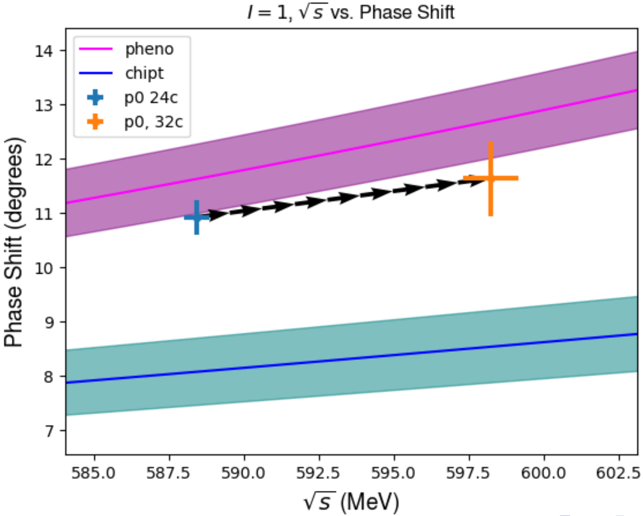


$I = 1$ insets (1/2)



I = 1, √s vs. Phase Shift
pheno
chipt
p0 24c
p0, 32c
Phase Shift (degrees)
75
70
65
60
55
50
45
40
35
700
710
720
730
740
750
760
770
√s (MeV)

$I = 1$ insets (2/2)



$I = 1$, $\sqrt{s}$ vs. Phase Shift
pheno
chipt
p0 24c
p0, 32c
Phase Shift (degrees)
$\sqrt{s}$ (MeV)
14
13
12
11
10
9
8
7
585.0
587.5
590.0
592.5
595.0
597.5
600.0
602.5

$I = 1$ Example Effective Mass Plot - 24^3 p0