Investigating Unitarity Violation With Chiral Perturbation Theory

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Introduction

- Will present work from the following two papers
 - "Applicability of the two-particle quantization condition to partially-quenched theories"^[1]
 - " $\pi\pi$ scattering in partially-quenched twisted-mass chiral perturbation theory"^[2]
- Will focus largely on [2] using results derived from [1]
 - $I = 0 \pi \pi$ scattering presents challenges the I = 1 and I = 2 channels do not
 - Will demonstrate existing results contain previously unknown errors



- [1] Z. T. Draper and S. R. Sharpe, Phys. Rev. D 104, 034510 (2021), 2107.09742.
- [2] Z. T. Draper and S. R. Sharpe, Phys. Rev. D 105, 034508 (2022), 2111.13975.
- [3] Y. Aoki et al., FLAG review 2021, arXiv:2111.09849.

- ETMC has calculated $\pi\pi$ scattering for I = 2, I = 1, and I = 0
 - Calculated using a twisted mass to get $\mathcal{O}(a)$ improvement
- I = 0 scattering most difficult numerically
 - Fully disconnected quark diagrams contribute
 - Isospin breaking from mass twist mixes I = 0 and I = 2, $I_3 = 0$ channels^[1]
- L. Liu et al. use partial quenching to prevent isospin mixing^[2]
 - In doing so, introduce unitarity violation to calculations
 - Lüscher's quantization condition, used to extract scattering lengths, is derived assuming a unitary theory

M. I. Buchoff, J.-W. Chen, and A. Walker-Loud, Phys. Rev. D 79, 074503 (2009), 0810.2464.
 L. Liu et al., Phys. Rev. D 96, 054516 (2017), 1612.02061.

Understanding Errors with χPT

- Our goal is to use Chiral Perturbation Theory (χ PT) to investigate potential I = 0 errors
- χPT can be made to incorporate
 - discretization errors
 - finite-volume effects
 - unphysical quark masses
 - unitarity violation
- Want a partially quenched (PQ) twisted mass (TM) version of χ PT to match work of L. Liu et al.

Formulating PQTM_xPT

Leading-order Lagrangian looks like that of leading-order χPT

•
$$\mathcal{L}_{\text{LO}} = \frac{f^2}{4} \operatorname{str} \left(\partial_{\mu} \Sigma \ \partial_{\mu} \Sigma^{\dagger} \right) - \frac{f^2}{4} \operatorname{str} \left(2B_0 (M^{\dagger} \Sigma + \Sigma^{\dagger} M) \right)$$

• The mass twist treats up and down quarks differently

•
$$M_0 = \operatorname{diag}(m_q, m_q) \rightarrow M = m_q e^{i\tau_3 \omega} \equiv m + i\mu\tau_3$$

- Hadronic fields are contained in $\Sigma = \exp(i\sqrt{2}\Pi/f)$
- Partial quenching introduces ghosts so that $\Pi = \begin{bmatrix} \phi & \eta_1 \\ \eta_2 & \tilde{\phi} \end{bmatrix}$
 - ϕ contains quark-quark NG bosons
 - $ilde{\phi}$ contains ghost-ghost NG bosons
 - η_1 , η_2 contain quark-ghost NG fermions



Partial Quenching to Prevent Isospin Mixing

• L. Liu et al. introduce additional valence and ghost u and d quarks

• $Q^{\mathrm{tr}} = \left(u_S, d_S, u_V, d_V, \tilde{u}_V, \tilde{d}_V \right)$

- Valence and ghost quarks come with twist opposite to sea quarks
 - (u_S, d_S) comes with twist τ_3
 - $(u_V, d_V), (\tilde{u}_V, \tilde{d}_V)$ comes with twist $-\tau_3$
- $SU(4 \mid 2)$ flavor symmetry broken by twisted mass
 - Left with $SU(2)_+ \times SU(2)_- \times U(1)$
 - For fields of positive twist, exact $SU(2)_+$ will prevent isospin mixing

PQTM χ *PT* Setup

• We can now formulate the LO Lagrangian using the standard power counting $m_q \sim p^2 \sim a^2$

•
$$\mathcal{L}_{LO} = \frac{f^2}{4} \operatorname{str}(\partial_{\mu}\Sigma \partial_{\mu}\Sigma^{\dagger}) - \frac{f^2}{4} \operatorname{str}(\chi^{\dagger}\Sigma + \Sigma^{\dagger}\chi) + \mathcal{V}_{a^2}$$

• $\mathcal{V}_{a^2} = -\hat{a}^2 W_6' \operatorname{str}(\Sigma + \Sigma^{\dagger})^2 - \hat{a}^2 W_7' \operatorname{str}(\Sigma - \Sigma^{\dagger})^2 - \hat{a}^2 W_8' \operatorname{str}(\Sigma^2 + \Sigma^{\dagger 2})$

• П now contains PGBs and PGFs of positive, negative, and mixed twist

$$\Pi = \begin{pmatrix} \pi_{++}^{0} + \frac{\eta_{4}}{2} + \frac{\phi_{1}}{2} & \pi_{-+}^{+} & \pi_{++}^{+} & \pi_{-+}^{uu} & \omega_{15} & \omega_{16} \\ (\pi_{-+}^{+})^{\dagger} & -\frac{\pi_{--}^{0}}{\sqrt{2}} - \frac{\eta_{4}}{2} + \frac{\phi_{1}}{2} & (\pi_{-+}^{dd})^{\dagger} & (\pi_{--}^{+})^{\dagger} & \omega_{25} & \omega_{26} \\ (\pi_{++}^{+})^{\dagger} & \pi_{-+}^{dd} & -\frac{\pi_{++}^{0}}{\sqrt{2}} + \frac{\eta_{4}}{2} + \frac{\phi_{1}}{2} & (\pi_{+-}^{+})^{\dagger} & \omega_{35} & \omega_{36} \\ (\pi_{-+}^{uu})^{\dagger} & \pi_{--}^{+} & \pi_{+-}^{+} & \frac{\pi_{--}^{0}}{\sqrt{2}} - \frac{\eta_{4}}{2} + \frac{\phi_{1}}{2} & \omega_{45} & \omega_{46} \\ \omega_{51} & \omega_{52} & \omega_{53} & \omega_{54} & \frac{\phi_{0}}{\sqrt{2}} + \phi_{1} & \phi_{56} \\ \omega_{61} & \omega_{62} & \omega_{63} & \omega_{64} & \phi_{56}^{\dagger} & -\frac{\phi_{0}}{\sqrt{2}} + \phi_{1} \end{pmatrix}$$

Z. T. Draper and S. R. Sharpe, Phys. Rev. D 105, 034508 (2022), 2111.13975.

• I = 2, I = 1, and I = 0 scattering calculated first at tree-level

$$\mathcal{A}_{I=2}^{\text{LO}} = \frac{1}{f^2} \left(-s + 2M_{\text{OS}}^2 \right) - \frac{64}{f^4} \hat{a}^2 W_7' - \frac{32}{f^4} \hat{a}^2 W_8'$$

$$\mathcal{A}_{OS}^{\text{LO}} \equiv 2B_0 m_q - \frac{16}{f^2} \hat{a}^2 W_8'$$

$$\mathcal{A}_{I=1}^{\text{LO}} = \frac{t-u}{f^2}$$

$$\mathcal{A}_{I=0}^{\text{LO}} = \frac{1}{f^2} \left(2s - M_{\text{OS}}^2 \right) - \frac{160}{f^4} \hat{a}^2 W_7' - \frac{80}{f^4} \hat{a}^2 W_8'$$

$$\mathcal{M}_{OS}^2 \equiv 2B_0 m_q - \frac{16}{f^2} \hat{a}^2 W_8'$$

$$(M_{SS}^{\pm})^2 \equiv 2B_0 m_q$$

- I = 0 amplitude contains unaccounted for $O(a^2)$ discretization errors
 - Could introduce O(100%) errors into calculation since $a^2 \sim M_{OS}^2$
- Lattice calculation of $\mathcal{A}_{I=2}^{LO}$ would allow discretization errors to be subtracted

•
$$\mathcal{A}_{I=0}^{\text{LO}} - \frac{5}{2}\mathcal{A}_{I=2}^{\text{LO}} = \frac{1}{f^2} \left(\frac{9}{2}s - 6M_{\text{OS}}^2\right)$$

1 (

- We turn our attention from discretization errors to unitarity violation
 - Unitarity can be violated when external and loop quarks differ due to partial quenching
- Lüscher's quantization condition is derived using s-channel unitarity
- The imaginary part of loop must be proportional to the squared magnitude of the tree-level amplitude
 - Proportionality constant related to the phase space available
- Multiple ways to check for possible violation
 - Quark line diagram analysis
 - Explicit computation



Quark Line Diagrams: I = 0

- Many diagrams contribute to I = 0 scattering
 - A single diagram with different external quarks and loop quarks is enough to violate unitarity
- Consider diagram contributing to s-channel at one-loop



- d and \overline{d} annihilate to produce valence, sea, or ghost quarks
 - Unless contributions cancel, process will violate unitarity

- An explicit calculation of the I = 0 amplitude confirms s-channel unitarity is violated
- The imaginary part of the loop is not proportional to the tree-level amplitude squared

$$\mathcal{A}_{I=0}^{\text{LO}} = \frac{1}{f^2} \left(2s - M_{\text{OS}}^2 \right) - 10w_7' - 5w_8' \text{ where } w_k' = \frac{16}{f^4} \hat{a}^2 W_k'$$

$$\mathcal{A}_{\text{OS},I=0}^{(s1)} = \frac{3s^2}{8f^4} J \left(s, M_{\text{SS}}^{\pm 2}, M_{\text{SS}}^{\pm 2} \right) + \frac{1}{8f^4} J \left(s, M_{\text{OS}}^2, M_{\text{OS}}^2 \right) \left(8M_{\text{OS}}^2 \left(8f^2w_7' + 26M_{\text{OS}}^2 + 5s \right) - 8M_{\text{SS}}^{\pm 2} \left(-8f^2w_7' + 44M_{\text{OS}}^2 + 7s \right) - 112f^2sw_7' + 256f^4w_7'^2 + 160M_{\text{SS}}^{\pm 4} + 13s^2 \right) - \frac{3}{f^4} \left(-3M_{\text{SS}}^{\pm 2} + 3M_{\text{OS}}^2 + M_{\text{SS}}^{02} \right)^2 J \left(s, M_{\text{OS}}^2, M_{\text{SS}}^{02} \right) + \frac{3}{2f^4} \left(3M_{\text{SS}}^{\pm 2} - 2 \left(M_{\text{OS}}^2 + M_{\text{SS}}^{02} \right) \right)^2 J \left(s, M_{\text{SS}}^{02}, M_{\text{SS}}^{02} \right) + \frac{5s}{12f^4} I \left(M_{\text{SS}}^{\pm 2} \right) + \frac{1}{36f^4} I \left(M_{\text{OS}}^2 \right) \left(-336f^2w_7' - 168M_{\text{SS}}^{\pm 2} + 120M_{\text{OS}}^2 + 65s \right)$$

What goes wrong?

• Consider an operator \mathcal{O} that annihilates a pair of pions

•
$$\mathcal{O}(t) = \pi^+(t)\pi^-(t)$$
 where $\pi^+(t) = \sum_{\vec{x}} \overline{d}\gamma_5 u(\vec{x},t)$ and $\pi^-(t) = \sum_{\vec{x}} \overline{u}\gamma_5 d(\vec{x},t)$

For a unitary theory, can extract finite volume energies using the following

• $\langle \mathcal{O}(\tau) \mathcal{O}^{\dagger}(0) \rangle = \sum_{n} c_{n} e^{-E_{n}\tau}$

Useful to consider a ratio of correlation functions

•
$$R(\tau) = \frac{\langle \mathcal{O}(\tau)\mathcal{O}^{\dagger}(0) \rangle}{\langle \pi(\tau)\pi(0) \rangle^2} = Ze^{-\delta E_0|\tau|} + \text{excited-state contributions}$$

• Allows for the extraction of $\delta E_0 = E_0 - 2M_{\pi}$

Lüscher's Quantization Condition

- Links finite-volume spectrum and infinite-volume scattering amplitude
- Liu et al. uses the threshold expansion for a unitary theory

• $\delta E_0 = -\frac{4\pi a_0}{M_{\pi}L^3} \left[1 + c_1 \frac{a_0}{L} + c_2 \frac{a_0^2}{L^2} + \mathcal{O}(L^{-3}) \right]$ where c_i are known constants

• Allows for extraction of scattering length, a_0

Computational Approach

• Neither of these two parts of Lüscher's formalism hold when s-channel unitarity is violated

•
$$R(\tau) = \frac{\langle \mathcal{O}(\tau)\mathcal{O}^{\dagger}(0) \rangle}{\langle \pi(\tau)\pi(0) \rangle^{2}} = Ze^{-\delta E_{0}|\tau|} + \dots = Z\left[1 - |\tau|\delta E_{0} + \frac{\tau^{2}}{2}(\delta E_{0})^{2}\right] + \dots$$

• $\delta E_{0} = -\frac{4\pi a_{0}}{M_{\pi}L^{3}}\left[1 + c_{1}\frac{a_{0}}{L} + c_{2}\frac{a_{0}^{2}}{L^{2}} + \mathcal{O}(L^{-3})\right]$

• Contributions to threshold expansion come from three diagrams



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$$R(\tau) = \frac{\langle \mathcal{O}(\tau)\mathcal{O}^{\dagger}(0) \rangle}{\langle \pi(\tau)\pi(0) \rangle^{2}} = Ze^{-\delta E_{0}|\tau|} + \dots = Z\left[1 - |\tau|\delta E_{0} + \frac{\tau^{2}}{2}(\delta E_{0})^{2}\right] + \dots$$

• $\delta E_{0} = -\frac{4\pi a_{0}}{M_{\pi}L^{3}}\left[1 + c_{1}\frac{a_{0}}{L} + c_{2}\frac{a_{0}^{2}}{L^{2}} + \mathcal{O}(L^{-3})\right]$

Contributions to threshold expansion come from three diagrams



Lüscher When S-Channel Unitarity Is Violated

- Can quantify errors that arise from applying Lüscher's formalism when not applicable
- Errors arise from two steps:
 - Extracting the energy spectrum from correlators

•
$$R(\tau) = Z \left[1 - |\tau| \delta E_0 + \frac{\tau^2}{2} (\delta E_0)^2 \right] + \cdots$$
 leads to $\leq 5\%$ error

• Extracting scattering amplitude from energy spectrum

•
$$\delta E_0 = -\frac{4\pi a_0}{M_{\pi}L^3} \left[1 + c_1 \frac{a_0}{L} + c_2 \frac{a_0^2}{L^2} + \mathcal{O}(L^{-3}) \right]$$
 leads to ~ 25% error

- Applying PQTM χ PT to study of $I = 0 \pi \pi$ scattering we found:
 - ${\sim}100\%$ uncontrolled error arising from discretization effects
 - A method of subtracting off these discretization errors
 - ~25% error arising from unitarity violation invalidating use of Lüscher's formalism
- One might hope to control ~25% error
 - Could forgo Lüscher's formalism and fit finite-volume correlators directly to $\ensuremath{\mathsf{PQTM}\chi\mathsf{PT}}$
 - Light states appearing in loops make analysis intractable
 - Intermediate OS π^0 and sea quark π^0 are lighter than two OS pions
 - Two sea quark π^0 s also lighter than two OS pions
- Leaves us with an essentially irreducible $\sim 25\%$ systematic error

$I = 0 \pi \pi$ Scattering in FLAG Report

- Reported in the 2021 Flavor Lattice Averaging Group (FLAG) report
- Uncertainty is underestimated

State of the second state								
Collaboration	Ref.	N_{f}	lignd	Chira Chira	ODX.	filli.	$a_0^0 M_\pi$	$\ell^0_{\pi\pi}$
Fu 17	[391]	2 + 1	А		0	*	0.217(9)(5)	45.6(7.6)(3.8)
Fu 13	[334]	2 + 1	А			*	0.214(4)(7)	43.2(3.5)(5.6)
Fu 11	[392]	2 + 1	А			*	0.186(2)	18.7(1.2)
Mai 19	[389]	2	Р			0	0.2132(9)	
ETM 16C	[335]	2	А	*		\star	0.198(9)(6)	30(8)(6)
Caprini 11	[332]						0.2198(46)(16)(64)	
Colangelo 01	[323]						$0.220(5)_{\mathrm{tot}}$	

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