Order of the Chiral and Continuum Limits in Staggered Chiral Perturbation Theory

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Abstract

Dürr and Hoelbling recently observed that the continuum and chiral limits do not commute in the two dimensional, one flavor, Schwinger model with staggered fermions. I point out that such lack of commutativity can also be seen in four-dimensional staggered chiral perturbation theory (SχPT) in quenched or partially quenched quantities constructed to be particularly sensitive to the chiral limit. Although the physics involved in the SχPT examples is quite different from that in the Schwinger model, neither singularity seems to be connected to the trick of taking the n$^{\text{th}}$ root of the fermion determinant to remove unwanted degrees of freedom ("tastes"). Further, I argue that the singularities in SχPT are absent in standard quantities in the unquenched (full) QCD case and do not imply any unexpected systematic errors in recent MILC calculations with staggered fermions.

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I. INTRODUCTION

The one-flavor Schwinger model in two dimensions (2D) has recently been studied by Dürr and Hoelbling [1] using both overlap and staggered fermions. The square root of the staggered determinant is used to eliminate the extra taste degree of freedom. This is basically the same trick that is employed in current MILC three-flavor QCD simulations [2, 3, 4, 5] (the fourth root is required in 4D). Although many of the results in Ref. [1] are encouraging for the use of "rooted" staggered quarks, there is one disturbing feature: The chiral and continuum limits of $\langle\bar{\psi}\psi\rangle$ do not commute. If the continuum limit is taken first, the known continuum result is reproduced. But if the chiral limit is first taken for the staggered quarks, the continuum limit then disagrees with the exact result. This leads to three key questions:

- Do similar singularities appear in 4D QCD with staggered fermions?
- If they do appear, do such singularities induce uncontrolled systematic errors in the results reported in, *e.g.*, Refs. [2, 3, 4, 5]?
- Are the singularities the result of the rooting procedure?

Here, I address these questions for 4D QCD in the context of staggered chiral perturbation theory (SχPT) [6, 7, 8, 9, 10]. In SχPT, singular quantities for which the chiral and continuum limits fail to commute can easily be found in the quenched or partially quenched cases. As explained in Sec. II, the way the non-commutativity comes about is simple: Taste violations split the masses of mesons, and the splitting becomes the dominant effect in the meson masses as the chiral limit is approached. When the physics is particularly sensitive to the chiral regime, the chiral and continuum limits do not commute. Quenching or partial quenching leads to such sensitivity through double poles in neutral meson propagators, which enhance the infrared (IR) regime in loop diagrams. In the context of SχPT, the lack of commutativity has nothing directly to do with the issue of taking the root of the staggered determinant, and occurs in normal, "un-rooted," staggered theories also.

In Sec. III, I discuss the issue of commutativity of limits for unquenched SχPT ("full SχPT"). I argue that the chiral and continuum limits of standard physical quantities always commute because the full theory has no double poles and is therefore better behaved in the

IR. In this sense it is very similar to full continuum chiral perturbation theory (χPT). However, one does have to be careful about how one defines "standard" quantities; furthermore there is at this point no proof, but only an intuitive argument for why the singularities are absent to all orders in the full case. However, as discussed in Sec. IV, even if one assumes that the argument breaks down and singularities actually appear at some higher order, the associated new errors in previously computed quantities would be negligible.

Finally, in Sec. V, I mention two other examples of lack of commutativity, one with Wilson fermions and one in the quenched 2D Schwinger model. I point out that the known examples seem to indicate that the rooting procedure and the commutativity issues are independent.

II. EXAMPLES FROM SχPT

The simplest example of non-commutativity of limits in SχPT occurs in the quenched pion mass, where the "pion" is made of two degenerate valence quarks of mass $m_{\text{ß}V}$. In continuum quenched χPT, we have at next-to-leading order (NLO) [11]:

$$\left(\frac{M_\pi^2}{2\mu m_{\text{ß}V}}\right)_{\text{cont}} = 1 + \frac{1}{16\pi^2 f^2}\,\frac{-2m_0^2}{3}\,\ln\left(\chi_{\text{ß}VV}/\Lambda\right) + \cdots\ , \tag{1}$$

where Λ is the chiral scale; m_0^2, the contribution to the η' mass from the anomaly; f, the decay constant normalized so that $f \approx 131\text{MeV}$; and $\chi_{\text{ß}VV}$, the tree-level pion mass squared, $\chi_{\text{ß}VV} = 2\mu m_{\text{ß}V}$. ($\mu$ is a constant with dimensions of mass.) The $\cdots$ represents less singular terms that do not lead to non-commutativity of limits. Here, and throughout this paper, I work in the infinite volume limit for simplicity.

The corresponding expression for the Goldstone pion in SχPT is [7]

$$\left(\frac{M_\pi^2}{2\mu m_{\text{ß}V}}\right)_{\text{stag}} = 1 + \frac{1}{16\pi^2 f^2}\,\frac{-2m_0^2}{3}\,\ln\left(\chi^I_{\text{ß}VV}/\Lambda\right) + \cdots\ , \tag{2}$$

where $\chi^I_{\text{ß}VV}$ is the squared tree-level mass of the taste-singlet pion,

$$\chi^I_{\text{ß}VV} = \chi_{\text{ß}VV} + a^2\Delta_I = 2\mu m_{\text{ß}V} + a^2\Delta_I \tag{3}$$

with $a^2\Delta_I$ the splitting of the taste-singlet pion from the Goldstone pion. In Eq. (2) the neglected terms include effects of the taste-violating hairpins [7]. These are suppressed by a^2 and cause no problems with the limits.

Taking the ratio of lattice to continuum results, we have, to this order,

$$\frac{(M_\pi^2/m_V)_{\rm stag}}{(M_\pi^2/m_V)_{\rm cont}} = 1 + \frac{1}{16\pi^2 f^2}\,\frac{-2m_0^2}{3}\,\ln\left(1+\frac{a^2\Delta_I}{\chi_{VV}}\right) + \cdots\ . \tag{4}$$

This ratio clearly goes to 1 if we take the continuum limit, $a \to 0$, first. But it blows up if the chiral limit ($m_V \to 0$, $\chi_{VV} \to 0$) is taken first, because the staggered theory gives the wrong answer in this case. Of course χPT breaks down once the correction term gets large. In this case the breakdown occurs because of the "quenched chiral log" in the continuum. The logarithm is cut off in the staggered theory by the taste splitting, $a^2\Delta_I$.

This quenched example makes my basic point, but it is not very similar with the effect seen in Ref. [1]. There, the staggered theory is found to give a finite result for either order of the limits $m_V \to 0$ and $a \to 0$; it is just that the result is incorrect (different from the continuum) when $m_V \to 0$ is taken first. An example that has this kind of behavior can be found in the partially quenched 4D theory.[1]

For simplicity, I take N_S degenerate sea quarks of mass m_S in the partially quenched theory, and again consider a pion made from degenerate valence quarks of mass m_V. In the continuum, the pion mass at NLO is [12]

$$\left(\frac{M_\pi^2}{2\mu m_V}\right)_{\rm cont} = 1 + \frac{1}{16\pi^2 f^2}\,\frac{2}{N_S}\,\left(2\chi_{VV} - \chi_{SS}\right)\ln\left(\chi_{VV}/\Lambda\right) + \cdots\ , \tag{5}$$

where $\chi_{SS} = 2\mu m_S$, and $\cdots$ represents analytic terms.

In the staggered case, consider N_F degenerate dynamical staggered fields with mass m_S. I define N_S here as the number of sea quarks in the continuum limit: $N_S = N_F$ if the fourth root of the determinant is taken; while $N_S = 4N_F$ if it is not. The result has the same form when written in terms of N_S, whether or not the root is taken. Putting sea and valence quarks separately degenerate in Eq. (48) of Ref. [7], one easily arrives at the one-loop mass of the Goldstone pion:

$$\left(\frac{M_\pi^2}{2\mu m_V}\right)_{\rm stag} = 1 + \frac{1}{16\pi^2 f^2}\,\frac{2}{N_S}\,\left(2\chi^I_{VV} - \chi^I_{SS}\right)\ln\left(\chi^I_{VV}/\Lambda\right) + \cdots\ , \tag{6}$$

where χ^I_{SS} is defined analogously to χ^I_{VV}, Eq. (3), and $\cdots$ represents analytic terms and the effects of taste-violating hairpins, which again cause no problem with the limits.

If the continuum limit is taken first, Eq. (6) reproduces Eq. (5), so the two will give identical results no matter how the chiral limit is subsequently taken. On the other hand, if

[1] But note that the example in Ref. [1] occurs in the *full* 2D theory.

first we take the valence chiral limit ($m_{\text{ß}V} \to 0$, with $m_{\text{ß}S}$ fixed), the lack of commutativity of limits exactly parallels the quenched case, with $\chi_{\text{ß}SS}$ playing the role of m_0^2. As before, $\mathcal{O}(a^2)$ terms in the staggered theory cut off a chiral log that is divergent in the continuum theory.

For my purposes, a more interesting chiral limit occurs when $m_{\text{ß}V}$ and $m_{\text{ß}S}$ both approach 0, but with $m_{\text{ß}S}$ vanishing much more slowly, so that

$$\chi_{\text{ß}SS} \sim \frac{-C}{\ln(\chi_{\text{ß}VV}/\Lambda)} \tag{7}$$

as $\chi_{\text{ß}VV} \to 0$, with C a positive constant. In this limit (with a fixed in the staggered case)

$$\left(\frac{M_\pi^2}{2\mu m_{\text{ß}V}}\right)_{\text{cont}} \to 1 + \frac{1}{16\pi^2 f^2}\,\frac{2}{N_{\text{ß}S}}\,C \tag{8}$$

$$\left(\frac{M_\pi^2}{2\mu m_{\text{ß}V}}\right)_{\text{stag}} \to 1 + \frac{1}{16\pi^2 f^2}\,\frac{2}{N_{\text{ß}S}}\,a^2\Delta_I \ln\left(a^2\Delta_I/\Lambda\right) + \cdots\ , \tag{9}$$

where $\cdots$ represents additional $\mathcal{O}(a^2\ln(a^2))$ or $\mathcal{O}(a^2)$ terms, coming from taste-violating hairpins or taste-violating analytic terms. If we now take the continuum limit,

$$\left(\frac{M_\pi^2}{2\mu m_{\text{ß}V}}\right)_{\text{stag}} \to 1\ , \tag{10}$$

in disagreement with Eq. (8). On the other hand, the staggered theory clearly reproduces Eq. (8) if the continuum limit is taken first in Eq. (6).

Note that the non-commutativity of limits has nothing to do with the fourth-root prescription, and has exactly the same form with or without the fourth root. Of course, for fixed number $N_{\text{ß}F}$ of dynamical staggered fields, the effective number of continuum sea quarks $N_{\text{ß}S}$ depends on whether the root is taken, so we could say in that sense that the rooting prescription trivially affects the the strength of the singularity, but not its existence.

III. COMMUTATIVITY IN FULL SχPT

The lack of commutativity of limits appears in the computed one-loop SχPT quantities [7, 8, 10] only in the quenched or partially quenched cases, which are enhanced in the IR relative to the full case and therefore especially sensitive to the chiral limit. This is due to the double pole structure that shows up in flavor-neutral meson propagators. In the full QCD case, there are only single poles, and I therefore do not expect non-commutativity.

For example, if we first go to full QCD ($m_{\text{ß}V} = m_{\text{ß}S} \equiv m$; $\chi_{\text{ß}VV} = \chi_{\text{ß}SS} \equiv \chi$) in Eqs. (5) and (6), the NLO corrections then always vanish in the subsequent $m \to 0$, $a \to 0$ limits, independent of their order.

The absence of the commutativity problem in full QCD quantities seems to be a general feature of SχPT. It is equivalent to the statement that the limit $m \to 0$ at fixed a is smooth in full SχPT, *i.e.*, that there are no IR divergences on shell in this limit. I believe this to be the case because, taking the additional limit $a \to 0$, one recovers the massless continuum χPT. Ordinary chiral power counting in this limit shows that IR divergences are absent: The derivative couplings suppress IR contributions and make loop effects finite even in the presence of massless particles.[2] If we now turn on the lattice-dependent ($\mathcal{O}(a^2)$ and higher) vertices of SχPT, these act as effective mass terms and should not induce IR divergences that were previously absent. Power counting applied to SχPT then implies that any logarithms of a^2 that appear in the $m \to 0$ limit are "protected" by powers of a^2, so they cause no problem in the subsequent $a \to 0$ limit.

Full SχPT in the chiral limit is in fact closely analogous to full continuum χPT with massless up and down quarks but a non-vanishing strange quark mass. In both cases there are terms giving mass to some, but not all, of the pseudoscalar mesons: The pions remain massless in the continuum example; while the taste-ξ_5 (Goldstone) meson remains massless in SχPT. And in both cases the mass or mass-like terms give rise to interactions lacking enough derivatives to suppress all IR divergences automatically. Yet, one expects no IR divergences in the continuum case as the strange quark mass turns on, and therefore I expect SχPT to be likewise well-behaved.

However, a detailed proof that the chiral limit of full SχPT is "safe" may be rather delicate. Although the lattice-dependent vertices give no non-derivative interactions purely among the taste-ξ_5 mesons [6, 7, 9] (the analogous statement is also true in the continuum example), potential problems may arise when external non-Goldstone mesons (taste different from ξ_5) scatter to give massless ξ_5 mesons in internal loops.

As a simple example, consider massless SχPT theory with two flavors, and take only the coefficient C_4 in the taste-violating, $\mathcal{O}(a^2)$, potential [6, 7] to be non-zero. This is sufficient

[2] Note that one needs to go on shell so that derivatives acting on external lines also suppress the diagrams in the massless limit.

to give mass to all the non-Goldstone mesons. Now consider the contribution shown in Fig. 1 to the scattering of two taste-singlet, flavor charged, mesons through the exchange of taste-ξ_5 mesons. If the two vertices come from the C_4 term, then there are no derivatives on the internal lines to suppress the logarithmic IR divergence. On shell, the momentum transfer through the loop will, in the generic case, provide a cutoff. However, with C_4 vertices, there is an IR divergence in this diagram in the forward direction, $p_1 = p_3$, $p_2 = p_4$. The divergence is canceled by the diagrams with one or both of the vertices replaced by kinetic energy vertices. The terms in the kinetic energy vertices where the derivatives act on the external lines provide the cancellation, possible because $p_1 = p_3$ implies $p_1 \cdot p_3 = -a^2\Delta_I = -64a^2C_4/f^2$. Terms where the derivatives act on the internal lines are clearly not IR divergent; neither is the corresponding "s-channel" diagram (on shell). Though the result of this example is positive (no IR divergence on shell), it also shows some of the issues that would need to be addressed in a completely proof that full SχPT is safe.

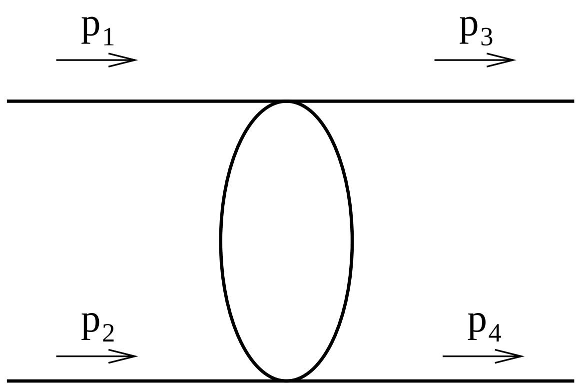

FIG. 1: A "t-channel" scattering diagram for the scattering of two taste-singlet mesons, with internal taste-ξ_5 mesons: $\pi_I^+(p_1) + \pi_I^-(p_2) \to \pi_I^+(p_3) + \pi_I^-(p_4)$.

A further subtlety is the following: When I suggest that full SχPT is "safe," I really only mean that certain standard quantities are safe, *i.e.*, they have commuting chiral and continuum limits. A sufficient number of derivatives (with respect to quark mass) of any safe quantity will certainly produce IR divergences and hence lack of commutativity of limits. Which quantities are likely to be safe? The above arguments suggest that any quantity which is free of IR divergences in the chiral limit of full continuum χPT will be safe in SχPT. This means, for example, that pseudoscalar masses and decay constants as computed in [2] will be safe. On the other hand, a quantity like the pion charge radius,[3] which is defined in terms of an external current with non-vanishing momentum transfer, is IR divergent in the continuum chiral limit [13]. The charge radius is therefore almost certain to have the wrong chiral limit at fixed a in SχPT; it should indeed behave much the same way as the quenched $M_\pi^2/2\mu m_{\text{ß}V}$, Eqs. (1) and (2).

Furthermore, since in the continuum one can differentiate the squared meson mass once with respect to the quark mass and still have a finite quantity in the chiral limit, I expect that the corresponding quantities in SχPT are safe. For the squared Goldstone (taste ξ_5) mass this is fairly obvious from the exact lattice $U_A(1)$; one can also divide by (instead of differentiating with respect to) the quark mass, as in the full SχPT version of Eq. (6). It is less obvious that one can differentiate the squared masses of non-Goldstone (taste other than ξ_5) mesons and still have a safe quantity. For example, how do we know that a term like $a^2\chi\ln\chi$ cannot appear in the squared non-Goldstone masses? Such terms are not divergent as $m \to 0$, but their derivatives are divergent, which would lead to non-commutativity. A one-loop calculation, similar to the scattering calculation described above, shows that such terms do in fact cancel for the taste-singlet mass. Whether this really persists beyond one loop remains to be seen. (Note that dividing a squared non-Goldstone mass by quark mass, rather than differentiating, is certainly unsafe, as is already clear at tree-level, Eq. (3).)

IV. ERRORS OF EXISTING NUMERICAL COMPUTATIONS

Dürr and Hoelbling [1] worry that the possible non-commutativity of limits with staggered fermions would induce new, uncontrolled, errors in the previously reported results with MILC staggered configurations [2, 3, 4, 5]. To the extent that SχPT describes the MILC simulations, we can argue that such errors are not present — even in the absence of a detailed proof that full SχPT is safe to all orders. That is because the extraction of physical results requires extrapolation only to the physical light quark masses, not to the chiral limit. The factor $\ln(\chi/\Lambda^2)$ is of order 3 or 4 at the physical point ($\chi \approx 140\,\text{MeV}$). Even should the logarithm not be "protected" by powers of χ in some higher order of SχPT and represent a divergence in the chiral limit at fixed a, it would still be suppressed, numerically, by the

[3] I thank S. Sharpe for this example

additional powers of a^2 at that order. By looking at the numerics of the calculations in Refs. [2, 3, 4, 5], it is not hard to convince oneself that any new errors would then be significantly smaller than the already-quoted systematic errors.

Note that my error estimate assumes that the "worst case" would be the existence of a singularity in full SχPT that would interfere with the extrapolation to the physical light quark masses. This is reasonable despite the fact that intermediate stages in the analysis in Refs. [2, 3, 4, 5] often involve fits to partially quenched lattice data, where we know that non-commutativity of limits does occur. The point is that the relevant NLO formulas such as Eq. (6) are known. We fit lattice data to them in a range of valence and sea masses that are far from the singularities. Since the light quark masses in the data are always more than a factor of three larger than the physical masses, the logarithms and the non-linearities associated with them are always significantly smaller than at the physical point. It is therefore not surprising that (as checked directly in the calculations) the NLO corrections in the fits are under control and of the expected magnitude. If unexpected new singularities were to occur in higher order, the resulting errors in the partially quenched fits would be smaller than those induced in the subsequent full SχPT extrapolation, simply because the logarithms are smaller.

Of course, if the staggered simulations had some additional non-commutativity of limits not captured by SχPT — having to do, say, with the fourth-root procedure — then an uncontrolled systematic error might in fact be present in the MILC results. However, recent advances in understanding the rooting procedure [14, 15, 16], coupled with the good fit of MILC data [2] to SχPT predictions [7, 8], make such a possibility seem increasingly unlikely.

V. ADDITIONAL REMARKS

The lack of commutativity of the chiral and continuum limits is not exclusively a property of staggered fermions. For Wilson fermions, it appears at one loop in a power counting for which $\mathcal{O}(m)$ and $\mathcal{O}(a^2)$ are treated as comparable [17]. At this order, a term of the form $a^2\chi\ln\chi$ is present in the squared meson mass in the full QCD case.[4] (The corresponding partially quenched case has not to my knowledge been studied.) After differentiating with

[4] I am grateful to O. Bär for pointing out to me this result in Ref. [17].

respect to (or dividing by) the quark mass, such a term leads to an IR divergence as $m \to 0$ for fixed a; whereas it clearly vanishes if the $a \to 0$ limit is taken first. The source of problem is the absence of an exact chiral symmetry in the massless limit. This means that massless Wilson pions can interact without derivative couplings [18], leading to IR singularities and failure of commutativity.

Note that the Wilson case is significantly worse than the staggered case: In the latter, self-interactions of the massless Goldstone (taste ξ_5) pion are always proportional to at least two powers of momentum. At finite a, the non-Goldstone staggered pions are not required to have derivative interactions, but neither are they massless.

My SχPT examples and certainly the Wilson case suggest that lack of commutativity has little or nothing to do with the rooting procedure. Is this also true of the 2D Schwinger models studied in Ref. [1]? The physics of the one-flavor 2D Schwinger model $\langle\bar{\psi}\psi\rangle$, where the non-commutativity is found, is quite distinct from the multiflavor 4D chiral theories discussed above. With one flavor, the "condensate" comes about because of the symmetry is violated by the anomaly, not because of spontaneous symmetry breaking. In the continuum, the anomaly leads to exact zero modes of the Dirac operator, which in turn saturate $\langle\bar{\psi}\psi\rangle$. Since staggered fermions have only near zero modes in complex pairs, their effect cancels in the $m \to 0$ limit, and $\langle\bar{\psi}\psi\rangle$ vanishes for fixed a. If the continuum limit is taken first, however, the complex pair of near zero modes becomes a pair of degenerate exact zero modes, and the rooting prescription works as desired, producing a single exact mode. (See Refs. [1, 19] for details.) Since the physics here is inextricably tied to having only one flavor, however, it is not possible to separate cleanly the issues of the lack of commutativity and the rooting procedure within this model.

In the two-flavor 2D Schwinger model, on the other hand, the rooting procedure is not required, yet I suspect that it would be possible to find non-commutativity in the masses of the "quasi-Goldstone bosons," of a similar nature to that seen in quenched or partially quenched 4D SχPT (Sec. II). That is because integration over a single (boson) pole in 2D has the same IR behavior as integration over a double pole in 4D. The problem here is that there is no true condensate in 2D, so there is no simple chiral theory: $\langle\bar{\psi}\psi\rangle$ and the quasi-Goldstone boson squared masses vanish as fractional powers of m as $m \to 0$ [20]. It is therefore a non-trivial problem to discover an analogue of SχPT that would allow one to calculate the discretization effects caused by staggered fermions. Thus I am not able at this point to make a specific proposal for where to look for non-commutativity in this model.

A simple alternative to the two-flavor theory in this context can be found in the quenched 2D Schwinger model, which does not require the rooting procedure either (trivially). Reference [19] studies the quenched theory with staggered fermions, but since $\langle\bar{\psi}\psi\rangle$ blows up as $1/m$ in the continuum, it is hard to see any non-commutativity cleanly. Recently, Dürr and Hoelbling have looked instead at $m\langle\bar{\psi}\psi\rangle/g^2$ (g is the coupling) for staggered fermions [21]. They find clear evidence that the chiral and continuum limits do not commute for this quantity. In addition, the behavior is is very similar, qualitatively, to that observed for $\langle\bar{\psi}\psi\rangle$ in the one-flavor Schwinger model. At the least, this shows that non-commutativity of limits is not inextricably tied to the rooting procedure in these 2D models.

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