QCD with rooted staggered fermions

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In this talk, I will give an overview of the theoretical status of staggered Lattice QCD with the “fourth-root trick.” In this regularization of QCD, a separate staggered quark field is used for each physical flavor, and the inherent four-fold multiplicity that comes with the use of staggered fermions is removed by taking the fourth root of the staggered determinant for each flavor. At nonzero lattice spacing, the resulting theory is nonlocal and not unitary, but there are now strong arguments that this disease is cured in the continuum limit. In addition, the approach to the continuum limit can be understood in detail in the framework of effective field theories such as staggered chiral perturbation theory.
1. Introduction

In the last few years, it has become possible to compute many hadronic quantities of phenomenological interest using Lattice QCD; for an overview of recent results, see the talk by Kronfeld at this conference [1]. Many of these results have been obtained using gauge configurations that include the effects of three light dynamical quarks, in which a (highly improved) staggered Dirac operator is used to discretize the quark action. Staggered fermions are attractive because of the relatively low expense required for reaching very light quark masses at very small lattice spacings. For most of these results, the claim is that all errors, statistical and systematic, are under control. However, as I will describe in more detail below, in order to remove a spurious four-fold redundancy inherent to staggered fermions, the fourth root of the fermion determinant for each physical flavor is taken inside the integral over the gauge field. This raises the critical question whether this method constitutes a valid regulator for QCD. In this talk, I will describe the problem in some detail, and then discuss the, in my view interesting and important, progress that has been made in answering this question. This talk is meant to give an overview, rather than a complete review of all work in this direction, as I do not have enough space to be complete. For other recent reviews, see Refs. [2, 3, 4, 5], which contain many more references to other relevant work.

Let me first very briefly recount the origin of the four-fold redundancy. A naive nearest-neighbor discretization of the free, massless Dirac operator, $S^1(p) = i\gamma_\mu \sin(ap_\mu)$, leads to an inverse lattice propagator of the form ($a$ is the lattice spacing)

$$S^1(p) = \sum_\mu \gamma_\mu \sin(ap_\mu):$$ (1.1)

In addition to the expected zero at $p = 0$, $S^1(p)$ has fifteen other zeros with at least one component of $p$ equal to $\pi/a$ on the Brillouin zone, from which it follows that this lattice fermion describes sixteen massless fermions in the continuum limit. This is an example of the well-known species doubling problem. There is a deep reason for the occurrence of these doublers in terms of the axial anomaly: a regulated theory with exact chiral symmetry has to produce an anomaly-free representation in the continuum limit [6].

Staggered fermions [7] reduce this multiplicity by four. They are constructed from naive lattice fermions by dropping the Dirac index, and replacing the $\gamma$-matrices by judiciously chosen, $x$-dependent phases. This reduces the sixteen-fold doubling to a four-fold doubling. In other words, each staggered fermion describes four degenerate relativistic flavors in the continuum limit, which we will henceforth refer to as the four “tastes” of each staggered fermion. The emergence of this continuum limit, which carries over to the interacting case, is a consequence of lattice symmetries and dimensional analysis: lattice symmetries guarantee that a continuum limit with SO(3,1) Lorentz and SU(4)$_L$ SU(4)$_R$ chiral “taste” symmetry is obtained without any tuning of the action [8]. A particularly important lattice symmetry is the U(1) transformation that rotates the fermion fields on even and odd lattice sites with opposite phases (“U(1)$_e$ symmetry”) [9], which is an exact axial symmetry, broken by a (single-site) mass term.

In practice, one uses the following method for simulating QCD with three light flavors. A separate staggered field is introduced for each physical flavor, with single-site mass terms for each, with masses $m_u$, $m_d$ and $m_s$. Each of these flavors thus comes in four tastes, and the the-
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ory would thus contain four up, four down and four strange quarks in the continuum limit, with a U(4)$_u$ U(4)$_d$ U(4)$_s$ taste symmetry. To eliminate this unphysical multiplicity, the fourth root of each staggered determinant is taken, motivated by the observation that, in the continuum limit, the staggered determinant should factorize as

$$\text{Det} (D_{\text{stag}}) = \text{Det} (D_{\text{cont}})^4.$$ \hspace{1cm} (1.2)

Since for all $m \neq 0$, $\text{Det} (D_{\text{stag}}) > 0$ (this determinant depends only on $\gamma$, because of $U(1)_e$ symmetry), it is clear that the positive fourth root should be taken, and that the resulting quark mass $m_q \propto \gamma$. This, then, constitutes a regularization of three-flavor QCD with all quark masses positive.

The topic of this talk is the validity of this regularization.

2. The problem

First, let us consider a continuum theory with exact $U(4)$ taste symmetry, i.e., with four fermions with equal positive quark masses. In this case, one can take the fourth root of the fermion determinant, and doing so reduces the partition function to that of a theory with one flavor, $N_f = 1$. In this rooted theory, one still has access to correlation functions with all four tastes on the external lines, e.g., correlation functions of the fifteen pions of the four-taste theory. It is thus interesting to ask in exactly what sense taking fourth root reduces the number of pions from fifteen to none.

The key observation is that, since rooting reduces the number of sea quarks from four to one, the correct number for the $N_f = 1$ theory, it is possible to construct consistent projections into the physical, unitary one-flavor theory [12]. I will illustrate this with an example in the meson sector.

For this, it is useful to describe rooting in terms of the replica rule: if we take $n_r$ copies of a $U(4)$-taste fermion field, so that the four-taste fermion determinant appears raised to the $n_r$-th power, then continuing $n_r! \rightarrow 1$ corresponds to taking the fourth root. Armed with this tool, let us consider, for example, the two-pion intermediate states in the taste-singlet scalar two-point function in chiral perturbation theory (ChPT) [13, 14]. These two-pion states produce a cut starting at $2m_{\pi}$, and in the theory with $n_r$ replicas, the "strength" of this cut is $16n_r^2$, because that is the number of pions in the theory with $n_r$ replicas, which has $SU_L(4n_r) \times SU_R(4n_r)$ chiral taste-replica symmetry for any positive integer $n_r$. If we now continue $n_r! \rightarrow 1$ (see also Sec. 5 below), we see that this factor vanishes, and the two-pion cut disappears, as it should; this follows from taste symmetry. Our example demonstrates how the theory is unitary for $n_r = N_f = 4$ for any positive integer $N_f$ even if $N_f < 4$, despite the presence of "too many" pions in the rooted theory.

On the lattice, taste symmetry is broken to a much smaller, discrete group, and the argument above no longer holds. This raises three questions that we will consider in the rest of this talk:

1) Is rooted staggered QCD a regularization like any other, or not? The answer is no, the theory is nonlocal and nonunitary at $a \neq 0$.

2) Can the continuum limit be taken, and is it in the correct universality class? Here the answer is most likely yes, and we will briefly review the renormalization-group (RG) based argument supporting this claim [15].
3) But this is not the end of the story. We work at $a \neq 0$, and scaling violations, while small, are still significant. Hence, in actual computations, the diseases are present, and one needs effective-field theory (EFT) techniques to parameterize the nonlocal effects (in addition to the need to control continuum and chiral extrapolations). The question is whether such an EFT framework exists. The claim is that it is provided by “Staggered ChPT plus the replica rule,” or rSChPT for short [16]. Two related, but different derivations have been given: The first derivation is entirely within the ChPT framework, and starts with the observation that rooting works trivially for a theory with four degenerate staggered fermions, i.e., an $N_f = 4$ theory. One then moves to the nondegenerate case by expanding around the degenerate case. This allows one, under certain assumptions, to decouple one or more of the fermions, thus arriving at the cases $N_f = 1, 2, \text{ or } 3$ [13]. The other is a direct derivation from the RG framework of Ref. [15], which we will describe below.

3. Nonlocality and nonunitarity from taste-symmetry breaking.

Taste symmetry is broken on the lattice, and we may thus split the staggered Dirac operator into two parts, $D_{stag} = D \mathbf{1}_4 + a \Delta$, with $\mathbf{1}_4$ the unit matrix in taste space, and $\Delta$ the taste-breaking part (with $\text{tr}_{\text{taste}}(\Delta) = 0$). The taste-breaking part vanishes linearly with $a$ in the classical continuum limit, which is why I factored out the explicit factor $a$. It follows that

\[
\log \text{Det}(D_{stag}) = 4 \log \text{Det}(D) + \log \text{Det} \left(1 + D^{-1} a \Delta\right) : \tag{3.1}
\]

While both $D$ and $a \Delta$ are local, clearly $D^{-1} a \Delta$ is not! This means that taste breaking, while local at the level of the action, has nonlocal consequences for the physics. Indeed, the second term on the right breaks taste symmetry, and lifts the degeneracy of the fifteen pions of the theory defined by $D \mathbf{1}_4$. The pion spectra of the $D_{stag}$ and $D \mathbf{1}_4$ theories do not match. From this observation, it is easy to prove that the rooted theory is nonlocal at $a \neq 0$ [17].

Lowest-order SChPT gives the pion masses of the staggered theory as

\[
(m_\pi^A)^2 = B m_{\text{quark}} + c^A a^2 A_{QCD}^4 ; \tag{3.2}
\]

in which the index $A$ labels the different pions, which fall into irreps of the exact remnant of taste symmetry on the lattice [18], with a different value of $c^A$ for each irrep.\(^3\) The pion-mass behavior predicted by Eq. (3.2) is clearly seen in numerical simulations [19]. Figure 1 shows the nondegeneracy of the various different pions, with the various labels corresponding to values of the index $A$ (for details, we refer to Ref. [19]), and Fig. 2 shows how the taste splittings scale with the lattice spacing ($r_1$ is a quantity used to set the scale).

This pattern implies that the $N_f = 1$ “pion counting” argument given at the beginning of the previous section for the continuum rooted theory is violated on the lattice. Exact cancellations that occurred because of full SU($4n_r$) taste symmetry no longer occur [14,13], and an $O(a^2)$ two-pion cut survives in the taste-singlet two-point function for $n_r = 1\cdots 4$. This example demonstrates that indeed rooted staggered fermions are not unitary at $a \neq 0$, and that this violation of unitarity occurs at physical scales, exhibiting the nonlocality of the theory.

\(^3\)There is only one exact Goldstone boson, for which $c^A = 0$ in Eq. (3.2), as a consequence of $U(1)_\epsilon$ symmetry.
While this discussion confirms the sickness of the rooted theory at $a \neq 0$, it teaches us several important things. First, if the taste-breaking operator $a \Delta$ is irrelevant (in the sense of the RG), the nonlocal and nonunitary behavior disappears in the continuum limit. In the unrooted theory, $a \Delta$ is indeed irrelevant, and taste symmetry is restored in the continuum limit. However, this is not obvious in the rooted theory, since it requires the extension of RG techniques to the nonlocal theory at $a \neq 0$. We will investigate this in the next section.

Another important observation is that pion masses are governed by two different IR scales: the physical quark mass $m$, and the unphysical taste splitting $(a \Lambda_{QCD}^2)^2$ that leads to unitarity violations in the $a \neq 0$ rooted theory. It is thus clear that (a) the limit $m \to 0$ at $a \neq 0$ is unphysical [20], and (b) that the limit $a \to 0$ has to be taken before continuation to Minkowski space.

4. Continuum limit: a renormalization-group framework.

It is natural to study the approach of the continuum limit in an RG framework. First, it gives us a tool for a precise definition of the continuum limit, making it possible to define what is meant by the intuitive factorization of the staggered determinant, Eq. (1.2). Second, in the unrooted theory, one expects that low-lying (IR) eigenvalues form taste quadruplets when $a$ becomes small, while this won’t happen for the UV (cutoff) eigenvalues. Here RG blocking helps: it gets rid of the UV eigenvalues.\footnote{For numerical investigations of staggered eigenvalues, see Ref. [21].}

A simple hypercubic blocking scheme can be set up [15] in which one takes the “coarse” lattice spacing $a_c = \Lambda_{QCD}$ arbitrarily small but fixed, and the fine lattice spacing $a_f$ to zero: after $n$ blocking steps, the relation between the two lattice spacings is given by $a_c = 2^n a_f$. The usual universality arguments imply that this will lead to the expected continuum limit for unrooted staggered fermions because they are local, and this is what we will assume in the rest of this talk.
In contrast, no direct RG blocking can be defined for the rooted theory, since the rooted theory is not formulated in terms of a path integral: the fourth root is taken inside the integral over gauge fields after the fermionic integral has been performed. However, it is possible to construct a bridge between the unrooted and rooted theory at each blocking step: these “reweighted” theories will be constructed to have the same $a_f = 0$ theory as the staggered theory, but they also will have exact taste symmetry [13].

This works as follows. After each blocking step, we split the (blocked) staggered Dirac operator $D_{stag n} = D_n \mathbb{1} + a_f \Delta_n$, with $a_f \Delta_n$ the taste-breaking part, just as before Eq. (3.1). The unrooted staggered theory defined by $D_{stag n}$ and the taste-invariant theory defined by $D_n \mathbb{1}$ have the same continuum limit, because $a_f \Delta_n$ will scale as expected in this case. The theory defined by $D_n \mathbb{1}$ has exact taste symmetry, and is local on the $n$-th lattice. This theory can thus be rooted, and one obtains a local one-taste theory with partition function

$$Z^{\text{reweigh}} = d\mu_{\text{gauge}} \text{Det} (D_n) :$$

(4.1)

The claim is now that for $n \to \infty$ (at fixed $a_c$) this local theory coincides with the nonlocal theory

$$Z^{\text{root}} = d\mu_{\text{gauge}} \text{Det}^{1/4} (D_{stag n}) :$$

(4.2)

Indeed, if $\langle a_f \Delta_n \rangle \lesssim a_f = a_c$, one has that

$$\text{Det}^{1/4} (D_n \mathbb{1} + a_f \Delta_n) = \text{Det} (D_n) \exp \left( \frac{1}{4} \text{tr} \log (1 + D_n^{-1} a_f \Delta_n) = \text{Det} (D_n) + O \left( \frac{a_f}{a_c^2} m \right) \right)$$

(4.3)

For this to work, it is necessary that $a_f \Delta_n$ scales like $a_f = a_c$ on an ensemble. We need this scaling between $1 = a_f$ and $1 = a_c$, and, since $1 = a_c = \Lambda_{\text{QCD}}$, this scaling should be calculable in perturbation theory. The conjecture here is that one can rely on this to work, because it concerns the scaling of a local operator ($\Delta_n$), in a renormalizable theory.

We may rephrase the RG argument as follows [3]:

- The starting point is that $a_f \Delta_n$ scales like $a_f$ in the unrooted staggered theory, because this theory is local. It has to, if the expected continuum limit for this theory exists.

- Therefore, $a_f \Delta_n$ scales like $a_f$ in the four-taste reweighted theory defined by $D_n \mathbb{1}$, which is U(4) taste invariant and local on the $n$-th lattice.

- One then expects that $a_f \Delta_n$ scales like $a_f$ in the one-taste reweighted theory; because of the exact taste symmetry of reweighted theories, the one-taste reweighted theory is still local.

- Finally, one may reconstruct the rooted staggered theory from the one-taste reweighted theory, using the expansion (4.3).

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5 One can “postpone” the integration over the gauge fields on the blocked lattices, so that the fermion integration remains gaussian at each step [15].

6 There is no space for a detailed discussion of this point, for which we refer to Ref. [15].
We end this section with the comment that, clearly, a necessary condition for all this to work is that rooting works in perturbation theory. Indeed, it does: in the theory with $N_f$ flavors and $n_r$ replicas, the total number of quarks on any closed loop is equal to $4N_f n_r$, which, for $n_r = 1$ to $N_f$ (which corresponds to taking the fourth root of each of the $N_f$ staggered determinants) is precisely equal to $N_f \prod_{i=2}^{N_f}$. It follows that indeed the rooted theory is (perturbatively) renormalizable, and thus standard power counting, according to which $a_f \Delta$ is irrelevant, applies.

5. Staggered ChPT from the RG approach.

After reviewing the RG-based argument for the validity of rooting in the continuum limit, we now use this framework to derive the existence of an EFT framework for the rooted staggered theory at nonzero $a$, thus addressing the concern expressed in the third question of Sec. 2 [23]. EFTs such as the Symanzik effective theory (SET) [24] and ChPT account for lattice artifacts through a systematic expansion in $a \Lambda_{QCD}$. An example may illustrate this as follows. The taste breaking at $a = 0$ leads to taste-breaking four-fermion operators in the effective continuum theory, much like “new physics” at a higher scale leads (for example) to effective four-fermion operators to be added to the Standard Model action. The “new physics” here is the taste (and rotational) symmetry breaking in the underlying lattice theory. For instance, the SET for the staggered theory contains an operator of the form

$$a^2 \left( \bar{\psi} R \bar{\xi}_5 \psi_L \right) \left( \bar{\psi} R \bar{\xi}_5 \psi_L \right) + h.c. : a^2 \text{tr} \left( \xi_5 \xi_5 \Sigma \xi_5 \xi_5 \Sigma \right) + h.c. ;$$

in which the $\xi_5$ are a set of $4 \times 4$ $\gamma$-matrices acting in taste space. On the right-hand side, I gave the translation of this four-fermion operator into ChPT, in terms of the nonlinear pion field $\Sigma$. Of course, all such operators, and their translation into ChPT, have to be systematically classified [16].

The key assumption on which the existence of EFTs is founded is that the underlying theory, in this case, the lattice theory, is local. Since the rooted staggered theory is not local, the construction of EFTs like the SET and ChPT along the lines described above is not automatic. The question is thus whether the construction of a SET and staggered ChPT can be extended to rooted staggered QCD.

The replica rule of Sec. 2 gives us an intuitive idea of what to do, but there is a catch. One starts with a theory with $n_r$ staggered fermions, with $n_r$ a positive integer. One constructs the desired EFT, and simply continues $n_r$! $N_f=4$ in this EFT, since this is precisely how one obtains the theory with $N_f$ flavors from staggered QCD through rooting (if $N_f$ itself is not a multiple of four). In other words, one continues the EFT from integer values of $n_r$, where the underlying theory is local, to quarter-integer values. This should work for the explicit dependence on $n_r$ that comes from calculating diagrams with loops in the EFT. The catch is, however, that the EFT depends on $n_r$ not only through loops, but also through the coupling constants that multiply the operators which build up the EFT. As long as $n_r$ is integer, these coupling constants are uniquely determined by the underlying local theory. But for quarter-integer values, they have to be obtained by continuation, and a unique continuation off the positive integers does not exist. Moreover, it might happen that the continuation will encounter a singularity precisely at $n_r = N_f/4$. All this implies that we need

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7I will restrict the discussion to $N_f < 4$ degenerate flavors; the generalization to nondegenerate masses is obvious.
more information about the dependence on \( n_r \) of the correlation functions of the underlying lattice theory.

This is where the RG framework of the previous section comes in. First, take \( n_r \) a positive integer, and carry out \( n \) RG blocking steps. The resulting theory has a partition function

\[
Z_{n_r} = \int d\mu_{gauge} \ Det^{a_f} (D_{stag} \mu) ; \tag{5.2}
\]

Now, we generalize this theory by replacing (recall, \( D_{stag} = D_n + a_f \Delta_n \))

\[
\Det^{a_f} (D_{stag}) / \Det^{a_f} (D_n) \cdot \Det^{a_f} (D_n + t a_f \Delta_n) / \Det^{a_f} (D_n) ; \tag{5.3}
\]

Here \( n_s \) is the desired number of physical flavors (with a given quark mass), and we thus need \( n_s = 4 \) staggered quarks. At this point, however, we still keep \( n_r \) integer, and not necessarily equal to \( n_s = 4 \).

Note the new “interpolating” parameter \( t \). We make the following observations:

- For \( n_s = 4 n_r \) and \( t = 1 \) this is the staggered theory with \( n_r \) replicas, hence the right-hand side of Eq. (5.3) indeed generalizes the theory (5.2);

- For \( t = 0 \) this is the (local!) reweighted, taste-invariant theory with \( n_s \) taste-singlet fermions;

- For \( n_s \neq 4 n_r \) (and \( t \neq 0 \)), this is a partially quenched theory \([22]\), in which the determinant in the denominator is obtained from a path integral over “ghost” quarks with opposite (i.e., bosonic) statistics.

As long as \( n_r \) and \( n_s \) are positive integers, and for any \( t \), this defines a local, but partially quenched theory. Our key assumption will be that for such theories EFTs like the SET and ChPT exist.\(^8\)

What this setup buys us is the following. Expanding the determinant ratio in Eq. (5.3) using

\[
\Det^{a_f} (D_n) \Det^{a_f} (D_n + t a_f \Delta_n) / \Det^{a_f} (D_n) = \Det^{a_f} (D_n) \exp n_r Tr \log (1 + t \Delta_n) ; \tag{5.4}
\]

one sees that, in this expansion, the power of \( n_r \) is smaller than the power of \( t \), which, in turn, is smaller than or equal to the power of \( a_f \) to which we expand. It follows that all correlation functions of the theory, when expanded to some fixed order in \( a_f \), are polynomial in \( n_r \)! Since this is true in the underlying lattice theory, it has to be true in any EFT representing this theory, and we may thus continue \( n_r \) to \( n_s = 4 \) in the EFT. In the end, we may also set \( t = 1 \), thus arriving at the EFT for the original staggered theory with \( n_r \) replicas, but now for any \( n_r = n_s = 4 \), with \( n_s \) a positive integer.

The correctness of rSChPT thus follows directly from the RG argument that supports the conjecture that rooted staggered fermions constitute a regularization of QCD in the correct universality class.

Note that the argument sketched above does not imply that we have to actually perform the continuation off integer values of \( n_r \) explicitly. The point is that our argument proves that the values of the coupling constants of the EFT are uniquely determined by the underlying lattice theory. It follows that the desired values (those at \( n_r = n_s = 4 \) and \( t = 1 \)) can then be determined by fits to the numerically computed correlation functions of the rooted theory itself.

\(^8\)This has become “standard lore” in lattice gauge theory, and there is now rather extensive numerical evidence supporting the validity of this assumption. This point has also been emphasized in Refs. [13, 2].
One may ask why this approach does not imply that the theory may be defined for any (real) value of \( n_r \). The key point here is that, as should be clear from the continuum example at the start of Sec. 2, only for \( n_r = n_s = 4 \) with positive integer \( n_s \) the continuum limit corresponds to a unitary theory.\(^9\) A corollary is that rSChPT should reproduce the sicknesses of the rooted staggered theory at \( a \neq 0 \), and indeed it does. A nontrivial test of this was performed in Ref. \([14]\), in which the \( a_0 \) and \( f_0 \) two-point functions were fitted to rSChPT. The values of low-energy constants found with this fit are in good agreement with those fitted from pion and kaon masses and decay constants.

6. Conclusions

While I have only been able to give a very schematic overview of (some of) the arguments, I conclude that, while at nonzero lattice spacing rooted staggered QCD is nonunitary, it is very likely to have the correct continuum limit. The RG-based arguments, in particular, tie the validity of the rooted theory very strongly to the — uncontested — validity of the local, unrooted theory.

In addition, I have shown how one can derive EFTs, such as rSChPT, which are valid at \( a \neq 0 \). This is necessary both because of the fact that scaling violations, while small, are not negligible at present, and also in order to test our understanding of the nonphysical effects of rooting numerically. The validity of rSChPT makes it possible to do numerical computations with pion masses down to \( m_\pi^2 \): \( \bar{Q}^4 \), which is crucial, with present resources, for reliable extrapolations to the physical values of the up and down quark masses. I emphasize that, since rSChPT follows directly from the RG argument for rooted staggered QCD, fits of numerical data using rSChPT constitute direct tests of this argument for the validity of rooting. An interesting test in this respect is an rSChPT fit in which \( n_r \) was kept as a free parameter in the fit, yielding \( n_r = 0.28(4) \) \([25]\).

In conclusion, there is now very good theoretical and numerical evidence that using the fourth-root trick works, despite the fact that for \( a \neq 0 \) the theory is sick. There is at present no valid argument that the fourth root trick fails (see the Appendix for an additional comment).

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Appendix

The only published arguments against rooting are those of Creutz (Ref. \([26]\) and refs. therein). I will not revisit the discussion of these arguments here again, since they have been proven incorrect \([12, 4]\) in all their incarnations. Indeed, none of our detailed arguments refuting his claims have been addressed by Creutz; in Ref. \([26]\) they are simply ignored. I emphasize that refuting Creutz’s arguments by itself does not prove rooting to be correct, and I have reviewed the current status of the evidence for the validity of rooting in this talk.

\(^9\)Perturbative renormalizability holds indeed for any \( n_r \).
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