On the foundations of partially quenched chiral perturbation theory

Claude Bernard and Maarten Golterman

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On the foundations of partially quenched chiral perturbation theory

Claude Bernard

Department of Physics, Washington University, St. Louis, MO 63130, USA

Maarten Golterman*

Institut de Física d'Altes Energies, Universitat Autònoma de Barcelona, E-08193 Bellaterra, Barcelona, Spain

Abstract

It has been widely assumed that partially quenched chiral perturbation theory is the correct low-energy effective theory for partially quenched QCD. Here we present arguments supporting this assumption. First, we show that, for partially quenched QCD with staggered quarks, a transfer matrix can be constructed. This transfer matrix is not Hermitian, but it is bounded, and it can be used to construct correlation functions in the usual way. Combining these observations with an extension of the Vafa–Witten theorem to the partially quenched theory allows us to argue that the partially quenched theory satisfies the cluster property. By extending Leutwyler's analysis of the unquenched case to the partially quenched theory, we then conclude that the existence and properties of the transfer matrix as well as clustering are sufficient for partially quenched chiral perturbation theory to be the correct low-energy theory for partially quenched QCD.

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* Permanent address: Department of Physics and Astronomy, San Francisco State University, San Francisco, CA 94132, USA

I. INTRODUCTION

Partially quenched chiral perturbation theory (PQChPT) has been extensively used in the analysis of numerical computations of hadronic quantities in lattice QCD. In such computations, one has the freedom to vary valence quark masses (masses of quark operators appearing explicitly in correlation functions) and sea quark masses (masses of quarks appearing in the fermion determinant of the theory) independently. This generalized version of QCD, which is commonly referred to as partially quenched QCD (PQQCD), contains full QCD as the special case in which valence and sea quark masses are set equal to each other (for each flavor) [1]. PQChPT is, correspondingly, the generalization of chiral perturbation theory to the partially quenched setting.[1]

The ability to vary valence and sea quark masses independently is useful for a variety of reasons. First, the computation of quark propagators needed for the contractions making up a correlation function is significantly less expensive in most applications than the generation of gauge field configurations, which depend on the sea quark mass. With fixed computational resources, it can thus be an advantage to generate data for a number of valence quark masses on an ensemble of gauge configurations with a given sea quark mass.

Second, PQQCD contains full QCD with the same set of sea quarks. It follows that the low-energy constants (LECs) of the effective theory for the partially quenched theory are those of the real world, because, by definition, the LECs do not depend on the quark masses [3].[2] It turns out that in a number of cases, it is easier to determine these LECs by varying the valence and sea quark masses independently; having more parameters to vary provides more "handles" on the theory.

Third, on the lattice, PQQCD can be generalized to QCD with a "mixed action," in which not only valence and sea quark masses are independently chosen, but also the discretization of the Dirac operator is different for valence and sea quarks [4]. The continuum limit of such a theory is a partially quenched theory; a fine tuning is generally required to make valence and sea quark masses equal in the continuum limit.

Fourth, lattice theories with staggered fermions that use the fourth-root procedure [5] to eliminate unwanted "taste" degrees of freedom are closely related to PQQCD because

[1] For a review, see Ref. [2].
[2] They do depend on the number of sea-quark flavors.

there is a mismatch between the (rooted) sea quarks and the (unrooted) valence quarks [6–8]. PQChPT plays an important role in the development of the effective chiral theory for rooted staggered fermions [9, 10], which in turn provides some evidence for the validity of the rooting procedure. For more discussion of these issues see Refs. [7, 11–13] and references therein.

However, it is less clear than in the case of full QCD that the partially quenched chiral theory is indeed the proper low-energy effective field theory. This is because PQQCD violates some of the properties of a healthy quantum field theory: The path integral definition of PQQCD includes an integral over ghost quarks, which have the same quantum numbers and masses as the valence quarks, but which have bosonic, rather than fermionic, statistics. The partially quenched theory thus violates the spin-statistics theorem. The reason for the presence of ghost quarks is that their determinant cancels the valence quark determinant [14]; it is this very cancellation that makes the gauge configurations independent of the valence mass.

In Ref. [15], Weinberg conjectured that the validity of chiral perturbation theory (ChPT) as a low-energy effective theory for the Goldstone sector of QCD follows from the basic properties of a healthy quantum field theory, which include analyticity, unitarity, cluster decomposition, and symmetry considerations. It was assumed that the S-matrix calculated with the most general local Lagrangian consistent with a certain symmetry group is the most general possible S-matrix consistent with these basic properties. This was then used as a starting point for the systematic development of ChPT to obtain S-matrix elements as an expansion in terms of the pion momenta and masses, following a well-defined power-counting scheme. The implicit reliance of this argument on unitarity, though, appears to be an obstruction to extending this line of reasoning to the partially quenched case, which is certainly not unitary.

A justification for ChPT as the low-energy effective theory for QCD based on a somewhat different set of arguments was presented by Leutwyler [16]. In this justification, the most important ingredients, in addition to symmetries, are locality and the cluster property of the underlying theory (full QCD), while unitarity is not used. Locality and clustering guarantee the existence of vertices in the effective theory that are independent of the correlation functions in which they appear, and, consequently, the existence of a loop expansion. We have found this approach more useful for the case of PQQCD than that of Ref. [15]. By construction, PQQCD is local. The question then becomes whether the theory also satisfies the cluster property. The main goal of the present article is to collect the theoretical evidence that this is indeed the case. Our argument will be based on three ingredients: the existence and properties of a transfer matrix for PQQCD, the observation that chiral symmetry breaking is expected to take place in PQQCD because it takes place in the full theory contained within PQQCD [17], and an extension of the Vafa–Witten theorem [18] about the absence of spontaneous symmetry breaking of vector-like global symmetries (this part of the argument extends the argument already given in Ref. [17]). The combination of these ingredients allows us to argue that the partially quenched theory satisfies the cluster property, under a set of mild additional assumptions similar to those used in Ref. [16]. With this result in hand, the justification for PQChPT as the low-energy effective theory for PQQCD then follows, much like it does for the case of full QCD. For technical reasons, we limit ourselves to lattice QCD with staggered quarks, but we believe that the extension to other discretizations of QCD is relatively straightforward.[3] An earlier account of part of this work appeared in Ref. [20].

As is well known, the partially quenched theory has more severe mass singularities than normal QCD. These arise in particular when valence and ghost masses vanish with sea masses held fixed and nonzero ("partially quenched chiral logarithms") and are caused by double poles in flavor-neutral propagators [1, 21]. The double poles are properties of PQQCD itself, not just of the chiral effective theory, as shown (with some assumptions) in Ref. [17]. Here, we will avoid these mass singularities by always working with all quark and ghost masses strictly positive. This has the further advantage that there are no massless particles (either from chiral symmetry breaking, or from breaking of other symmetries, which we show cannot occur). Thus "clustering" in this article means, "exponential clustering," with correlation functions of widely separated Euclidean points falling exponentially with distance. We emphasize that we do not need to take the limit of vanishing masses in order to show that pseudo-Goldstone bosons (pions) exist in the partially quenched theory; as mentioned above, this is a consequence of their existence in unquenched QCD and the (extended) Vafa–Witten theorem.

In constructing the PQQCD transfer matrix, we begin with a theory of ghost (bosonic)

[3] For instance, see Ref. [19] for Wilson ghost quarks.

quarks only, coupled to background gluons. This is clearly the nontrivial part of the problem, since transfer matrices for ordinary quarks and gluons are standard. Our approach makes it unnatural to demand that ghost-quark and valence-quark masses (call them m_q and m_v, respectively) are equal from the outset, as they are in the usual numerical application of PQQCD. Thus we are led to a more general setting, where all three types of quark masses (valance quark, sea quark, and ghost quark) may be different. This general setting has some interesting features, most of which seem to be of purely academic interest, since the limit of equal ghost-quark and valence-quark masses is the useful one. However, it does provide one important insight: The double poles, which are considered to be characteristic of PQQCD and PQChPT, arise from the near-cancelation of single poles in the limit $m_g \to m_v$. It is crucial here that the poles associated with ghosts have residues with opposite signs from those of the valence quarks. These unusual signs are associated with the bosonic nature of the ghost quarks, which also causes the ghost-quark Hamiltonian to be non-Hermitian. The ensuing violations of unitarity (see Sec. III C) thus appear to be a more fundamental feature of PQQCD than the existence of double poles *per se*, which appear only in the special case $m_g = m_v$.

Instead of using bosonic quarks to cancel the unwanted valence-quark determinant, Damgaard and Splittorff [22] proposed a replica approach, in which each valence quark is replicated n_r times, and one attempts to continue n_r to zero from the positive integers at the end in order to remove the determinant. It is interesting to consider whether further progress in justifying PQChPT can be made using that approach. The main obstacle in that direction seems to be the absence of a proof that the replica approach is indeed equivalent to PQQCD nonperturbatively. If that obstacle were overcome, many other steps would be straightforward, since the theory has a conventional chiral theory for each positive integer n_r. However, a similar problem would also remain on the chiral side of the argument, since one also has no proof that the replica version of the chiral theory is nonperturbatively equivalent to PQChPT when n_r is continued to zero.

This article is organized as follows. In Sec. II we construct the transfer matrix for PQQCD with staggered quarks. We find that the transfer matrix is not Hermitian, but is nevertheless bounded. It turns out to be instructive to consider the free theory in some detail, and this is done in Sec. III. In particular, the free theory clearly demonstrates that unitarity is violated in PQQCD.

Then, in Sec. IV, we turn to the effective theory, PQChPT. We first give a brief recapitulation of Leutwyler's arguments for the unquenched case in Sec. IV A, focusing on the use of clustering. In the partially quenched case, the exponential clustering "almost" follows from the existence of a bounded transfer matrix, but the possibility of massless particle from spontaneous symmetry breaking is a significant loophole. In Sec. IV B, we argue that the extension of the Vafa–Witten theorem about vector-like global symmetries in QCD implies (up to certain mild assumptions) that the cluster property does in fact hold in PQQCD. We discuss the role of rotational symmetry in Sec. IV C, and synthesize all our observations into an argument for the correctness of PQChPT as the low-energy effective theory for PQQCD in Sec. IV D. For technical reasons, we need to assume that the pion masses remain real in PQQCD, despite the fact that the corresponding transfer-matrix Hamiltonian is not Hermitian. This assumption is strongly supported by numerical evidence. In Sec. IV E, we use CPT symmetry to argue that all low energy constants in PQChPT have the same phases (real, with usual conventions) as they would in a Hermitian theory. This supports our assumption that the masses are real. Nevertheless, as we show in Sec. IV F, in the nonstandard case where ghost-quark masses are not degenerate with valence-quark masses, the effective theory shows that complex masses may arise in some ranges of quark and ghost masses, as may a new phase transition. The effective theory also shows how double poles arise from single poles in the $m_g \to m_v$ limit. Our conclusions are contained in Sec. V. There are two appendices, both concerned with the free theory. In App. A we show completeness of a basis of (right or left) eigenstates, and App. B discusses a path integral formulation of the free theory.

II. TRANSFER MATRIX

In this section, we construct the transfer matrix for a gauge theory coupled to fermionic and bosonic or "ghost" staggered quarks. Each of these quarks can have an arbitrary mass, but we will require all masses to be positive.[4] In Sec. II A we construct the transfer matrix for ghost quarks in a background gauge field. In Sec. II B we discuss some properties of the ghost transfer matrix; in particular, we show that it is bounded. Then, in Sec. II C

[4] The phase of a ghost-quark mass cannot be changed by chiral transformations [19, 23].

we combine this with the transfer matrix for a gauge theory with only fermionic quarks to arrive at the complete transfer matrix, and show that it is invariant under PT and CPT symmetry. We will use the "double time-slice" construction for both fermionic and ghost quarks [24, 25].

A. Ghost sector

The staggered action is

$$S = \sum_x \left\{ \frac{1}{2} \sum_\mu \eta_\mu(x) \left(\chi^\dagger(x) U_\mu(x) \chi(x+\mu) - \chi^\dagger(x+\mu) U_\mu^\dagger(x) \chi(x) \right) + m \chi^\dagger(x) \chi(x) \right\} , \tag{2.1}$$

in which

$$\eta_\mu(x) = (-1)^{x_1 + \dots x_{\mu-1}} , \tag{2.2}$$

and where χ and $\chi^\dagger$ are the staggered fields, $U_\mu(x)$ are the link variables, and color indices are suppressed. We will denote a lattice gauge field consisting of all link variables $U_\mu(x)$ by $\mathcal{U}$. If χ and $\chi^\dagger$ are Grassmann, they are independent of each other, and $\chi^\dagger$ can then also be denoted as $\overline{\chi}$, as is often done. However, here we are interested in the ghost-quark sector of the theory, for which we take $\chi(x)$ to be a c-number. In order that the path integral over the ghost fields be convergent, we need to take $\chi^\dagger(x)$ to be the Hermitian conjugate of $\chi(x)$. With this choice, the partition function

$$Z(\mathcal{U}) = \int \prod_x d\chi_x^\dagger d\chi_x \exp(-S) \tag{2.3}$$

is well-defined, as long as we take $m > 0$, which we will assume throughout this article.

In order to construct the transfer matrix representation of Z, we find it convenient to introduce real fields ϕ_1 and ϕ_2 through

$$\chi(x) = \eta_4(x)\phi_1(x) + i\phi_2(x) , \qquad \chi^\dagger(x) = \eta_4(x)\phi_1(x) - i\phi_2(x) . \tag{2.4}$$

Choosing temporal gauge, $U_4(x) = 1$, and splitting $x \to (\vec{x},\, t = x_4)$, we rewrite S as[5]

$$
\begin{aligned}
S \;=\; \sum_x \Bigg\{ & i\Big(\phi_1(\vec{x},t)\phi_2(\vec{x},t+1) - \phi_2(\vec{x},t)\phi_1(\vec{x},t+1)\Big) \\
+i\sum_j \eta'_j(\vec{x}) & \left(\phi_1(\vec{x},t) \;\mathrm{Re}\; U_j(\vec{x},t)\phi_2(\vec{x}+\vec{j},t) + \phi_2(\vec{x},t) \;\mathrm{Re}\; U_j(\vec{x},t)\phi_1(\vec{x}+\vec{j},t)\right) \\
+i\sum_j \eta_j(\vec{x}) & \left(-\phi_1(\vec{x},t) \;\mathrm{Im}\; U_j(\vec{x},t)\phi_1(\vec{x}+\vec{j},t) + \phi_2(\vec{x},t) \;\mathrm{Im}\; U_j(\vec{x},t)\phi_2(\vec{x}+\vec{j},t)\right) \\
& +m\left(\phi_1(x)^2 + \phi_2(x)^2\right) \Bigg\} \;,
\end{aligned} \tag{2.5}
$$

in which

$$
\eta'_j(\vec{x}) = \eta_j(\vec{x})\eta_4(\vec{x}) \;, \tag{2.6}
$$

and

$$
\begin{aligned}
\mathrm{Re}\; U_k(x) \;&=\; \frac{1}{2}(U_k(x) + U_k^*(x)) \;, \\
\mathrm{Im}\; U_k(x) \;&=\; \frac{1}{2i}(U_k(x) - U_k^*(x)) \;.
\end{aligned} \tag{2.7}
$$

Next, we divide the lattice into even and odd time slices, and rename the fields Φ, respectively Π, defining

$$
\begin{aligned}
t = 2k: \qquad & \phi_1(\vec{x},t) = \Phi_{1,k}(\vec{x}) \;, \qquad \phi_2(\vec{x},t) = -\Phi_{2,k}(\vec{x}) \;, \\
t = 2k+1: \;\; & \phi_1(\vec{x},t) = \Pi_{2,k}(\vec{x}) \;, \qquad \phi_2(\vec{x},t) = \Pi_{1,k}(\vec{x}) \;.
\end{aligned} \tag{2.8}
$$

Accordingly, the action can be rewritten as

$$
\begin{aligned}
S \;=\; & \sum_k \Bigg\{ \sum_{\vec{x}} i\left(\Phi_{1,k}(\vec{x})\Pi_{1,k}(\vec{x}) + \Phi_{2,k}(\vec{x})\Pi_{2,k}(\vec{x})\right) \\
& \qquad +\mathcal{H}_-[\Phi_{1,k}, \Phi_{2,k}; \mathcal{U}(2k)] + \mathcal{H}_0[\Phi_1, \Phi_2; m] \Bigg\} \\
& + \sum_k \Bigg\{ \sum_{\vec{x}} -i\left(\Pi_{1,k}(\vec{x})\Phi_{1,k+1}(\vec{x}) + \Pi_{2,k}(\vec{x})\Phi_{2,k+1}(\vec{x})\right) \\
& \qquad +\mathcal{H}_+[\Pi_{1,k}, \Pi_{2,k}; \mathcal{U}(2k+1)] + \mathcal{H}_0[\Pi_1, \Pi_2; m] \Bigg\} \;,
\end{aligned} \tag{2.9}
$$

[5] The fields ϕ_1 and ϕ_2 are always transposed when they appear as the first factor in a bilinear in these fields. We also use that $\eta_4(\vec{x}+\vec{j}) = -\eta_4(\vec{x})$.

in which $\mathcal{U}(t)$ denotes the gauge field at a time slice t, and

$$\begin{aligned}
\mathcal{H}_{\pm}[\Psi_1,\Psi_2;\,\mathcal{U}(t)] \;=\; \sum_{\vec{x}}\Bigg\{ &\pm\sum_j i\eta'_j(\vec{x})\,\Big(\Psi_1(\vec{x})\,\mathrm{Re}\,U_j(\vec{x},t)\Psi_2(\vec{x}+\vec{j})+(1\leftrightarrow 2)\Big)\\
&-\sum_j i\eta_j(\vec{x})\,\Big(\Psi_1(\vec{x})\,\mathrm{Im}\,U_j(\vec{x},t)\Psi_1(\vec{x}+\vec{j})-(1\rightarrow 2)\Big)\Bigg\}\ ,\\
\mathcal{H}_0[\Psi_1,\Psi_2;m] \;=\; m\sum_{\vec{x}}&\left(\Psi_{1,k}(\vec{x})^2+\Psi_{2,k}(\vec{x})^2\right)\ .
\end{aligned}\tag{2.10}$$

After shifting k to $k+1$ in the $\mathcal{H}_-$ term, we define a kernel

$$\begin{aligned}
T(\Phi_{1,k+1}\Phi_{2,k+1};\Phi_{1,k}\Phi_{2,k}) = &\int\prod_{\vec{y}} d\Pi_{1,k}(\vec{y})\int\prod_{\vec{y}} d\Pi_{2,k}(\vec{y})\ \times\\
\exp\Bigg[-\Bigg\{&\sum_{\vec{x}} i\left(\Phi_{1,k}(\vec{x})\Pi_{1,k}(\vec{x})+\Phi_{2,k}(\vec{x})\Pi_{2,k}(\vec{x})-\Pi_{1,k}(\vec{x})\Phi_{1,k+1}(\vec{x})-\Pi_{2,k}(\vec{x})\Phi_{2,k+1}(\vec{x})\right)\\
&+\mathcal{H}_-[\Phi_{1,k+1},\Phi_{2,k+1};\,\mathcal{U}(2(k+1)]+\mathcal{H}_+[\Pi_{2,k},\Pi_{1,k};\,\mathcal{U}(2k+1)]\\
&+\mathcal{H}_0[\Phi_1,\Phi_2;m]+\mathcal{H}_0[\Pi_1,\Pi_2;m]\Bigg\}\Bigg]\ .
\end{aligned}\tag{2.11}$$

The claim is then that

$$T(\Phi_{1,k+1}\Phi_{2,k+1};\Phi_{1,k}\Phi_{2,k}) = \langle\Phi_{1,k+1}\Phi_{2,k+1}|\hat{T}_{G,k}(\mathcal{U})|\Phi_{1,k}\Phi_{2,k}\rangle\ , \tag{2.12}$$

with

$$\hat{T}_{G,k}(\mathcal{U}) = e^{-\mathcal{H}_-[\hat{\Phi}_1,\hat{\Phi}_2;\,\mathcal{U}(2(k+1)]-\mathcal{H}_0[\hat{\Phi}_1,\hat{\Phi}_2;m]}\ e^{-\mathcal{H}_+[\hat{\Pi}_2,\hat{\Pi}_1;\,\mathcal{U}(2k+1)]-\mathcal{H}_0[\hat{\Pi}_1,\hat{\Pi}_2;m]}\ , \tag{2.13}$$

in which the Hermitian operators $\hat{\Phi}_a(\vec{x})$ and $\hat{\Pi}_a(\vec{x})$ obey the commutation rules

$$[\hat{\Phi}_a(\vec{x}),\hat{\Pi}_b(\vec{y})] = i\delta_{\vec{x},\vec{y}}\,\delta_{ab}\ . \tag{2.14}$$

This is proven by inserting a complete set of states into the right-hand side of Eq. (2.12):

$$\begin{aligned}
\langle\Phi_{1,k+1}\Phi_{2,k+1}|\hat{T}_{G,k}(\mathcal{U})|\Phi_{1,k}\Phi_{2,k}\rangle \;=\;&\\
\int d\Pi_{1,k}\int d\Pi_{2,k}\ &\langle\Phi_{1,k+1}\Phi_{2,k+1}|e^{-\mathcal{H}_-[\hat{\Phi}_1,\hat{\Phi}_2;\,\mathcal{U}(2(k+1))]}\ e^{-\mathcal{H}_+[\hat{\Pi}_2,\hat{\Pi}_1;\,\mathcal{U}(2k+1)]}|\Pi_{1,k}\Pi_{2,k}\rangle\\
&\times\ \langle\Pi_{1,k}\Pi_{2,k}|\Phi_{1,k}\Phi_{2,k}\rangle\\
=\int d\Pi_{1,k}\int d\Pi_{2,k}\ &e^{-\mathcal{H}_-[\Phi_{1,k+1},\Phi_{2,k+1};\,\mathcal{U}(2(k+1))]}\ e^{-\mathcal{H}_+[\Pi_{2,k},\Pi_{1,k};\,\mathcal{U}(2k+1)]}\\
&\times\ e^{i\left(\Phi_{1,k+1}\Pi_{1,k}+\Phi_{2,k+1}\Pi_{2,k}-\Phi_{1,k}\Pi_{1,k}-\Phi_{2,k}\Pi_{2,k}\right)}\ ,
\end{aligned}\tag{2.15}$$

where we omitted the explicit arguments $\vec{x}$ from the fields. Restoring these, the last line of Eq. (2.15) coincides precisely with Eq. (2.11). The ghost partition function in a gauge-field background $\mathcal{U}$ is now given by

$$Z_G(\mathcal{U}) = \mathrm{Tr}\left(\prod_{k=1}^{T/2} \hat{T}_{G,k}(\mathcal{U})\right) , \tag{2.16}$$

if T is the time extent of the lattice.

B. Properties of the ghost transfer matrix

The transfer matrix (2.13) is not Hermitian, but it is bounded. The proof is as follows. The operator $\mathcal{H}_-[\hat{\Phi}_1, \hat{\Phi}_2; \mathcal{U}(2(k+1))] + \mathcal{H}_0[\hat{\Phi}_1, \hat{\Phi}_2; m]$ consists of a positive semi-definite part (if $m > 0$), and an anti-Hermitian part containing the gauge field. Moreover, it commutes with its Hermitian conjugate, because all $\hat{\Phi}_a(\vec{x})$ commute among themselves. Therefore, the operator

$$\hat{T}_1(\mathcal{U}) = e^{-\mathcal{H}_-[\hat{\Phi}_1,\hat{\Phi}_2;\,\mathcal{U}(2(k+1))]-\mathcal{H}_0[\hat{\Phi}_1,\hat{\Phi}_2;m]} \tag{2.17}$$

is normal and bounded,[6]

$$\| \hat{T}_1(\mathcal{U}) \| \leq 1 . \tag{2.18}$$

A similar argument applies to

$$\hat{T}_2(\mathcal{U}) = e^{-\mathcal{H}_+[\hat{\Pi}_2,\hat{\Pi}_1;\,\mathcal{U}(2k+1)]-\mathcal{H}_0[\hat{\Pi}_1,\hat{\Pi}_2;m]} , \tag{2.19}$$

and thus it follows that $\hat{T}_G$ itself is bounded,

$$\| \hat{T}_G(\mathcal{U}) \| \leq \| \hat{T}_1(\mathcal{U}) \| \| \hat{T}_2(\mathcal{U}) \| \leq 1 . \tag{2.20}$$

This establishes that all eigenvalues of $\hat{T}_G$ have an absolute value less than or equal to one. If, moreover, the eigenvalue λ_0 with maximal absolute value is unique, correlation functions in this theory decay exponentially with distance.

The transfer matrix (2.13) may be assumed to have a complete set of right and left eigenstates. This is equivalent to saying that, if we block-diagonalize $\hat{T}_G$ (put it in Jordan

[6] We use the Euclidean norm, which, for a matrix A, is defined as the positive square root of the largest eigenvalue of $A^\dagger A$.

normal form), there are no blocks of the form

$$\begin{pmatrix} \lambda & \kappa \\ 0 & \lambda \end{pmatrix} , \tag{2.21}$$

with $\kappa \neq 0$ (or generalizations of this form with higher degeneracies). We will see in Sec. III (and App. A) that this situation does not occur in the free theory. The condition that it happens on some nontrivial gauge field in the interacting case then restricts such fields to a subspace of co-dimension one (or more) in the full space of gauge-field configurations. Therefore, for "most" (meaning all gauge fields except a set of zero measure in the space of all gauge fields), the transfer matrix $\hat{T}_{G,k}(\mathcal{U})$ can be completely diagonalized, and complete sets of right and left eigenstates exist.

There is a caveat, however. In the next section, we will incorporate the ghost transfer matrix we have constructed thus far into a transfer matrix for the entire theory, including quantized quarks and gauge fields as well as ghosts. In order to conclude that the total transfer matrix does not have any nontrivial Jordan blocks of the form (2.21) (or generalizations thereof, *cf.* App. A), we would have to construct the full Hilbert space for the entire matrix, something we do not know how to do.[7] One might, however, consider a hybrid construction of the entire theory, in which fermions and ghosts are treated in a canonical formalism, and gauge fields are taken into account through the path integral. What this means is that correlation functions with quarks or ghosts on the external lines are first constructed in the transfer-matrix formalism, in an arbitrary fixed gauge-field background. The full QCD correlation functions are then obtained by integrating these correlation functions over the gauge fields. We first exclude from this integral the measure-zero set of gauge fields for which the Jordan normal form of the transfer matrix in a fixed gauge-field background may be nondiagonal. Since we then have a complete set of eigenstates in each background field, we think it reasonable to assume that the entire transfer matrix has a complete set of eigenstates.

[7] For the free theory it is obvious that it can be completely diagonalized, because in that case the Hilbert space is the direct product of the free Hilbert spaces for the quark and ghost sectors.

C. Full transfer matrix

It is straightforward to combine the transfer matrix for ghost quarks constructed in Sec. II A with the transfer matrix for lattice QCD with staggered fermions. First, from Refs. [24, 25], the fermionic transfer matrix for a staggered quark in a fixed background gauge field $\mathcal{U}$ can be written in the form

$$\hat{T}_{F,k}(\mathcal{U}) = e^{\hat{A}^\dagger[\mathcal{U}(2(k+1))]}\, e^{\hat{B}[m]}\, e^{\hat{A}[\mathcal{U}(2k+1)]} \ , \tag{2.22}$$

with $\hat{B}$ Hermitian. This translates the system from double time slice k (*cf.* Eq. (2.8)), with gauge fields $\mathcal{U}(2k)$ and $\mathcal{U}(2k+1)$, to the next double time slice $k+1$, with gauge fields $\mathcal{U}(2(k+1))$ and $\mathcal{U}(2(k+1)+1)$. In more detail, the factor $e^{\hat{A}}$ takes care of the hop within the double slice, connecting slice $2k$ to slice $2k+1$ (and it contains spatial terms on slice $2k+1$), whereas the factor $e^{\hat{A}^\dagger}$ hops from slice $2k+1$ to slice $2(k+1)$ in the next double slice (and it contains spatial terms on the slice $2(k+1)$).

The ghost transfer matrix of Eq. (2.13) can be written similarly as:

$$\hat{T}_{G,k}(\mathcal{U}) = e^{-\mathcal{H}_-[\hat{\Phi}_1,\hat{\Phi}_2;\,\mathcal{U}(2(k+1))]}\, e^{-\hat{\mathcal{H}}[m]}\, e^{-\mathcal{H}_+[\hat{\Pi}_1,\hat{\Pi}_2;\,\mathcal{U}(2k+1)]} \ , \tag{2.23}$$

where

$$e^{-\hat{\mathcal{H}}[m]} \equiv e^{-\mathcal{H}_0[\hat{\Phi}_1,\hat{\Phi}_2;m]}\, e^{-\mathcal{H}_0[\hat{\Pi}_1,\hat{\Pi}_2;m]} \ . \tag{2.24}$$

We can then write the transfer matrix for the total theory of QCD with staggered quarks and ghost quarks in the form

$$\hat{T}_{total} = \hat{T}_U^{1/2}\, e^{\hat{A}^\dagger}\, e^{-\mathcal{H}_-[\hat{\Phi}_1,\hat{\Phi}_2;\hat{\mathcal{U}}]}\, \hat{T}_U\, e^{-\hat{\mathcal{H}}[m]}\, e^{\hat{B}}\, e^{\hat{A}}\, e^{-\mathcal{H}_+[\hat{\Pi}_1,\hat{\Pi}_2;\hat{\mathcal{U}}]}\, \hat{T}_U^{1/2} \ , \tag{2.25}$$

with $\hat{T}_U$ the transfer matrix of the pure gauge theory constructed in Ref. [26]. The gauge field transfer matrix hops between single time slices, and therefore a factor $\hat{T}_U$ needs to be inserted between $e^{\hat{A}}\, e^{-\mathcal{H}_+[\hat{\Pi}_1,\hat{\Pi}_2;\hat{\mathcal{U}}]}$ and $e^{\hat{A}^\dagger}\, e^{-\mathcal{H}_-[\hat{\Phi}_1,\hat{\Phi}_2;\hat{\mathcal{U}}]}$, with matrix elements

$$\langle \mathcal{U}(2(k+1))|\hat{T}_U|\mathcal{U}(2k+1)\rangle \ . \tag{2.26}$$

Then, when one writes the partition function as a trace over a power of the transfer matrix, the factors $\hat{T}_U^{1/2}$ combine to hop the gauge field from slice $2k$ to $2k+1$ (on the right of Eq. (2.25)), or from slice $2(k+1)$ to slice $2(k+1)+1$ (on the left of Eq. (2.25)).

Although $\hat{T}_{total}$ is not Hermitian, and therefore is not required to have only real eigenvalues, there are significant restrictions on the eigenvalues coming from discrete symmetries. Most importantly, $\hat{T}_{total}$ is invariant under the antiunitary symmetry PT, the product of parity and time-reversal symmetries. Under PT, the ghost fields in Eq. (2.25) transform according according to

$$\begin{aligned} \mathcal{PT}\ \hat{\Phi}_1(\vec{x})\ (\mathcal{PT})^\dagger &= \hat{\Phi}_2(-\vec{x})\ , \\ \mathcal{PT}\ \hat{\Phi}_2(\vec{x})\ (\mathcal{PT})^\dagger &= \hat{\Phi}_1(-\vec{x})\ , \\ \mathcal{PT}\ \hat{\Pi}_1(\vec{x})\ (\mathcal{PT})^\dagger &= -\hat{\Pi}_2(-\vec{x})\ , \\ \mathcal{PT}\ \hat{\Pi}_2(\vec{x})\ (\mathcal{PT})^\dagger &= -\hat{\Pi}_1(-\vec{x})\ , \end{aligned} \tag{2.27}$$

where $\mathcal{PT}$ is the antiunitary operator that generates the symmetry. Note that, because it is antiunitary, PT it leaves the commutation rules, Eq. (2.14), unchanged. In the free case ($U_j(\vec{x},t) = 1$), the invariance of the ghost part of the transfer matrix, $\hat{T}_G$, under PT can be easily checked using the definitions of $\mathcal{H}_\pm$ and $\mathcal{H}_0$, Eq. (2.10), and the relations $\eta_j(\vec{x}+\vec{j}) = \eta_j(\vec{x})$ and $\eta'_j(\vec{x}+\vec{j}) = -\eta'_j(\vec{x})$. In the interacting case, the ghost transfer matrix $\hat{T}_G(\mathcal{U})$ is of course not invariant under Eq. (2.27) for fixed background fields $U_j(\vec{x},t)$; we must also let the time-slice gauge field operators transform. The transformation rule is standard:

$$\mathcal{PT}\ \hat{U}_j(\vec{x})\ (\mathcal{PT})^\dagger = \hat{U}_{-j}(-\vec{x}) \equiv \hat{U}_j^\dagger(-\vec{x}-\vec{j})\ . \tag{2.28}$$

Of course the quark and pure gauge parts of $\hat{T}_{total}$ are also invariant under PT.

Since $\hat{T}_{total}$ is invariant under PT,

$$\mathcal{PT}\ \hat{T}_{total}\ (\mathcal{PT})^\dagger = \hat{T}_{total}\ , \tag{2.29}$$

each eigenvalue of $\hat{T}_{total}$ must be either real or one of a complex conjugate pair:

$$\hat{T}_{total}|\Psi\rangle = \lambda|\Psi\rangle \quad \Rightarrow \quad \hat{T}_{total}(\mathcal{PT}|\Psi\rangle) = \lambda^*(\mathcal{PT}|\Psi\rangle)\ . \tag{2.30}$$

Non-Hermitian Hamiltonians with PT symmetry have been studied extensively by Bender and others [27]. PT-symmetric theories may often be redefined to give an acceptable unitary theory. Here, however, we do not want to make any such redefinitions, since the path integral is given, and the unitarity violations due to a non-Hermitian transfer matrix (or Hamiltonian) are as expected for a theory with spin-1/2 bosons.

For future reference, we note that $\hat{T}_{total}$ is also invariant under charge conjugation symmetry, C, and hence under the combined symmetry CPT, with

$$\begin{aligned}
\mathcal{CPT}\ \hat{\Phi}_1(\vec{x})\ (\mathcal{CPT})^\dagger &= \hat{\Phi}_1(-\vec{x})\ , \\
\mathcal{CPT}\ \hat{\Phi}_2(\vec{x})\ (\mathcal{CPT})^\dagger &= \hat{\Phi}_2(-\vec{x})\ , \\
\mathcal{CPT}\ \hat{\Pi}_1(\vec{x})\ (\mathcal{CPT})^\dagger &= -\hat{\Pi}_1(-\vec{x})\ , \\
\mathcal{CPT}\ \hat{\Pi}_2(\vec{x})\ (\mathcal{CPT})^\dagger &= -\hat{\Pi}_2(-\vec{x})\ .
\end{aligned} \tag{2.31}$$

The gauge field transforms under CPT as

$$\mathcal{CPT}\ \hat{U}_j(\vec{x})\ (\mathcal{CPT})^\dagger = \hat{U}_j^{\mathrm{T}}(-\vec{x}-\vec{j})\ , \tag{2.32}$$

with T the matrix transpose.

From Eq. (2.31), we can find the CPT transformation rules for the c-number fields $\chi(x)$ and $\chi^\dagger(x)$, which are, from Eqs. (2.8) and (2.4), the eigenvalues of (linear combinations of) the operators $\hat{\Phi}_1(\vec{x})$, $\hat{\Phi}_2(\vec{x})$, $\hat{\Pi}_1(\vec{x})$, and $\hat{\Pi}_2(\vec{x})$ on each time slice. Note that, since the time-translation operator in Euclidean space is $\exp(-Hx_4)$, we should not send $x_4 \to -x_4$ under this symmetry if we want the Euclidean action, as opposed to merely the Hamiltonian, to be invariant.[8] We then have

$$\begin{aligned}
\mathrm{CPT}:\quad \chi(\vec{x},x_4) &\to (-1)^{x_4}\ \chi^{\dagger\mathrm{T}}(-\vec{x},x_4)\ , \\
\mathrm{CPT}:\quad \chi^\dagger(\vec{x},x_4) &\to (-1)^{x_4}\ \chi^{\mathrm{T}}(-\vec{x},x_4)\ ,
\end{aligned} \tag{2.33}$$

where the factors of $(-1)^{x_4}$ arise from the minus signs in the last two equations in Eq. (2.31). It is straightforward to check that the action, Eq. (2.1), is unchanged by this transformation.

For staggered quarks, the action is

$$S = \sum_x \left\{ \frac{1}{2} \sum_\mu \eta_\mu(x) \left(\bar{q}(x)U_\mu(x)q(x+\mu) - \bar{q}(x+\mu)U_\mu^\dagger(x)q(x) \right) + m\bar{q}(x)q(x) \right\}\ , \tag{2.34}$$

where now $q(x)$ and $\bar{q}(x)$ are independent Grassmann-valued fields. Starting from the naive-quark transfer matrix Hamiltonian [25] or the "reduced-staggered" transfer matrix in [24],

[8] There is however a *linear* time-inversion symmetry of the action in Euclidean space, which is simply the time-direction equivalent of the spatial inversions. We focus instead on the antiunitary symmetry of the Hamiltonian because it will be useful to us in constraining the chiral theory.

one can derive the transformation rules for $q(x)$ and $\bar{q}(x)$ that correspond to Eq. (2.33):

$$\begin{aligned} \mathrm{CPT}: \quad & q(\vec{x}, x_4) \;\to\; (-1)^{x_4}\, \bar{q}^{\mathrm{T}}(-\vec{x}, x_4)\ , \\ \mathrm{CPT}: \quad & \bar{q}(\vec{x}, x_4) \;\to\; -(-1)^{x_4}\, q^{\mathrm{T}}(-\vec{x}, x_4)\ . \end{aligned} \tag{2.35}$$

The extra minus sign in the second equation in Eq. (2.35) (as compared to Eq. (2.33)) makes up for the minus sign coming from Fermi statistics when taking the transpose of the action.

We end this section with a few comments. First, implicitly, we have only considered one flavor of quarks and one flavor of ghost quarks. The generalization to arbitrary numbers of each is immediate. In addition, we have generalized beyond PQQCD by choosing an arbitrary (positive) mass for each quark or ghost quark. In PQQCD, each ghost quark mass is equal to the mass of one of the fermionic quarks, thus turning that quark into a valence quark. Sea quarks appear as fermionic quarks without ghost partners. A further issue arises from the use of the staggered action (without rooting) for the ghosts and quarks, which implies that each flavor comes in four tastes. This is actually not a serious restriction for PQQCD, since extra (unwanted) species of valence quarks and ghosts are harmless: they have no effect on any processes if we choose not to put them on external lines (in the standard case where valence quarks and ghosts are degenerate). Further, if one wishes to avoid extra tastes in the sea, it would be completely straightforward to use any alternative discretization for the sea quarks that has a transfer matrix, such as unimproved Wilson quarks.

III. THE FREE THEORY

This section focuses on the ghost transfer matrix, Eq. (2.13), in the free theory, *i.e.*, in the case where the background gauge field $U_j(\vec{x}, t) = 1$. We work in the limit of vanishing temporal lattice spacing. We first follow the standard momentum-space construction for staggered fermions [24, 28] to identify the eight degrees of freedom that arise from spatial doubling (the doubling associated with the time direction is already explicitly taken into account in our two-time-slice construction of the transfer matrix).[9] We diagonalize the Hamiltonian in spin-taste space, and proceed to determine the eigenstates and eigenvalues using a generalized Bogoliubov transformation. Two-point correlators can then be easily

[9] The 16 degrees of freedom are identified as the four tastes of Dirac fermions, each with four spin degrees of freedom.

found; they clearly show the expected violations of unitarity in the ghost sector of the theory. The explicit calculations below and in App. A demonstrate that $\hat{T}_G$ has a complete set of (right or left) eigenstates in the free theory. In other words, they show that, when $U_j(\vec{x},t) = 1$, blocks of the form of Eq. (2.21) do not occur in the Jordan normal form of the transfer matrix. As an alternative to the Bogoliubov-transformation approach, a path-integral construction of the correlators is given in App. B.

A. The free Hamiltonian

Setting $U_j(\vec{x},t) = 1$, writing[10]

$$\hat{T}_{G,k}(\mathcal{U}=1) \equiv \exp\left(-2a_t H\right) \ , \tag{3.1}$$

and taking the limit $a_t \to 0$, we find the Hamiltonian H in that limit:[11]

$$\begin{aligned} H \ = \ & \frac{1}{2}\sum_{\vec{x}}\Big\{ m\left(\Phi_1(\vec{x})^2 + \Phi_2(\vec{x})^2 + \Pi_1(\vec{x})^2 + \Pi_2(\vec{x})^2\right) + \sum_j i\eta'_j(\vec{x}) \ \times \\ & \left(-\Phi_1(\vec{x})\Phi_2(\vec{x}+\vec{j}) - \Phi_1(\vec{x}+\vec{j})\Phi_2(\vec{x}) + \Pi_2(\vec{x})\Pi_1(\vec{x}+\vec{j}) + \Pi_2(\vec{x}+\vec{j})\Pi_1(\vec{x})\right)\Big\} \ . \end{aligned} \tag{3.2}$$

Introducing creation and annihilation operators $a_1^\dagger$, a_1, $a_2^\dagger$, a_2 through

$$\begin{aligned} \Phi_1(\vec{x}) \ &= \ \int_k \frac{1}{\sqrt{2}}\left(a_1(\vec{k}) + a_1^\dagger(-\vec{k})\right) e^{i\vec{k}\cdot\vec{x}} \ , \\ \Pi_1(\vec{x}) \ &= \ \int_k \frac{-i}{\sqrt{2}}\left(a_1(\vec{k}) - a_1^\dagger(-\vec{k})\right) e^{i\vec{k}\cdot\vec{x}} \ , \\ \Phi_2(\vec{x}) \ &= \ \int_k \frac{-i}{\sqrt{2}}\left(a_2(-\vec{k}) - a_2^\dagger(\vec{k})\right) e^{i\vec{k}\cdot\vec{x}} \ , \\ \Pi_2(\vec{x}) \ &= \ \int_k \frac{-1}{\sqrt{2}}\left(a_2(-\vec{k}) + a_2^\dagger(\vec{k})\right) e^{i\vec{k}\cdot\vec{x}} \ , \end{aligned} \tag{3.3}$$

in which

$$\int_k \equiv \int \frac{d^3k}{(2\pi)^{\frac{3}{2}}} \ , \tag{3.4}$$

---

[10] The factor 2 appears because $\hat{T}_G$ is a double time-slice transfer matrix.

[11] From now on we drop hats on operators.

this can be re-expressed as

$$
\begin{aligned}
H \;=\; & \frac{1}{2}\sum_{\vec{x}}\int_k\int_\ell e^{i(\vec{k}+\vec{\ell})\cdot\vec{x}} \;\times \\
& \Bigg\{ m\left(a_1^\dagger(-\vec{k})a_1(\vec{\ell})+a_1(\vec{k})a_1^\dagger(-\vec{\ell})+a_2^\dagger(\vec{k})a_2(-\vec{\ell})+a_2(-\vec{k})a_2^\dagger(\vec{\ell})\right) \\
& +\sum_j e^{i\ell_j}\; e^{i\vec{\pi}_{\eta'_j}\cdot\vec{x}}\left(-a_1(\vec{k})a_2(-\vec{\ell})+a_1^\dagger(-\vec{k})a_2^\dagger(\vec{\ell})-a_2(-\vec{k})a_1(\vec{\ell})+a_2^\dagger(\vec{k})a_1^\dagger(-\vec{\ell})\right)\Bigg\}\;.
\end{aligned}
\tag{3.5}
$$

Here the factors $e^{i\vec{\pi}_{\eta'_j}\cdot\vec{x}}$ are equal to the sign factors $\eta'_j(\vec{x})$ in Eq. (3.2), if we choose

$$
\vec{\pi}_{\eta'_1}=(\pi,\pi,\pi)\;,\quad \vec{\pi}_{\eta'_2}=(0,\pi,\pi)\;,\quad \vec{\pi}_{\eta'_3}=(0,0,\pi)\;. \tag{3.6}
$$

The creation and annihilation operators have commutation rules

$$
[a_\alpha(\vec{k}),a_\beta^\dagger(\vec{\ell})]=\delta(\vec{k}-\vec{\ell})\;\delta_{\alpha\beta}\;. \tag{3.7}
$$

We now split up the (spatial) Brillouin zone as in Refs. [24, 28] for staggered fermions:[12]

$$
\vec{k}=\vec{p}+\vec{\pi}_A\;,\qquad \vec{\ell}=\vec{q}+\vec{\pi}_B\;, \tag{3.8}
$$

with

$$
\vec{\pi}_A,\vec{\pi}_B\in\{(0,0,0),(\pi,0,0),\dots,(\pi,\pi,\pi)\}\;, \tag{3.9}
$$

such that $-\pi/2<p_j,q_j\le\pi/2$. Operators get relabeled as in

$$
a_\alpha(\vec{k})=a_\alpha(\vec{p}+\vec{\pi}_A)\equiv a_\alpha^A(\vec{p})\;, \tag{3.10}
$$

etc. Performing the sum over $\vec{x}$ in Eq. (3.5) we find the delta functions

$$
\begin{aligned}
\delta(\vec{p}+\vec{q}+\vec{\pi}_A+\vec{\pi}_B) \;&=\; \delta(\vec{p}+\vec{q})\delta_{AB}\;, \\
\delta(\vec{p}+\vec{q}+\vec{\pi}_A+\vec{\pi}_B+\vec{\pi}_{\eta'_j}) \;&=\; \delta(\vec{p}+\vec{q})X^j_{AB}\;,
\end{aligned}
\tag{3.11}
$$

where the second of these equations defines three symmetric matrices X^j. In the Hamiltonian these matrices occur in combination with the factors $e^{i\pi_{Bj}}$ coming from $e^{i\ell_j}$, and we define another set of matrices

$$
\alpha^j_{AB}=X^j_{AB}\,e^{i\pi_{Bj}}\;. \tag{3.12}
$$

[12] See also Ref. [2] for a review.

The matrices α^j are real, and antisymmetric:

$$\alpha^j_{BA} = X^j_{BA}\, e^{i\pi_{Aj}} = X^j_{AB}\, e^{i(\pi_B+\pi_{\eta'_j})_j} = -X^j_{AB}\, e^{i\pi_{Bj}} = -\alpha^j_{AB}\ , \tag{3.13}$$

because $(\pi_{\eta'_j})_j = \pi$. Hence the α^j are anti-Hermitian. Using all this, we can simplify the expression for the Hamiltonian to

$$\begin{aligned} H \ =\ \int_p \Bigg\{ & \frac{1}{2}m\left(a_1^\dagger(\vec{p})a_1(\vec{p}) + a_1(\vec{p})a_1^\dagger(\vec{p}) + a_2^\dagger(\vec{p})a_2(\vec{p}) + a_2(\vec{p})a_2^\dagger(\vec{p})\right) \\ & +i\sum_j \sin\left(p_j\right)\left(a_1(\vec{p})\alpha^j a_2(\vec{p}) - a_2^\dagger\alpha^j a_1^\dagger(\vec{p})\right)\Bigg\}\ . \end{aligned} \tag{3.14}$$

Note that the integral over $\vec{p}$ is over the reduced Brillouin zone.

Finally, the eigenvalues of the 8×8 matrix $\sum_j \sin\left(p_j\right)\alpha^j$ are equal to $\pm is(\vec{p})$ with $s^2(\vec{p}) = \sum_j \sin^2\left(p_j\right)$. Dropping a constant proportional to $1/a^3$, we can thus write H as a sum and integral over terms of the form

$$h(\vec{p}) = m\left(a_1^\dagger(\vec{p})a_1(\vec{p}) + a_2^\dagger(\vec{p})a_2(\vec{p})\right) \pm s(\vec{p})\left(a_1(\vec{p})a_2(\vec{p}) - a_2^\dagger(\vec{p})a_1^\dagger(\vec{p})\right)\ . \tag{3.15}$$

B. Eigenvalues and eigenstates

Dropping the dependence on $\vec{p}$ in Eq. (3.15), our next step is to find eigenvalues and left and right eigenstates of the non-Hermitian Hamiltonian

$$h = m(a_1^\dagger a_1 + a_2^\dagger a_2) + s(a_1 a_2 - a_2^\dagger a_1^\dagger)\ , \tag{3.16}$$

in which $a_{1,2}$ and $a_{1,2}^\dagger$ are a set of bosonic annihilation and creation operators, $m>0$ and s is real. (Taking s real without restriction on its sign takes care of both signs in Eq. (3.15).) Adapting the method of Ref. [29], we introduce new operators

$$\begin{aligned} b_1 &= \cos\theta\ a_1 - \sin\theta\ a_2^\dagger\ , \\ b_2 &= \cos\theta\ a_2 - \sin\theta\ a_1^\dagger\ , \\ \tilde{b}_1 &= \cos\theta\ a_1^\dagger + \sin\theta\ a_2\ , \\ \tilde{b}_2 &= \cos\theta\ a_2^\dagger + \sin\theta\ a_1\ , \end{aligned} \tag{3.17}$$

which obey the commutation rules

$$[b_\alpha, \tilde{b}_\beta] = \delta_{\alpha\beta}\ , \tag{3.18}$$

while all other commutators vanish. Note that the operators $\tilde{b}_\alpha$ are not the Hermitian conjugates of the operators b_α, which is why this is a "generalized" Bogoliubov transformation. Expressed in terms of these operators h becomes

$$\begin{aligned} h \;=\; & (m\cos(2\theta) + s\sin(2\theta))\,(\tilde{b}_1 b_1 + \tilde{b}_2 b_2) \\ & + (-m\sin(2\theta) + s\cos(2\theta))\,(b_1 b_2 - \tilde{b}_2\tilde{b}_1) + \text{constant}\;. \end{aligned} \tag{3.19}$$

Requiring the term proportional to $b_1 b_2 - \tilde{b}_2\tilde{b}_1$ to vanish yields

$$\theta = \frac{1}{2}\arctan(s/m)\;, \tag{3.20}$$

where we picked the solution that vanishes for $s \to 0$. Substituting this solution into Eq. (3.19) gives

$$h = \sqrt{m^2+s^2}\,(\tilde{b}_1 b_1 + \tilde{b}_2 b_2) + \text{constant}\;. \tag{3.21}$$

Even though $\tilde{b}_\alpha \neq b_\alpha^\dagger$, the operators $N_\alpha = \tilde{b}_\alpha b_\alpha$ are still number operators, and we can find a set of right eigenstates $|n_1, n_2\rangle_R$ such that

$$\begin{aligned} N_1|n_1,n_2\rangle_R \;&=\; n_1|n_1,n_2\rangle_R\;, \\ N_2|n_1,n_2\rangle_R \;&=\; n_2|n_1,n_2\rangle_R\;, \end{aligned} \tag{3.22}$$

and

$$\begin{aligned} b_1|n_1,n_2\rangle_R &\propto |n_1-1,n_2\rangle_R\;, \\ b_2|n_1,n_2\rangle_R &\propto |n_1,n_2-1\rangle_R\;. \end{aligned} \tag{3.23}$$

Because of the upper bound (2.20) on the absolute values of the eigenvalues of $\hat{T}_G$, which implies a lower bound on the real part of the eigenvalues of h, we find that there exists a "right vacuum" state $|0,0\rangle_R$ annihilated by b_1 and b_2; otherwise n_1 and n_2 could be lowered indefinitely, violating this bound. Therefore, it follows that N_1 and N_2 vanish on $|0,0\rangle_R$. The right eigenstates of h are then given by

$$\begin{aligned} |n,m\rangle_R \;&=\; \frac{1}{\sqrt{n!m!}}\,\tilde{b}_1^n\tilde{b}_2^m|0,0\rangle_R\;, \\ h|n,m\rangle_R \;&=\; (n+m)E|n,m\rangle_R\;, \qquad E \equiv \sqrt{m^2+s^2}\;, \end{aligned} \tag{3.24}$$

where we have dropped the constant in Eq. (3.21). The normalization of the states we have chosen is convenient but arbitrary, since the only relevant normalization condition relates right to left states (Eq. (3.26) below). A similar reasoning leads to a left ground state ${}_L\langle 0,0|$, and a construction of the left eigenstates

$$
\begin{aligned}
{}_L\langle n,m| &= {}_L\langle 0,0|\frac{1}{\sqrt{n!m!}}\, b_1^n b_2^m \ , \\
{}_L\langle n,m|h &= {}_L\langle n,m|E(n+m) \ ,
\end{aligned}
\tag{3.25}
$$

where the normalization here follows from Eq. (3.24) if we demand that

$$
{}_L\langle n_1,m_1|n_2,m_2\rangle_R = \delta_{n_1,n_2}\,\delta_{m_1,m_2} \ . \tag{3.26}
$$

We note that

$$
{}_L\langle n,m| \neq (|n,m\rangle_R)^\dagger \tag{3.27}
$$

because $\tilde{b}_\alpha \neq b_\alpha^\dagger$; there is no simple relation between left- and right-eigenstates. However, we do have a completeness relation:

$$
\sum_{n,m} |n,m\rangle_R\ {}_L\langle n,m| = 1 \ . \tag{3.28}
$$

Completeness is not obvious, since our Hamiltonian is not Hermitian. We refer to App. A for a proof.

Under PT symmetry, $h(\vec{p},s)\to h(-\vec{p},-s)$, so it is actually the sum $h(\vec{p},s)+h(-\vec{p},-s)$ that is PT symmetric. Since, from Eq. (3.21), $h(\vec{p},s)$ and $h(-\vec{p},-s)$ have identical eigenvalues, PT symmetry implies that those eigenvalues must either be real or come in complex-conjugate pairs. In fact all the eigenvalues are real, as seen in Eq. (3.24), and all energy eigenstates of the sum may be chosen to be eigenstates of PT. In the PT literature [27] this situation is referred to as "unbroken PT symmetry." This is somewhat different from standard field-theory usage of the terms broken and unbroken symmetry, which refer to the properties of the ground state only.

C. Two-point correlators

The free ghost partition function Z is the trace of the (Euclidean) evolution operator, which we may write, using Eq. (3.28), as

$$
Z = \sum_{n,m} {}_L\langle n,m|e^{-Th}|n,m\rangle_R = \sum_{n,m} e^{-(n+m)ET} = \frac{1}{(1-e^{-ET})^2} \ . \tag{3.29}
$$

From Eqs. (3.24), (3.25) and the commutation rules (3.18), it is straightforward to show that (with no sum over α)

$$\langle b_\alpha(t)\tilde{b}_\alpha(0)\rangle = \frac{1}{Z}\sum_{n,m} {}_L\langle n,m|e^{-(T-t)h}b_\alpha e^{-th}\tilde{b}_\alpha|n,m\rangle_R = \frac{e^{-Et}}{1-e^{-ET}} \ , \tag{3.30}$$

and likewise

$$\langle \tilde{b}_\alpha(t)b_\alpha(0)\rangle = \frac{e^{-E(T-t)}}{1-e^{-ET}} \ , \tag{3.31}$$

where we used

$$\sum_{n=0}^{\infty} n\ e^{-nET} = -\frac{\partial}{\partial(ET)}\sum_{n=0}^{\infty} e^{-nET} = -\frac{\partial}{\partial(ET)}\frac{1}{1-e^{-ET}} = \frac{e^{-ET}}{(1-e^{-ET})^2} \ . \tag{3.32}$$

More interesting are the two-point correlation functions involving the original creation and annihilation operators a_α and $a_\alpha^\dagger$. For these we find from Eqs. (3.30) and (3.31), using the inverse of Eq. (3.17),

$$\langle a_i(t)a_j(0)\rangle = \delta_{i+j,3}\ \frac{s}{2E}\ \frac{e^{-Et}+e^{-E(T-t)}}{1-e^{-ET}} = -\langle a_i^\dagger(t)a_j^\dagger(0)\rangle \ , \tag{3.33}$$

and

$$\langle a_i(t)a_j^\dagger(0)\rangle \ = \ \delta_{ij}\left(\frac{E+m}{2E}\ \frac{e^{-Et}}{1-e^{-ET}} - \frac{E-m}{2E}\ \frac{e^{-E(T-t)}}{1-e^{-ET}}\right) \ , \tag{3.34a}$$

$$\langle a_i^\dagger(t)a_j(0)\rangle \ = \ \delta_{ij}\left(-\frac{E-m}{2E}\ \frac{e^{-Et}}{1-e^{-ET}} + \frac{E+m}{2E}\ \frac{e^{-E(T-t)}}{1-e^{-ET}}\right) \ . \tag{3.34b}$$

Equation (3.34b) is a clear indication of the violation of unitarity in this theory: In the limit $T\to\infty$, this correlator is negative (for $s\neq 0$). In a normal theory, it would be a sum of decaying exponentials times positive coefficients.

An alternative, path-integral derivation of the correlators Eqs. (3.33) and (3.34) is given in App. B. That approach also makes possible a direct comparison between our treatment of this nonunitary theory, and a treatment of a similar Hamiltonian in the PT symmetry literature [30], where unitarity is restored through a redefinition of the theory.

IV. THE EFFECTIVE THEORY

We now return to the interacting theory defined by the transfer matrix T_{total} given in Eq. (2.25). We want to argue that the there exists a corresponding chiral effective theory, and that it is given by PQChPT. We will follow the discussion of Ref. [16] as closely as possible, so we first give a brief overview of the arguments there. Two key ingredients are the identification of the light degrees of freedom (which we will collectively refer to as "pions") and clustering. For each of these ingredients, an extension of the Vafa–Witten theorem [18] turns out to be useful, as discussed in Sec. IV B. In the case of clustering, we are then able to close the loophole that remains after constructing a bounded transfer matrix: we can argue that there is a gap (for strictly positive quark and ghost masses) between the ground state and the lowest excited state, so that clustering is in fact exponential. The fact that an extended Vafa–Witten theorem allows one to identify the light degrees of freedom has already been noted in Refs. [17, 31]. In the case of unquenched QCD, Lorentz invariance also plays an important role [16]. Our setting is Euclidean, and we instead have hypercubic invariance, which we assume to enlarge to $O(4)$ in the continuum limit, as usual. We use this to argue in Sec. IV C that our pions satisfy the expected dispersion relation.

We then put all the ingredients together to write down the effective theory in Sec. IV D. A subtlety absent in the unquenched theory arises because, in our theory with arbitrary fermionic and ghost quark masses, pion masses can in general be complex. In Sec. IV E, we use CPT invariance, already introduced in Sec. II C, in order to show that the phases of LECs in our theory are the same as in normal ChPT. This does not preclude the occurrence of complex masses in the effective theory, but the effective theory can now be used to investigate this issue in more detail, as we do in Sec. IV F.

As before, we will assume that all quark masses are always positive, both in the mass-degenerate and mass-nondegenerate cases considered below, as this is the setting for which the path integral (2.16) is well-defined, and the arguments of Ref. [18] apply. For simplicity, we will also assume that the continuum limit has been taken, so that we can ignore the peculiarities of the staggered quark formalism with respect to species doubling. In particular, our arguments will apply to QCD with any number of continuum quarks.

A. Recapitulation of Leutwyler's arguments

Reference [16] attempts to justify standard ChPT as the effective theory for low-energy QCD. The argument is, roughly speaking, divided into two parts. In the first, which is largely qualitative, it is argued that there is an effective chiral description of QCD in terms of a Lagrangian that describes pions being exchanged between local vertices. This is based on a few observations and assumptions:

- Pions are the lightest particles, so the low energy theory is dominated by pion exchange. In Minkowski space, this is the statement of "pion pole dominance."

- Clustering, either power-law (when pions are massless) or exponential (when pions are massive), implies that the interaction among pions in a local region of space is independent of what is going on far away. Thus the local interactions of pions may be described by vertices that do not depend of the particular Green's function being considered.

- The vertices are assumed to be expandable in a power series in the momenta of the pions. Note that one needs to *assume* this in the case of massless pions, since Green's functions are themselves not expandable in a power of series in momenta, due to the infrared singularities that would result. The assumption is that, once the singularities are accounted for by the exchange of massless pions, the vertices may be expanded. However, this assumption seems to be unnecessary in the massive case, because no infrared singularities would result from a momentum expansion.

- Because more than one pion may be exchanged between any two given vertices, pion loops must be included. The fact that these loops can be expressed as the usual four-dimensional momentum integrations of a quantum field theory is not explained in detail. However, the point seems to be that the underlying theory has a complete set of states, and the sum over (on shell) states can be turned into four-dimensional loop integrals over off-shell states, by the standard arguments that relate old-fashioned perturbation theory to the Feynman diagram approach. (See, for example, Ref. [32], Sec. 9.5.)

The second, and much more lengthy, part of the discussion in Ref. [16] is a demonstration that the chiral Lagrangian, with vector sources inserted that transform like gauge fields, can be chosen to have local chiral symmetry (up to anomalies, which must be dealt with separately). The main ingredient here is the chiral Ward–Takahashi identities. This part of the argument is crucial for showing that the chiral Lagrangian has the standard form of ChPT.

B. Pion spectrum and clustering: extension of the Vafa–Witten theorem

An extension of the Vafa–Witten theorem serves two purposes here. First of all, it shows that, due to spontaneous breaking of chiral symmetry, pions exist in PQQCD, so that any effective theory must be based on the exchange and interaction of pions. Second, it shows that pions are the *only* light particles (absent particles that are light for accidental reasons, which cannot be ruled out except by assumption). This allows us to argue that the fall off of correlation functions with distance, which follows from the existence of a bounded transfer matrix, is actually exponential. In other words, the theory obeys exponential clustering.

PQQCD contains unquenched QCD. Concretely, this means that if we consider correlation functions of operators made out of sea quarks (and gluons) only, these correlation functions coincide exactly with those of QCD with only sea quarks, *i.e.*, unquenched QCD. Therefore, we know that PQQCD has excitations which correspond to pions made only out of sea quarks, and that all correlation functions made out of sea-pion operators behave as they should in a healthy quantum field theory.

First, consider PQQCD in which all quark masses are equal; *i.e.*, $m_s = m_v = m_g$.[13] In this case, we have a vector flavor symmetry group[14] $SU(N_s + N_v|N_v)$, which, if it is unbroken, relates the two-point (and other) correlation functions of all pions in the theory to each other, and thus implies that there is a fully degenerate multiplet of pions in the adjoint representation of $SU(N_s + N_v|N_v)$. As already observed in Ref. [17], the vector-flavor group $SU(N_s + N_v|N_v)$ is unbroken because of an extension of the Vafa–Witten theorem [18].

Reference [18] contains two proofs. The first proof is based on a consideration of quark bilinears, and goes through without modification in the partially quenched case. It implies immediately that valence condensates are equal to sea condensates, because with $m_v = m_s$ there is in fact no distinction between these two types of fermions. One ingredient that is needed is that the measure in the path integral is positive, but this is not changed by the

[13] For the rest of this article we will use the subscripts s, v, and g to refer to sea, valence, and ghost quarks, respectively.

[14] Until further notice, we use for simplicity the language of the "fake symmetries" introduced in Ref. [1], which do not take into account all the subtleties coming from the ghost sector, rather than the correct symmetries introduced in Refs. [17, 19, 23]. The subtleties do not affect the general argument. In Sec. IV E, where the details of the chiral Lagrangian matter, we use the nonperturbatively correct form. See Ref. [2] for a review of the issues arising from the ghost sector.

fact that the valence part of the fermion determinant is missing. It is also straightforward to prove that no flavor-symmetry breaking can take place between the valence and ghost sectors, at the level of order parameters made out of quark bilinears [31].

As Ref. [18] points out, spontaneous breaking of flavor symmetry could occur without quark-bilinear order parameters. A more general proof that it does not considers the current-current correlation functions for the conserved flavor currents. If spontaneous symmetry breaking took place, these correlation functions would couple to the corresponding massless Goldstone excitations, and would therefore show a power-like fall-off. The idea is to show that such correlation functions instead satisfy an exponential bound that is uniform in the gauge-field configuration. This implies that no Goldstone mesons exist, and thus that flavor symmetry is unbroken. Since this argument is based on the Ward–Takahashi identities for flavor symmetry, the framework also applies to the Euclidean partially quenched theory, because these identities can also be worked out from the Euclidean path integral.

In fact, Ref. [18] establishes a somewhat more complicated bound by considering a smeared, gauge-invariant quark propagator. But the key point for our discussion is that this bound is obtained for a fixed gauge-field background, and independent of that gauge-field background. Since the only difference between the standard QCD case and the PQQCD case is the relative weight of all gauge-field backgrounds in the Euclidean path integral, the analysis of Ref. [18] carries over to the partially quenched case.

Therefore, we conclude that the Vafa–Witten theorem applies to the PQQCD case with fully degenerate quarks [17]. PQQCD contains a complete $SU(N_s + N_v|N_v)$ multiplet of pseudo-Goldstone mesons in the mass-degenerate case. As in full QCD, if there are no other excitations that are accidentally light, one can consider the low-energy regime, in which this partially quenched pion multiplet contains the only light excitations below a certain scale. Since we know that the pions in the sea sector have a nonzero mass, all pions in the partially quenched theory are massive, and thus all correlation functions of pion operators fall off exponentially, with a rate equal to the pion mass.

In the partially quenched theory, there are other states, made for example from multiple valence quarks, that have no analogue in the sea sector, so these states are not constrained by the Vafa–Witten argument above. The absence of spontaneous symmetry breaking means that there is no fundamental reason for these states to be light, but we cannot eliminate the possibility that they are accidentally light or massless. As in Ref. [16], this possibility can be excluded only by assumption: we assume that the pions are the only light states in the theory.

With this additional assumption, all correlation functions must decay exponentially, which we may call "cluster-like." This result is supported by overwhelming numerical evidence from lattice QCD computations. For true clustering it is necessary in addition that a vacuum state exists and that this state is nondegenerate. The existence of a complete set of states follows from the existence of a transfer matrix for the partially quenched theory, *cf.* Sec. II C.[15] A state with a maximal absolute eigenvalue of the transfer matrix must also exist, because the transfer matrix is bounded. We cannot, however, prove uniqueness. For example, we must by assumption exclude the possibility that some breaking of a discrete symmetry (*e.g.* parity) occurs, resulting in two vacua, but without Goldstone bosons. With these assumptions, which are closely analogous to the assumptions required in Ref. [16], it follows that the degenerate partially quenched theory obeys exponential clustering.

Next, we consider the nondegenerate case, always keeping all quark masses nonzero. When we move away from the degenerate point by taking the valence, ghost, and sea masses unequal (including, but not limited to, the partially quenched case where valence and ghost masses remain degenerate), we can still apply the bounds of Ref. [18] on correlation functions directly, even if the vector symmetries are broken explicitly by the mass differences. The gauge measure remains positive in this case because it is just a product of two positive determinants (valence and sea determinants) divided by the positive ghost determinant. Thus the bounds go through, and all connected correlation functions from point x to point y decay exponentially. Here "connected" means they are formed out of one or more quark propagators that go from x to y. For connected correlation functions, we thus automatically have behavior which is "cluster-like," in that correlators decay exponentially.

There are however many disconnected correlators in the partially quenched theory (made using many valence flavors so that x to y contractions do not occur), and once again most of these have no pure-sea analogue. We need to assume, as before, that such correlators do not have power-law or anomalously light decay. With this assumption, the nondegenerate partially quenched theory has exponential decay in all channels. If we further assume

[15] At least this is true at nonzero lattice spacing; we will ignore subtleties with defining a Hilbert space in the continuum limit. We also will follow Sec. II B in assuming that any gauge configuration on which $\hat{T}_G$ does not have a complete set of eigenstates can be ignored.

that there is a unique lowest state, then the partially quenched theory obeys exponential clustering, even with nondegenerate masses.

C. The dispersion relation

We will assume that the continuum limit of the Euclidean partially quenched theory has $O(4)$ "space-time" invariance. What we wish to argue next is that this leads to the expected form of propagators for one-particle pion states, and thus to the usual relation between energy, mass and spatial momentum.

The transfer matrix for the full theory has (right) eigenstates, which can be classified according to their eigenvalues. In addition, since the theory is invariant under spatial translations, spatial momentum is conserved, and the eigenstates of the transfer matrix can simultaneously be labeled by their spatial momentum. This follows because the transfer matrix, even if it is not Hermitian, generates translations in the time direction, and thus commutes with the generators of spatial translations, *i.e.*, spatial momentum.

Consider first a pion two-point correlator with zero spatial momentum. We know from the preceding section that this correlator falls off exponentially for large times:

$$C_\pi(t) \propto e^{-m_\pi |t|} \ . \tag{4.1}$$

Here the parameter m_π might in principle be complex, since the Hamiltonian is not Hermitian, and it is possible at this stage that m_π is one of a complex pair of eigenvalues. However we do know that m_π has a positive real part, as required by the exponential damping of correlation functions. There may also be other states that contribute to $C_\pi(t)$, which would lead to other exponentially damped contributions, with a faster decay rate (for instance, three-pion states).

The Fourier transform of $C_\pi(t)$ is

$$f(p_4) = \int_{-\infty}^{\infty} dt\, e^{ip_4 t - m_\pi |t|} = \frac{2m_\pi}{p_4^2 + m_\pi^2} \ . \tag{4.2}$$

We now consider the correlator of a pion with a nonzero spatial momentum $\vec{p}$. By $O(4)$ invariance, the Fourier transform of this correlator has to be equal to

$$f(p) = \frac{2m_\pi}{p^2 + m_\pi^2} \ , \tag{4.3}$$

where $p^2 = \sum_\mu p_\mu p_\mu$. If we now Fourier transform back, we obtain the leading exponential of the pion correlator with nonzero spatial momentum,

$$C_\pi(t,\vec{p}) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dp_4\, \frac{2m_\pi e^{-ip_4 t}}{p_4^2+\vec{p}^2+m_\pi^2} = \frac{m_\pi}{E}\, e^{-E|t|}\ , \tag{4.4}$$

with $E = \sqrt{m_\pi^2+\vec{p}^2}$. It follows that the dispersion relation for pions in PQQCD is the usual one, even though this theory is only defined in Euclidean space and even though the "mass" m_π may in principle be complex.

D. The chiral effective theory

We now have all the needed ingredients to extend the arguments of Ref. [16] to the partially quenched case. The existence of the transfer matrix, together with the arguments and assumptions discussed in Sec. IV B, tell us that the theory clusters, and that the lowest states are pions. From Sec. IV C, the pion states have arbitrary momentum, with the usual dispersion relation for energy in terms of spatial momentum and (possibly complex) mass. Further, from Sec. II, the transfer matrix has a complete set of eigenstates, under the mild assumption discussed at the end of Sec. II C.

We then just follow Ref. [16] step by step. The low-energy theory is dominated by exchange of the lightest particles, the pions (*i.e.*, one has "pion pole dominance," although of course there are no poles in Euclidean space). Pion interactions in a small region of space are described by vertices, which do not depend on the overall process due to clustering. These vertices are strictly local, *i.e.*, they may be expanded in powers of momenta. In fact, since we are not concerned here with the massless case, this strict locality would appear to follow from the absence of infrared singularities in Green's functions, and thus not require a separate assumption as it does in the massless case considered in Ref. [16]. However, the relevant mass scale in this argument is the pion mass, m_π, and this argument would not exclude an expansion parameter p/m_π, with p a typical momentum. What we need instead is that vertices can be expanded in p/Λ_{QCD}, and we thus end up having to make the same assumption as in Ref. [16]. Long-distance correlation function then involve the exchange of pions between local vertices. Since the vertices are strictly local building blocks in correlation functions in the effective theory, two (or more) vertices can be joined by more than one pion propagator, leading to loops. And because the set of eigenstates is complete, the correlation functions can be written as sums over intermediate states, which can be turned into four-dimensional loop integrals as in the normal QCD case. Note that the existence of double poles is not a problem for this argument, because we can work with ghost and valence masses unequal, where we have only single poles, and take the limit of equal ghost and valence masses only after the loop expansion is in place. However, a subtlety could arise if the possibility of complex masses is realized, because the standard arguments to relate sums over intermediate (on-shell) states to four-dimensional loop integrals would seem to depend on knowing the locations of poles and cuts in Green's functions, and these singularities will not be in the normal places if there are complex masses. We will assume that no complex masses arise, and then note that this assumption is confirmed *a posteriori* by the effective theory of PQChPT both in the conventional (and most important) limit of degenerate valence-quark and ghost masses, and for appropriate choices of masses in the more general theory that allow us to take that limit. As discussed in Sec. IV F, however, complex masses do seem to be possible in PQChPT with some choices of nondegenerate valence- and ghost-quark masses. Thus the reader should keep in mind that the foundations of the effective theory are less secure at present if such nondegenerate masses are allowed.

Following the first part of the discussion in Ref. [16], the above ingredients (which we may roughly summarize as "pions, vertices, and loops"), are all that are needed to argue that there is an effective chiral theory describing the low energy behavior of the theory. To get the *standard* chiral theory (ordinary ChPT in the full QCD case, PQChPT in the partially quenched case), a further technical argument, based on the chiral Ward–Takahashi identities, is needed to show that one may choose the chiral theory to have *local* chiral symmetry. However, we claim that this part of the argument goes through in the partially quenched case exactly as in the full QCD case, since the partially quenched theory Ward–Takahashi identities are just like those of the ordinary theory, but with the chiral group extended to a graded chiral group. The role of Lorentz invariance in this argument in Ref. [16] is of course played by Euclidean invariance in our case.

Note that we do not have to build the existence of double poles into the chiral theory from the beginning, even though they can be shown to occur already at the fundamental PQQCD level when valence and ghost masses are equal [17] . Their existence in the appropriate limit follows automatically from the effective theory, PQChPT.

E. The effective theory and constraints from CPT

We now work with the nonperturbatively-correct partially quenched chiral Lagrangian introduced in Refs. [17, 19, 23]. The Lagrangian is a function of the chiral fields $\Sigma(x)$ and $\Sigma^{-1}(x)$. Σ is parameterized as

$$\Sigma(x) = \exp(2\Phi(x)/f) \; ; \qquad \Phi(x) = \begin{pmatrix} i\phi(x) & \omega(x) \\ \bar{\omega}(x) & \tilde{\phi}(x) \end{pmatrix} \tag{4.5}$$

where f is the pion decay constant, and where $\phi(x)$ are the quark-antiquark mesons, $\tilde{\phi}$ are the ghost-antighost mesons, and ω and $\bar{\omega}$ are quark-antighost and ghost-antiquark mesons, respectively. While ϕ and $\tilde{\phi}$ are commuting fields, ω and $\bar{\omega}$ are Grassmann valued. At leading order (and in the continuum limit), the Euclidean effective Lagrangian is [19]

$$\mathcal{L}_{\text{eff}} = \frac{f^2}{8} \,\text{str}\,(\partial_\mu \Sigma \partial_\mu \Sigma^{-1}) - v\, \text{str}\,(M\Sigma + \Sigma^{-1} M^\dagger) \tag{4.6}$$

where str denotes the supertrace, M is the quark and ghost mass matrix, and v is a LEC. We have assumed that the super-η' field $\Phi_0 \equiv -i\,\text{str}\,\ln\Sigma = \text{tr}\,(\phi + i\tilde{\phi})$ has been integrated out, which is possible as long as the theory is not completely quenched [17].

In the past, it has been assumed that the LECs in the partially quenched chiral Lagrangian are real, just as the corresponding ones are in the ordinary Hermitian chiral Lagrangian for full, unitary QCD. For most LECs, such as v above, this follows from the fact that QCD is a special case of PQQCD, and LECs that the two effective theories share (for the same number of sea-quark flavors) are equal [3]. However there are additional LECs that are unique to the partially quenched theory, and vanish for pure sea quantities [33]. We would like to be able to argue that those LECs are real too, in order to see that complex meson masses will in general not occur.[16] The antiunitary CPT symmetry of the theory, introduced in Sec. II C, can be used to show this.

We must first determine the transformation properties of ϕ, $\tilde{\phi}$, ω and $\bar{\omega}$ under CPT symmetry. This is a bit subtle since the discrete symmetries of staggered quarks (or ghosts) include additional discrete taste transformations (see for instance the discussion of spatial inversion symmetry in Ref. [28]). Since we want the transformation laws of pseudoscalar

[16] They may still occur in the flavor-diagonal sector, as we will see in the next section.

mesons under continuum CPT (without additional taste transformations), we must look on the lattice at taste-singlet mesons.

From Ref. [34],[17] a staggered quark-antiquark bilinear with spin Γ and taste Ξ is

$$\frac{1}{64}\sum_{A,B}\bar{q}(x+A)\; q(x+B)\mathrm{tr}\left(\Omega^\dagger(A)\;\Gamma\;\Omega(B)\;\Gamma_\Xi^\dagger\right) \tag{4.7}$$

where A and B hypercube vectors (with components 1 or 0 in each of the four directions), $\Gamma_\Xi = \Xi^*$, $\Omega(x) \equiv \gamma_1^{x_1}\gamma_2^{x_2}\gamma_3^{x_3}\gamma_4^{x_4}$, and we have omitted gauge links for simplicity. For the quark-antiquark meson field ϕ_{jk}, with j and k the quark and antiquark flavors, respectively, we have:

$$\begin{aligned}\phi_{jk}(y) \;&\doteq\; \frac{i}{64}\sum_{A,B}\bar{q}_k(x+A)\; q_j(x+B)\mathrm{tr}\left(\Omega^\dagger(A)\;\gamma_5\;\Omega(B)\right)\\ &=\; \frac{i}{16}\sum_{A,B}\big(\delta_{A+B,D}\;(-1)^{B_1+B_3}\;\bar{q}_k(x+A)\;q_j(x+B)\big)\end{aligned} \tag{4.8}$$

where $\doteq$ should be read as "has the same renormalized matrix elements as," $D=(1,1,1,1)$ is the diagonal of a hypercube, and $y \equiv x + D/2$ is defined for convenience to be the middle of the hypercube. The taste-singlet pseudoscalar meson is thus created by a "four-link" operator that joins opposite corners of a hypercube. The overall factor of i in Eq. (4.8) is crucial; it is required to make the propagator $\langle\phi_{jk}(y)\;\phi_{kj}(y')\rangle$ positive, which follows at the chiral level from the definitions Eqs. (4.5) and (4.6).[18]

For ghost-ghost mesons, the corresponding relation is

$$\tilde{\phi}_{jk}(y) \;\doteq\; \frac{1}{16}\sum_{A,B}\Big(\delta_{A+B,D}\;(-1)^{B_1+B_3}\;\chi_k^\dagger(x+A)\;\chi_j(x+B)\Big)\;. \tag{4.9}$$

Here there is no factor of i because there is no minus sign in the propagator due to statistics; by the definitions in Eqs. (4.5) and (4.6), ϕ and $\tilde{\phi}$ have equal propagators. Similarly the

[17] The following argument can also be given in the language of Ref. [35].

[18] The positivity of this propagator in the continuum limit can be most easily seen by noting that the corresponding propagator for taste ξ_5 (taste-pseudoscalar) pions is a sum of absolute squares, which in turn follows from the fact that the staggered Dirac operator obeys $\mathcal{D}^\dagger = \epsilon\mathcal{D}\epsilon$, where ϵ is a diagonal matrix in position space with $\epsilon(x) = (-1)^{x_1+x_2+x_3+x_4}$ along the diagonal. The two factors of i in the propagator cancel the minus sign from Fermi statistics. In the continuum limit, the propagators for (flavor-charged) mesons of arbitrary taste will be equal.

quark-antiqhost and ghost-antighost mesons are given by

$$\omega_{jk}(y) \doteq \frac{1}{16}\sum_{A,B}\Big(\delta_{A+B,D}\,(-1)^{B_1+B_3}\,\chi^\dagger_k(x+A)\,q_j(x+B)\Big)$$
$$\bar\omega_{jk}(y) \doteq \frac{1}{16}\sum_{A,B}\big(\delta_{A+B,D}\,(-1)^{B_1+B_3}\,\bar q_k(x+A)\,\chi_j(x+B)\big)\ . \tag{4.10}$$

Again, no factor of i is needed here to make the $\langle\omega_{jk}(y)\,\bar\omega_{kj}(y')\rangle$ propagator have the same sign as the corresponding ϕ propagator, which is required by Eqs. (4.5) and (4.6).

We can now determine the CPT transformation rules for the meson fields by using the ghost and quark transformation rules, Eqs. (2.33) and (2.35). We find

$$\begin{aligned}
\mathrm{CPT}: &\quad \phi(\vec y, y_4) \;\to\; \phi^{\mathrm{T}}(-\vec y, y_4)\ ,\\
\mathrm{CPT}: &\quad \tilde\phi(\vec y, y_4) \;\to\; -\,\tilde\phi^{\mathrm{T}}(-\vec y, y_4)\ ,\\
\mathrm{CPT}: &\quad \omega(\vec y, y_4) \;\to\; -\,\bar\omega^{\mathrm{T}}(-\vec y, y_4)\ ,\\
\mathrm{CPT}: &\quad \bar\omega(\vec y, y_4) \;\to\; \omega^{\mathrm{T}}(-\vec y, y_4)\ ,
\end{aligned} \tag{4.11}$$

with T the transpose, which acts on flavor indices. The factors of $(-1)^{x_4}$ in Eqs. (2.33) and (2.35), combined with the fact that the spin-1/2 fields in the taste-singlet mesons are on different time-slices, are important to getting the above signs under CPT. The fact that the quark-antiquark meson field is even under CPT is standard.

From the definition of Φ in Eq. (4.5) we then have

$$\mathrm{CPT}: \quad \Phi(\vec x, x_4) \to -\Phi^{\mathrm{t}}(-\vec x, x_4) \tag{4.12}$$

where t denotes a graded transpose defined on a matrix with commuting diagonal blocks and anticommuting off-diagonal blocks by

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{\mathrm{t}} = \begin{pmatrix} a^{\mathrm{T}} & c^{\mathrm{T}} \\ -b^{\mathrm{T}} & d^{\mathrm{T}} \end{pmatrix}\ . \tag{4.13}$$

The operation t has the useful property that

$$\mathrm{str}\,\left(E^{\mathrm{t}}\,F^{\mathrm{t}}\,G^{\mathrm{t}}\,\ldots\,K^{\mathrm{t}}\right) = \mathrm{str}\,\left(\left[K\,\ldots\,G\,F\,E\right]^{\mathrm{T}}\right) \tag{4.14}$$

where E, F, G, K are matrices of the form in Eq. (4.13). The property can be proved by writing both sides as index sums, counting the number of interchanges of anticommuting numbers between the left and right sides, and showing that the sign resulting from the interchanges is the same as the sign coming from the factors of -1 in the definition of t. Note that, unlike the normal rule for the transpose of a product of matrices with commuting entries, this equality is only true under the supertrace. It is not true for the matrices themselves, as is already obvious from considering a single matrix instead of a product.

We can now investigate the consequences of CPT for the chiral theory. Our definitions have ensured that antiunitary CPT symmetry leaves the Euclidean action of the fundamental theory invariant, so it will also leave the Euclidean chiral action invariant. We will see that this implies that the phases of all LECs in the partially quenched chiral Lagrangian are the same as they would be in normal ChPT. For a term that is special to the partially quenched case (because in the normal case with the given number of sea-quark flavors it is not independent due to Cayley-Hamilton relations), the phase of the LEC is the same as it would be in the ChPT theory for a QCD-like theory with sufficient numbers of flavors to make the term independent. The argument goes as follows:

1. Since Euclidean rotational invariance requires derivative operators to be contracted as $\partial_\mu \partial_\mu$ we may redefine $\vec{x} \to -\vec{x}$ on the right-hand-side of Eq. (4.12) without changing sign of any term. (We postpone discussion of anomaly terms, which may have the form $\epsilon_{\mu\nu\lambda\sigma}\partial_\mu\partial_\nu\partial_\lambda\partial_\sigma$, until item 5, below.)

2. Chiral symmetry demands that any term in the Lagrangian be formed from one or more supertraces. Therefore Eq. (4.12) and the rule Eq. (4.14) mean that CPT effectively interchanges Σ and Σ^{-1} and inverts the order of products of arbitrary numbers Σ and Σ^{-1} matrices. The overall transpose on the right-hand side of Eq. (4.14) of course has no effect inside a supertrace.

3. Because CPT is antiunitary it complex-conjugates all LECs.

4. Thus the effect of CPT on the Lagrangian is exactly the same as the effect of taking the Hermitian conjugate would be in a theory where Σ is unitary. The phases are therefore the same as in normal ChPT.

5. For anomaly terms with $\epsilon_{\mu\nu\lambda\sigma}\partial_\mu\partial_\nu\partial_\lambda\partial_\sigma$, an extra minus sign results from taking $\vec{x} \to -\vec{x}$, since we are not flipping the sign of x_4 in Euclidean space. Therefore such terms require an overall factor of i (relative to what they would have in Minkowski space) in order to be CPT invariant. However, this factor of i is precisely the factor that

automatically arises in going from Minkowski space to Euclidean space in any term with a single time derivative. Thus the LEC again has the same phase as it would be ordinary ChPT.

A consequence of this result is that all parameters in the chiral effective Lagrangian corresponding to the square of a meson mass are real (in the usual convention in which they would also be real in the case of a normal theory). Further, all mass terms shared by the PQ and normal theory must have signs that ensure that squared meson masses are positive. This means that as one turns on partial quenching by moving away from a point where valence and ghost masses are degenerate with sea quark masses, the squared meson mass terms must stay positive, at least until the valence, ghost and sea mass differences become large.[19] As we will see in the next section, this still does *not* preclude complex masses from appearing in the theory for small perturbations, due to subtleties in the flavor-diagonal sector. However, "trivial" complex masses, coming directly from complex LECs, are ruled out.

F. Masses in the chiral theory

As mentioned in Sec. IV D, the possibility of complex masses is a concern for our derivation. Once we have the chiral effective theory, however, we can study this possibility in more detail.

Consider, for instance, the two-point function of a flavor-diagonal valence pion and a flavor-diagonal ghost pion, in the mass nondegenerate case. Extending the results of Ref. [1], this two-point function is given by

$$D_{vg}(p) = -\frac{p^2 + M_s^2}{N_v(p^2 + M_s^2)(M_g^2 - M_v^2) + N_s(p^2 + M_v^2)(p^2 + M_g^2)} , \tag{4.15}$$

where we have chosen the number of ghost flavors, N_g, equal to the number of valence flavors, N_v, while allowing $m_g \neq m_v$, and where we have sent the singlet part of the η' mass to infinity. $M_{v,g,s}$ are the masses of (flavor nondiagonal) valence, ghost, and sea pions; in

[19] Negative squared masses would not imply imaginary masses, but rather signal a phase transition and the need to find a new vacuum state. We believe such transitions, driven by possible mass terms special to the partially quenched theory, cannot occur in the usual PQ case of degenerate valence and ghost masses, since the dynamics of such a theory are controlled by the sea masses. We have not however ruled out the existence of such transitions when valence and ghost mass differences are large.

this subsection we use capital letters to distinguish meson masses from quark masses. The denominator of this expression is a quadratic form in $-p^2$ of the form

$$A(-p^2)^2 + B(-p^2) + C \ , \tag{4.16}$$

with

$$\begin{aligned} A &= N_s \ , \\ B &= -N_v(M_g^2 - M_v^2) - N_s(M_g^2 + M_v^2) \ , \\ C &= N_v M_s^2(M_g^2 - M_v^2) + N_s M_g^2 M_v^2 \ . \end{aligned} \tag{4.17}$$

The discriminant of this quadratic form is

$$B^2 - 4AC = (N_v + N_s)^2(M_g^2 - M_v^2)^2 + 4N_v N_s(M_g^2 - M_v^2)(M_v^2 - M_s^2) \ . \tag{4.18}$$

Note that the discriminant vanishes in the limit $M_g = M_v$, and Eq. (4.15) has a double pole in that case as expected, unless also $M_s = M_v$. The double pole is coming from cancellations between ghost and valence terms, which arise in turn because "wrong sign" contributions from the ghosts due ultimately to their non-Hermitian Hamiltonian.

In order to obtain only real single poles, $B^2 - 4AC$ needs to be positive, and this turns out not to be always the case. For simplicity, take $N_v = N_s \equiv N$, so that

$$\left(B^2 - 4AC\right)|_{N_v=N_s=N} = 4N^2(M_g^2 - M_v^2)(M_g^2 - M_s^2) \ . \tag{4.19}$$

This is only positive if $M_g < M_v$ and $M_g < M_s$, or if $M_g > M_v$ and $M_g > M_s$. This means that even a small perturbation from the degenerate case can lead to a situation in which the discriminant is negative, leading to a conjugate pair of complex zeros of Eq. (4.16). The real part of these zeros is given by $-B/(2A) = M_g^2$. The two-point function is still well defined, but the effective theory implies that it is possible to be in the situation that energies of states become complex (with a positive real part). Note that the existence of a conjugate pair of energies is consistent with the PT symmetry of the theory. The reality of M_g^2, M_v^2 and M_s^2, which follows from the reality of the LECs of theory, does however not guarantee that the poles of this real propagator occur at real values of $-p^2$. We emphasize, though, that it is always possible to take the limit $M_g \to M_v$ in such a way that the energies remain real. In particular, if $M_v < M_s$, we can take $M_g \to M_v$ from below, and if $M_v > M_s$, we can take $M_g \to M_v$ from above.

Another instructive example is to take $M_v = M_s \neq M_g$ (while leaving N_v and N_s arbitrary), which keeps $B^2 - 4AC > 0$. Now the zeros $-p_\pm^2$ of the quadratic form are

$$\begin{aligned} -p_-^2 &= M_v^2 \ , \\ -p_+^2 &= M_g^2 + \frac{N_v}{N_s}(M_g^2 - M_v^2) \ . \end{aligned} \tag{4.20}$$

However, the zero $-p_+^2$ becomes negative for

$$M_v^2 > M_g^2 \left(1 + \frac{N_s}{N_v}\right) > M_g^2 \ . \tag{4.21}$$

This would make the Fourier transform of Eq. (4.15) ill-defined, but this can only happen if one perturbs M_v far enough away from M_g. This suggests that for a choice of M_v such that $M_v^2 = M_g^2(1 + N_s/N_v)$ a phase transition takes place. In that case, the effective partition function would have to be evaluated by performing a different saddle-point expansion than the one assumed in writing down Eq. (4.15). Of course, as already remarked above, no such problems, and no complex energies, appear when $M_g = M_v$, which is the "physical" case of PQQCD, because in that case $B^2 - 4AC = 0$, and we recover the usual double pole. We therefore do not pursue the possibilities arising for $M_g \neq M_v$ further.

V. CONCLUSION

In this article, we have presented the theoretical evidence that PQChPT provides the correct low-energy effective theory for PQQCD. Our starting point is the discussion by Leutwyler [16] of the foundations of chiral perturbation theory in the case of full QCD. The cluster property of a Lorentz invariant, local quantum field theory plays a central role in Ref. [16]; unitarity, in contrast, appears not to be needed. This starting point is essential in any attempt to extend the validity of ChPT to the partially quenched case, in which unitarity is lost. Therefore, our main task has been to see to what extent the cluster property can be established in PQQCD as well.

The key ingredients are the existence of a bounded transfer matrix, as well as an extension of the Vafa–Witten theorem to the partially quenched case. The existence of the transfer matrix allows us to identify a complete set of states in the theory, even though the transfer matrix and the corresponding states do not have all the usual properties they possess in a unitary theory. An important point, however, is that the pion states do satisfy a rotationally invariant dispersion relation. The Vafa–Witten theorem [18] allows us to connect the space-time dependence of correlation functions in the partially quenched theory with those of correlation functions of the corresponding full QCD theory with the same set of sea quarks. While these ingredients together are not sufficient to provide a rigorous proof of clustering, we have identified the further assumptions needed to establish the cluster property in PQQCD, assuming that it holds in the full theory.[20]

Once the cluster property is established, the argument for the correctness of PQChPT as the low-energy effective theory for PQQCD follows mainly along the same lines as that given in Ref. [16]. While in both cases some additional assumptions are needed (such as the assumption that no other accidentally light states exist in the theory), these additional assumptions in general have little to do with the "sickness" of the partially quenched theory, and we thus believe them to be equally plausible in both the full and partially quenched cases. One issue unique to the partially quenched case is the possibility of complex energies, which could make it difficult to write effective-theory loops as normal four-dimensional integrals, and require instead three-dimensional integrals over on-shell states. The arguments presented in Sec. IV support the assumption that this situation does not occur in the only case of practical interest, in which ghost quark masses are chosen equal to the corresponding valence quark masses, *i.e.*, the case usually referred to as partial quenching. Section IV E shows that CPT symmetry requires the effective theory to have real low energy constants. This restricts the problem of complex masses to the flavor-diagonal sector. As demonstrated in Sec. IV F, complex masses (or poles located at negative values of (Euclidean) $-p^2$) do not occur when all ghost quark masses are chosen equal to the corresponding valence quark masses. The only "sickness" is the familiar occurrence of double poles, at positive values of $-p^2$, in the valence sector.

Our framework for the construction of the effective low-energy theory generalizes to the fully nondegenerate case, in which ghost-quark masses are not equal to valence-quark masses. It turns out that this generalized theory contains some new properties absent in the partially quenched case; these properties can be investigated in the corresponding effective field theory. In particular, one can choose values for ghost and valence masses such that complex

[20] We are not aware of a rigorous proof of the cluster property for full QCD either; for a discussion of the cluster property in quantum field theories, see Ref. [36].

poles appear in the disconnected propagator. We leave open the question of the validity of the standard loop expansion of the effective theory for this case. Of course, as already emphasized above, this issue is primarily of academic interest, since, by construction, ghost and valence quark masses are always equal in numerical applications of PQQCD.

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Appendix A: Completeness

In this appendix, we prove completeness in the free theory of the basis of right eigenstates given by Eq. (3.24), or the left eigenstates given by Eq. (3.25). The argument has three steps. First, we prove that $|0,0\rangle_R$, ${}_L\langle 0,0|$ are the unique right and left vacuum states. We then show that all right eigenstates are obtained by acting with the raising operators $\tilde{b}_1$ and $\tilde{b}_2$ on $|0,0\rangle_R$ (and similarly for left eigenstates). Finally, we prove that that no blocks of the form of the form (2.21), or larger generalizations thereof, occur in the Jordan normal form of the Hamiltonian matrix of the free theory.

The uniqueness of the right and left vacua can be proved by working in position space and solving the differential equations corresponding to the definitions of $|0,0\rangle_R$ and ${}_L\langle 0,0|$, which are given in operator form by

$$\begin{aligned} b_1\,|0,0\rangle_R \;&=\; (\cos\theta\; a_1 - \sin\theta\; a_2^\dagger)\,|0,0\rangle_R = 0\;, \\ b_2\,|0,0\rangle_R \;&=\; (\cos\theta\; a_2 - \sin\theta\; a_1^\dagger)\,|0,0\rangle_R = 0\;, \end{aligned} \tag{A1}$$

and

$$
\begin{aligned}
{}_L\langle 0,0|\,\tilde{b}_1 &= {}_L\langle 0,0|\,(\cos\theta\ a_1^\dagger + \sin\theta\ a_2) = 0\ , \\
{}_L\langle 0,0|\,\tilde{b}_2 &= {}_L\langle 0,0|\,(\cos\theta\ a_2^\dagger + \sin\theta\ a_1) = 0\ ,
\end{aligned}
\tag{A2}
$$

where we used Eq. (3.17).

Using x for the position associated with oscillator described by a_1, $a_1^\dagger$ and y for the oscillator described by a_2, $a_2^\dagger$, we have

$$
\begin{aligned}
a_1 &= \frac{1}{\sqrt{2}}(x + \frac{\partial}{\partial x}), \qquad & a_1^\dagger &= \frac{1}{\sqrt{2}}(x - \frac{\partial}{\partial x}) \\
a_2 &= \frac{1}{\sqrt{2}}(y + \frac{\partial}{\partial y}), \qquad & a_2^\dagger &= \frac{1}{\sqrt{2}}(y - \frac{\partial}{\partial y})\ .
\end{aligned}
\tag{A3}
$$

Now let

$$
\langle x, y|0,0\rangle_R = \psi(x,y), \qquad {}_L\langle 0,0|x,y\rangle_R = \chi^*(x,y)
\tag{A4}
$$

be the position-space wavefunctions for the vacua. The equations for $\psi(x,y)$ and $\chi(x,y)$ are

$$
\begin{aligned}
\left[\cos\theta\left(x + \frac{\partial}{\partial x}\right) - \sin\theta\left(y - \frac{\partial}{\partial y}\right)\right]\psi(x,y) &= 0\ , \\
\left[-\sin\theta\left(x - \frac{\partial}{\partial x}\right) + \cos\theta\left(y + \frac{\partial}{\partial y}\right)\right]\psi(x,y) &= 0\ , \\
\left[\cos\theta\left(x + \frac{\partial}{\partial x}\right) + \sin\theta\left(y - \frac{\partial}{\partial y}\right)\right]\chi(x,y) &= 0\ , \\
\left[\sin\theta\left(x - \frac{\partial}{\partial x}\right) + \cos\theta\left(y + \frac{\partial}{\partial y}\right)\right]\chi(x,y) &= 0\ .
\end{aligned}
\tag{A5}
$$

The solutions are (recalling Eq. (3.20))

$$
\begin{aligned}
\psi(x,y) &= A\exp\left(-\frac{E}{2m}(x^2+y^2) + \frac{s}{m}\,xy\right)\ , \\
\chi(x,y) &= A\exp\left(-\frac{E}{2m}(x^2+y^2) - \frac{s}{m}\,xy\right)\ .
\end{aligned}
\tag{A6}
$$

Since the only free parameter in these solutions is the normalization A, we have shown that the right and left vacua are unique.

It is now clear (following the argument after Eq. (3.23)) that any right eigenstate of h can be repeatedly lowered by application of b_1 and b_2 until we reach $|0,0\rangle_R$. This is all we need in order to show that the eigenstate can, in turn, be obtained by operating with $\tilde{b}_1$ and $\tilde{b}_2$ on the vacuum, and is therefore just proportional to one of the states $|n,m\rangle_R$ in Eq. (3.24).

For example, consider an eigenstate $|1', 0'\rangle_R$, with

$$\begin{aligned}\tilde{b}_1 b_1 \, |1', 0'\rangle_R &= |1', 0'\rangle_R \ , \\ \tilde{b}_2 b_2 \, |1', 0'\rangle_R &= 0 \ .\end{aligned} \tag{A7}$$

By uniqueness of the vacuum,

$$b_1 \, |1', 0'\rangle_R \propto |0, 0\rangle_R \ . \tag{A8}$$

Operating on both sides of this equation with $\tilde{b}_1$ and using Eq. (A7) then proves that

$$|1', 0'\rangle_R \propto \tilde{b}_1 \, |0, 0\rangle_R = |1, 0\rangle_R \ . \tag{A9}$$

It is straightforward to extend this step to a proof by induction that, similarly,

$$|n', m'\rangle_R \propto |n, m\rangle_R \ , \tag{A10}$$

for an eigenstate $|n', m'\rangle_R$ of the number operators $\tilde{b}_1 b_1$ and $\tilde{b}_2 b_2$ with eigenvalues n' and m' respectively. An analogous argument extends this first step to left eigenstates as well.

The fact that we have shown that all right and left eigenstates are of the form of Eq. (3.24) and (3.25) does not yet quite prove completeness of these states. Since the Hamiltonian (3.21) is not Hermitian, it is possible that its Jordan normal form has nontrivial blocks of the form (2.21), with $\kappa \neq 0$. We now prove that this does not happen in the free theory. First, the Hamiltonian is proportional to the sum of two number operators, $N_1 = \tilde{b}_1 b_1$ and $N_2 = \tilde{b}_2 b_2$, which commute with each other. Therefore, the matrix representation of the sum is a direct product of the two matrices representing N_1 and N_2. It is thus sufficient to show that no nontrivial Jordan blocks occur in the matrix representation of $N = \tilde{b} b$, where $b = b_i$ and $\tilde{b} = \tilde{b}_i$, with $i = 1$ or 2.

Now assume that a hypothetical Jordan block of arbitrary size $p \times p$ occurs, with $p > 1$. Such blocks have an eigenvalue on the diagonal, and an arbitrary constant κ on the "superdiagonal." The block is trivial if $\kappa = 0$; nontrivial otherwise. We already know that possible eigenvalues of the number operator N are $n = 0, 1, 2, \ldots$. So, for example, a block for eigenvalue n and $p = 4$ would look like

$$\begin{pmatrix} n & \kappa & 0 & 0 \\ 0 & n & \kappa & 0 \\ 0 & 0 & n & \kappa \\ 0 & 0 & 0 & n \end{pmatrix} \ . \tag{A11}$$

We will prove by induction on n that no such blocks can exist for any n, and any size p. For any such hypothetical block, let $|n\rangle_R$ be the true right eigenvector and $|A^{(n)}\rangle_R$ be the first nontrivial generalized right eigenvector. These states obey

$$\begin{aligned} N\,|n\rangle_R &= n|n\rangle_R \ , \\ N\,|A^{(n)}\rangle_R &= n|A^{(n)}\rangle_R + \kappa|n\rangle_R \ . \end{aligned} \tag{A12}$$

For example, in the $p = 4$ case above, $|n\rangle_R$ and $|A^{(n)}\rangle_R$ could be represented by

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \gamma \\ 1 \\ 0 \\ 0 \end{pmatrix} \ , \tag{A13}$$

respectively, with γ arbitrary.

The theorem that we will prove is:

> If, for any n, there exists a state $|A^{(n)}\rangle_R$ that is linearly independent of the eigenvector $|n\rangle_R$ and obeys
>
> $$N\,|A^{(n)}\rangle_R = n|A^{(n)}\rangle_R + \kappa|n\rangle_R \ , \tag{A14}$$
>
> then $\kappa = 0$.

Thus $|A^{(n)}\rangle_R$ is a right eigenstate degenerate with $|n\rangle_R$. However, since we showed above that the eigenstates of N are nondegenerate, $|A^{(n)}\rangle_R$ would have to be proportional to $|n\rangle_R$, which contradicts the assumption of linear independence. Thus, no state $|A^{(n)}\rangle_R$ can exist, and the Jordan block is not only trivial ($\kappa = 0$) but is actually one-dimensional ($p = 1$).

We first show the theorem is true for $n = 0$. For a nontrivial Jordan block with $n = 0$ we would have

$$N\,|A^{(0)}\rangle_R = \kappa|0\rangle_R \ , \tag{A15}$$

which implies

$$Nb\,|A^{(0)}\rangle_R = (bN - b)|A^{(0)}\rangle_R = -b\,|A^{(0)}\rangle_R \ . \tag{A16}$$

So $b\,|A^{(0)}\rangle_R$ would have to be an eigenstate of N with eigenvalue -1, which is impossible since N is positive semidefinite. Thus $b\,|A^{(0)}\rangle_R$ must vanish, which implies

$$N\,|A^{(0)}\rangle_R = \tilde{b}b\,|A^{(0)}\rangle_R = 0 \ . \tag{A17}$$

Comparing with Eq. (A15), we see that $\kappa = 0$, as desired.

We now assume that the theorem is true for eigenvalue n, and prove it is also true for eigenvalue $n+1$. Suppose we have a state $|A^{(n+1)}\rangle_R$ that is linearly independent of $|n+1\rangle_R$ and satisfies

$$N\,|A^{(n+1)}\rangle_R = (n+1)|A^{(n+1)}\rangle_R + \kappa|n+1\rangle_R \ . \tag{A18}$$

Then

$$Nb\,|A^{(n+1)}\rangle_R = (bN-b)|A^{(n+1)}\rangle_R = nb\,|A^{(n+1)}\rangle_R + \sqrt{n+1}\;\kappa|n\rangle_R \ . \tag{A19}$$

So the state $b|A^{(n+1)}\rangle_R$ satisfies Eq. (A14) for eigenvalue n, with κ replaced by $\kappa' = \sqrt{n+1}\;\kappa$. Furthermore, $b|A^{(n+1)}\rangle_R$ is linearly independent of $|n\rangle_R$. If not, $b\,|A^{(n+1)}\rangle_R = \alpha|n\rangle_R$ for some constant α, which implies by Eq. (A18) that

$$\tilde{b}b\,|A^{(n+1)}\rangle_R = (n+1)|A^{(n+1)}\rangle_R + \kappa|n+1\rangle_R = \tilde{b}\,\alpha|n\rangle_R = \sqrt{n+1}\;\alpha|n+1\rangle_R \ , \tag{A20}$$

contradicting the assumption that $|A^{(n+1)}\rangle_R$ is linearly independent of $|n+1\rangle_R$. Therefore, $b\,|A^{(n+1)}\rangle_R$ satisfies the conditions of the induction hypothesis, which implies $\kappa' = 0$, and hence $\kappa = 0$.

This concludes the proof of our theorem, and hence completeness of the free theory as in Eq. (3.28).

Appendix B: Path integral for the free ghost theory

Starting from Eq. (3.16), we reconstruct a path integral which yields the same correlation functions as those generated by the transfer matrix defined in terms of h. This is an alternative to the operator analysis based on the generalized Bogoliubov transformation, Eq. (3.17). For simplicity, we take $T \to \infty$ from the beginning.

We start by defining new fields ψ_i and conjugate momenta ρ_i

$$\psi_i = \frac{1}{\sqrt{2m}}(a_i + a_i^\dagger) \ , \qquad \rho_i = -i\sqrt{\frac{m}{2}}(a_i - a_i^\dagger) \ , \tag{B1}$$

which are conventionally normalized,

$$[\psi_i, \rho_j] = i\,\delta_{ij} \ . \tag{B2}$$

The Hamiltonian then may be written

$$h = \frac{1}{2}\left(\rho_1^2 + \rho_2^2 + m^2(\psi_1^2 + \psi_2^2)\right) + is\,(\psi_1\rho_2 + \psi_2\rho_1) + \text{constant} \ . \tag{B3}$$

Introducing sources J_i for ψ_i and K_i for ρ_i, the partition function in the Hamiltonian form of the path integral is

$$Z[J_i, K_i] = \int \mathcal{D}\psi_1\, \mathcal{D}\psi_2\, \mathcal{D}\rho_1\, \mathcal{D}\rho_2\, \exp(i\rho_j\dot{\psi}_j - h + J_j\psi_j + K_j\rho_j) , \tag{B4}$$

with a sum over the repeated index j, and with $\dot{\psi}_j \equiv d\psi_j/dt$. The quadratic integrals over ρ_1 and ρ_2 are easily done,[21] and the result is

$$Z[J_i, K_i] = \int \mathcal{D}\psi_1\, \mathcal{D}\psi_2\, e^{-\mathcal{L}_E[J_i,K_i]} , \tag{B5}$$

with the Euclidean Lagrangian $\mathcal{L}_E[J_i, K_i]$ given by

$$\begin{aligned} \mathcal{L}_E[J_i, K_i] \;=\; & \frac{1}{2}\left(\dot{\psi}_1^2 + \dot{\psi}_2^2 + E^2(\psi_1^2 + \psi_2^2)\right) - iK_1(\dot{\psi}_i - s\psi_2) - iK_2(\dot{\psi}_2 - s\psi_1) \\ & -J_1\psi_1 - J_2\psi_2 - \frac{1}{2}(K_1^2 + K_2^2) - s\frac{d}{dt}(\psi_1\psi_2) . \end{aligned} \tag{B6}$$

The terms quadratic in K_j are standard, and just give contact terms that we drop from now on. We will also drop the final, total-derivative term, since we want to calculate a partition function with periodic boundary conditions on ψ_j. Note, however, that for computing transition amplitudes between ψ_j eigenstates, dropping the total derivative would be incorrect; indeed that term leads to violations of unitarity. Violations arise because the Minkowski-space transition amplitude

$$T_{ba} = \langle \psi_{1,b}\psi_{2,b}; t_b | \psi_{1,a}\psi_{2,a}; t_a \rangle \tag{B7}$$

is proportional to $\exp[s(\psi_{1,b}\psi_{2,b} - \psi_{1,a}\psi_{2,a})]$ and does therefore does not obey $T_{ba} = T_{ab}^*$.

If we focused only on correlation functions of ψ_j, the sources K_j could also be dropped completely, and one would immediately see that the correlation functions are the completely normal correlators of two harmonic oscillators with frequency E. One could in fact *change* the rules at this point, and write down a standard (double) harmonic oscillator Hamiltonian h' that gives these same ψ_j correlators:

$$h' = \frac{1}{2}\left(\rho_1^2 + \rho_2^2 + E^2(\psi_1^2 + \psi_2^2)\right) \tag{B8}$$

The analogous step for the Hamiltonian of Ref. [29] is taken in Ref. [30]. However, this is really a change of rules, because it changes the correlators involving ρ_j. As we will see below, nonunitary effects we already obtained in Sec. III C show up in those correlators.

[21] The ρ_j have open boundary condition, as is always the case in the path integral formulation.

From Eqs. (B5) and (B6), we can easily compute all two-point correlators by taking derivatives with respect to J_j and K_j. The results are:

$$\langle\psi_i(t)\psi_j(0)\rangle = \delta_{ij}\,\frac{e^{-Et}}{2E} \qquad \left[= \delta_{ij}\,\frac{e^{-Et}}{2E}\right], \tag{B9a}$$

$$\langle\psi_i(t)\rho_j(0)\rangle = \delta_{ij}\,\frac{ie^{-Et}}{2} + \delta_{i+j,3}\,\frac{-ise^{-Et}}{2E} \qquad \left[= \delta_{ij}\,\frac{ie^{-Et}}{2}\right], \tag{B9b}$$

$$\langle\rho_i(t)\psi_j(0)\rangle = \delta_{ij}\,\frac{-ie^{-Et}}{2} + \delta_{i+j,3}\,\frac{-ise^{-Et}}{2E} \qquad \left[= \delta_{ij}\,\frac{-ie^{-Et}}{2}\right], \tag{B9c}$$

$$\langle\rho_i(t)\rho_j(0)\rangle = \delta_{ij}\,\frac{m^2e^{-Et}}{2E} \qquad \left[= \delta_{ij}\,\frac{Ee^{-Et}}{2}\right]. \tag{B9d}$$

Here, the corresponding results in the standard theory defined by h' are shown in square brackets. For both our theory and the standard theory, these correlators satisfy the conditions required by the commutators Eq. (B2) in the limit $t \to 0$. (The relevant correlators are unaffected by the dropped contact terms.)

Aside from the off-diagonal terms in the ψ-ρ correlators, the difference between our theory and the standard theory appears in the normalization of the ρ-ρ correlator in Eq. (B9d). From Eq. (B1) and Eq. (B9), we can easily check that we reproduce the correlators Eqs. (3.33) and (3.34) for the creation and annihilation operators in the limit $T \to \infty$. In particular, the unitarity-violating negative result for $\langle a_i^\dagger(t)a_j(0)\rangle$ shows up here because of the incomplete cancellation of the various contributions from Eqs. (B9a) through (B9d). (Note that, in order to recover expected results for correlators of creation and annihilation operators in the standard theory, one must replace the definitions Eq. (B1) by letting $m \to E$, so that the Hamiltonian h' takes its standard form in terms of a_i and $a_i^\dagger$.)

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