

Singlets in gauge theories with fundamental matter

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We provide the first determination of the mass of the lightest flavor-singlet pseudoscalar and scalar bound states (mesons) in the $Sp(4)$ Yang-Mills theory coupled to two flavors of fundamental fermions, using lattice methods. This theory has applications both to composite Higgs and strongly interacting dark matter scenarios. We find the singlets to have masses comparable to those of the light flavored states, which might have important implications for phenomenological models. We focus on regions of parameter space corresponding to a moderately heavy mass regime for the fermions. We compare the spectra we computed to existing and new results for $SU(2)$ and $SU(3)$ theories, uncovering an intriguing degree of commonality. As a by-product, in order to perform the aforementioned measurements, we implemented and tested, in the context of symplectic lattice gauge theories, several strategies for the treatment of disconnected-diagram contributions to two-point correlation functions. These technical advances set the stage for future studies of the singlet sector in broader portions of parameter space of this and other lattice theories with a symplectic gauge group.

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I. INTRODUCTION

The possible existence of new strongly interacting sectors that extend the standard model (SM) of particle physics has been the subject of a long-standing history of theoretical studies. In recent years, this idea has been prominently featured in the context of composite Higgs

models (CHMs) in which the Higgs fields of the SM originate as pseudo-Nambu-Goldstone bosons (PNGBs) of the underlying theory [1–3].¹ A parallel development has led to strongly coupled gauge theories being considered as the dynamical origin of hidden sectors in which dark matter consists of strongly interacting massive particles (SIMPs) [64–73]. This scenario can address observational problems, such as the “core vs cusp” [74] and “too big to fail” [75] ones, and have implications for gravitational wave experiments [76–93]—see, e.g., Refs. [94–99], as well as Refs. [100–104]. Both CHMs and SIMPs give rise to particles, the PNGBs, carrying nontrivial quantum numbers of non-Abelian global (flavor) symmetries, that suppress and protect their masses.

In general, strongly coupled theories also yield bound states that are flavor singlets. Composite models with a

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¹The recent literature is vast. See, e.g., the reviews in Refs. [4–6], the summary tables in Refs. [7–9], and the selection of papers in Refs. [10–48] and Refs. [49–63].

strongly coupled origin can in particular give rise to a light dilaton [105–107], the PNGB associated with (approximate) scale invariance. The striking phenomenological implications of this possibility [108] have also been studied extensively (see, e.g., Refs. [109–120]), and the low energy effective field theory (EFT) of the dilaton [121,122] and the other PNGBs can be combined in the dilaton EFT [123–138]. Numerical evidence supporting this possibility has emerged in the context of SU(3) lattice gauge theories with special field content [139–151]. The singlet sector of a strongly coupled theory contains also pseudoscalar composite states, the phenomenology of which is the subject of dedicated studies [9,23,27,152–154]. Their EFT treatment follows closely that of axionlike particles (ALPs) [155–157].

The phenomenological consequences of such theories depend crucially on the mass spectrum of the lightest states and on the (model dependent) couplings to the standard model. While an efficient tool in treating the latter is provided by the EFT methodology, even the construction of such EFTs requires a good understanding of the lightest portion of the spectrum. Whatever the original motivation and application envisioned for such new strongly coupled physical sectors is, they have a plethora of bound states, some of which can be either stable or long lived, and potentially light. It is then desirable to gain a broad nonperturbative understanding of their spectroscopy, for all bound states, and in the largest possible portions of the parameter space. The instrument of choice for this endeavor is that of (numerical) lattice gauge theories. There has been a wide variety of investigations into the spectrum of many such theories, especially those with SU(N) group, with matter in various numbers and representations. Besides the aforementioned work, and Refs. [143,144,158–162] on SU(3), see, e.g., Refs. [163–171] for SU(2) theories, Refs. [172–175] for SU(4) in multiple representations, and [176] for G_2 , as well as the reviews in Refs. [177–180].

Gauge theories with a symplectic group play a special role in all these contexts, because of the peculiar properties of Sp($2N$) groups and their representations. For example, the model in Ref. [16] provides the simplest realization of a CHM that combines it with top partial compositeness [181] and consists of a Sp($2N$) gauge theory with mixed-representation fermion content. Likewise, Refs. [64,66] use it for the construction of a SIMP-“miracle”. A number of recent lattice studies started to characterize them [182–198], following the pioneering effort in Ref. [199]. While much such work has focused on the spectroscopy of bound states carrying flavor, with this paper, we report on progress in the singlet sector.

The present study explores the flavor-singlet bound state sector in the Sp(4) gauge theory coupled to two fermions in the fundamental representation, a theory that has gathered substantial interest in the CHM context and also provides a minimal realization of the SIMP

mechanism [67,69,71,72,200]. This study is complementary to the available nonsinglet hadron spectrum found in Refs. [182,184–187,189,190,197]. Within the general aim of understanding universal features of the low-lying spectrum across different gauge groups, this is also a step toward understanding how the approach to the large- N limit of Sp($2N$) gauge theories differs from that of SU(N) gauge theories, especially with respect to the axial anomaly and topology. Our results could in the future help to understand the anomaly-mediated decays of singlets into SM particles.

We supplement this publication with numerical results obtained in two other theories. The first is the closely related SU(2) theory with two fundamental fermions, for which earlier studies exist [163,201], and for which we perform additional, new calculations. In the case of the SU(3) theory coupled to fermions in the fundamental representation, the pseudoscalar singlet has been studied in Refs. [202–214]. The determination of the mass (and width) of the lightest scalar singlet has proven to be particularly challenging, and a number of studies in SU(3) with dynamical fermions exists both in the context of real-world QCD [215–224] and more general field content [141,143,144,158–161]. We borrow results from this extensive literature for the purpose of comparing with our own results.

The paper is organized as follows. The pseudo-real nature of the fundamental representation of Sp(4)—as for SU(2)—leads to symmetry enhancement by modifying the flavor symmetry and symmetry-breaking pattern. The structure of the low-lying spectrum is hence different from the more familiar QCD case. We briefly comment on the most striking such features in Sec. II, as we define the continuum theory of interest. In Sec. III, we describe the lattice methods that we use to study the flavor-singlet states, putting some emphasis on the implications for the construction of suitable operators, in Sec. III A. The study of correlations functions involving singlets is affected by notorious difficulties, poor signal-to-noise ratio featuring prominently among them. This required the adoption of advanced techniques to obtain a nonzero signal, as we explain in Sec. III B, and in more detail in the Appendices.

We present the body of our numerical results in Sec. IV. Section IV A is devoted to the lightest pseudoscalar singlet state, in both the Sp(4) and SU(2) theories, for degenerate masses. We report on the case of nondegenerate flavor masses for Sp(4) (which realizes a scenario relevant to dark matter models) in Sec. IV B. The scalar singlet sector, in the degenerate case for the Sp(4) theory, is the subject of Sec. IV C, though we anticipate that, because of the bad signal-to-noise ratio, only a rough estimate with unclear finite-spacing systematics can be established at this stage. Finally, we assess our results by a comparison to the SU(3) case and report the results in Sec. IV D. Our general conclusion, exposed more critically in Sec. V, is that for

the available range of fermion masses the singlets are indeed light enough to affect phenomenology and low-energy EFT considerations. We add several technical appendices, covering further details. We note that some preliminary results are available in Ref. [225].

II. FLAVOR SINGLETs IN SYMPLECTIC GAUGE THEORIES

We start the presentation by defining explicitly the (continuum) field theories of interest. We provide both their microscopic definition, in terms of elementary fields, and their salient long-distance properties, which can be explained in EFT terms. In doing so, we emphasize the role of the symmetries of the theory.

A. Microscopic theory and global symmetries

The $\text{Sp}(2N)$ gauge theories of interest are characterized by a Lagrangian density, \mathcal{L} , which in this section, we write using a metric with Lorentzian signature $(+1, -1, -1, -1)$, and takes the form:

$$\mathcal{L} = -\frac{1}{2} \text{Tr}[G_{\mu\nu}G^{\mu\nu}] + \bar{u}(i\gamma^\mu D_\mu - m_u)u + \bar{d}(i\gamma^\mu D_\mu - m_d)d, \quad (1)$$

where $G_{\mu\nu} \equiv \sum_A G_{\mu\nu}^A t^A$ are the field strength tensors, and t^A are the generators of $\text{Sp}(2N)$, normalized so that $\text{Tr}T^A T^B = \frac{1}{2}\delta^{AB}$, while u and d are four-component Dirac spinors, denoting the two flavors of fermion fields transforming in the fundamental representation of $\text{Sp}(2N)$. The Lagrangian is real and Lorentz invariant, as $\bar{u} \equiv u^\dagger \gamma^0$, and $\bar{d} \equiv d^\dagger \gamma^0$. The covariant derivatives are defined in terms of the gauge fields $A_\mu \equiv A_\mu^A t^A$ as

$$D_\mu u \equiv \partial_\mu u + igA_\mu u, \quad D_\mu d \equiv \partial_\mu d + igA_\mu d, \quad (2)$$

where g is the gauge coupling. Explicitly, the field-strength tensor is given by

$$G_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu], \quad (3)$$

where $[\cdot, \cdot]$ denotes the commutator.

The fundamental representation of $\text{Sp}(2N)$ is pseudo-real. As a result, the global symmetry is enhanced: One can show explicitly, by rewriting Eq. (1) in terms of two-component fermions,² that for each Dirac fermion, the $U(1)_L \times U(1)_R$ Abelian global symmetry acting on its chiral projections is enhanced to a non-Abelian $U(2)$ global

²This somewhat tedious exercise can be found in all its details in the literature, for instance, in Refs. [168,185] and references therein.

symmetry. The fermion kinetic terms hence, written in terms of covariant derivatives, exhibit an enhanced (classical) $U(4) = U(1)_A \times SU(4)$ global symmetry; we will return to the effect of anomalies in the next subsection.

The fermion mass terms break explicitly the global symmetry. If the masses are degenerate, $m_u = m_d$, as will be the case throughout most of this paper, then the global symmetry is explicitly broken to $\text{Sp}(4)$. The bilinear, nonderivative operator appearing in the Lagrangian density as a mass term is also expected to condense so that the same symmetry breaking pattern appears also in spontaneous symmetry breaking effects. For generic choices of fermion masses, $m_u \neq m_d$, the approximate global symmetry is further broken to $\text{Sp}(2)^2 \sim \text{SU}(2)^2$ [197].

B. Light meson spectrum for two fundamental fermions

We summarize here the main properties of the bound states of interest, guided by gauge invariance and symmetry arguments, starting from the case in which the fundamental fermions have degenerate mass, $m_u = m_d$. We observe that the group structure has an even number of colors; hence baryons are bosons. Furthermore, because the matter content consists only of fermions transforming in the pseudo-real fundamental representation, and as a result, the global symmetry is enhanced, ordinary baryon number is a subgroup of the enhanced $SU(4)$ and is unbroken in the vacuum of the theory, and hence objects that one might be tempted to classify as having different baryon number (e.g., mesons and diquarks) belong to the same $\text{Sp}(4)$ multiplet.

We restrict the discussion from here onward to mesons made of two fundamental fermions. It may be convenient to think of the mesons in terms of their two-component fermion field content in order to classify them by their $\text{Sp}(4)$ transformations and attribute their J^P quantum numbers.³ As the two-component fermions transform as a 4 of $\text{Sp}(4)$, the multiplication properties imply that there exist mesons transforming as a 1, 5, and 10 of $\text{Sp}(4)$.

Starting from the spin-0 states, one expects to find in the spectrum 5 PNBGs, spanning the $SU(4)/\text{Sp}(4)$ coset, and transforming as a 5 of $\text{Sp}(4)$, to become massless in the $m_u = m_d \rightarrow 0$ limit.⁴ These states have parity partners, generalizing what in QCD literature are usually denoted as a_0 particles. Some numerical lattice evidence exists that at high

³We define the parity P so that flavor eigenstates are also parity eigenstates. See Refs. [165,185,197] for extended discussions of the subtleties involving twisting between space and flavor in the definition of parity.

⁴These are the states playing a role in CHMs; in their EFT description in terms of weakly coupled fields, four of them are identified with the components of the SM Higgs doublet because the $SU(2)_L \times SU(2)_R$ approximate symmetry of the electroweak theory is identified with the $SO(4)$ subgroup of $\text{Sp}(4)$, and hence $5 = 4 \oplus 1$ [16]. The 1 is an additional state that carries no SM gauge quantum numbers, but in the EFT description of the strong coupling sector, it is degenerate with the 4. Likewise, these states are the dark matter candidates in SIMP models [64,65,197].

temperature, these two sets of states become degenerate—see Ref. [226] for SU(2) and Ref. [227] for SU(3), both with two flavors of fundamental fermions—because the $U(1)_A$ symmetry relating them is restored, but at zero temperature the scalar 5 is expected to be heavy, the mass of the particles being of the order of the confinement scale, even in the $m_u = m_d \rightarrow 0$ limit.

Classically, one would expect also two singlet scalars to be light: the axion and the dilaton. Indeed, the classical Lagrangian for $m_u = m_d = 0$ is invariant also under the action of a $U(1)_A$ symmetry and of dilatations, the condensates breaking both of them spontaneously, and these two additional light states can be thought of as the PNGBs associated with these two Abelian symmetries. Alas, besides being explicitly broken by the fermion masses, both these symmetries are also anomalous. The $U(1)_A$ and scale anomalies hence provide masses for the axion-dilaton system, related to the scale of confinement of the theory. Mixing effects between these states and other vacuum excitations (e.g., glueballs with the same J^P quantum numbers) are present as well, given that no symmetry argument can be invoked rigorously to forbid them. The precise determination of such masses, hence, is nontrivial, and to large extent this paper is about setting the stage for its future large-scale, high-precision calculation. Furthermore, in confining theories with large numbers of degrees of freedom, and when approaching the lower edge of the conformal window, nonperturbative effects might suppress the mass of the axion and dilaton, respectively; this is a very active field of research in itself, for a potential phenomenological role both of this axion and of the dilaton, as we mentioned in the introduction; the technology we developed and tested for this paper could play an important future role in either case.

The spin-1 part of the meson spectrum is more rich. In analogy with the case of QCD, one expects the lightest of such states to generalize the ρ mesons; they transform as a 10 of Sp(4) and have $J^P = 1^-$, and their properties have been studied elsewhere [184]. They have the peculiar property that they can be sourced by two different interpolating operators, with the schematic structures $\bar{\psi}\gamma_\mu\psi$ and $\bar{\psi}\sigma_{\mu\nu}\psi$, respectively. In addition, the generalizations of the a_1 and b_1 from QCD transform as a 5 and a 10 of Sp(4), respectively; these additional states are heavier than the aforementioned 10-plet with $J^P = 1^-$ —see the discussions in Refs. [168,185]. It is worth noticing that some spin-1 singlet mesons of QCD are actually part of these multiplets because of the symmetry-enhancement pattern—noticeably, the particle that corresponds to ω in QCD.

In the presence of nondegenerate fermion masses, $m_u \neq m_d$, the global symmetry breaks further from Sp(4) down to $Sp(2) \times Sp(2) = SU(2) \times SU(2) \sim SO(4)$. Consequently, the multiplets decompose with respect to the smaller flavor symmetry [197]. The 5-plets split into a 4-plet

and a singlet, whereas the 10-plet decomposes into a 6-plet and a 4-plet. This implies that an additional singlet appears in states that would have been a 5-plet in the mass-degenerate theory, such as the PNGBs and the axial vectors. This is the familiar scenario in QCD: In the presence of a mass difference between up and down quark, isospin is explicitly broken, and the flavor-neutral pion π^0 becomes a singlet, with different mass from the charged π^\pm states. The main difference with QCD is that, as the pseudo-reality of the representation results in additional flavor neutral states, which microscopically can be written as di-quark states, the multiplet is enlarged.

This differs for mesons in the 10-plet representation, such as the vector meson. The 10 decomposes in a 4-plet (with the same flavor structure as in the case of the PNGBs) and a 6-plet. The latter consists of two states sourced by ordinary meson operators (in the QCD analogy, they are the ρ^0 and the ω particles with $J^P = 1^-$) and four other states that are sourced by diquark operators. A further splitting of these multiplets is possible, for example, by gauging a U(1) subgroup of the SO(4) symmetry [197], but we do not consider it here.

III. LATTICE SETUP

We perform lattice simulations using the standard plaquette action and standard Wilson fermions [228]. We use the HiRep code [229,230] extended for Sp(2N) gauge theories [231] to generate configurations and to perform the measurements. In the case of degenerate fermions, we use the hybrid Monte Carlo (HMC) [232] algorithm, and for non-degenerate fermions, we use the rational HMC (RHMC) [233] algorithm. The latter case does not guarantee positivity of the fermion determinant. In this case, we have monitored the lowest eigenvalue of the Dirac operator, which we always found to be positive. Thus, we do not see any hints of a sign problem for the fermion masses studied in this work. Results for the nonsinglet spectrum for two fundamental fermions were first reported in Refs. [185,197]. We give simulation details of our ensembles in Tables I and II.

We perform simulations on Euclidean lattices of size $T \times L^3$ and define the bare inverse gauge coupling as $\beta = 8/g^2$. We implement periodic boundary conditions for the gauge fields. For the Dirac fields, we impose periodic boundary conditions in the spatial directions and antiperiodic boundary conditions in the temporal direction.

A. Interpolating operators and two-point functions

We use fermion bilinear operators for sourcing both singlet and nonsinglet mesons. From here onward, with some abuse of notation, we denote as η' and σ , respectively, the pseudoscalar and scalar, flavor-singlet states. While the mesonic sectors are enlarged in Sp(2N) with fundamental fermions, every nonsinglet or singlet state can still be

TABLE I. List of all ensembles with degenerate fermion masses used in this work. We report the number of configurations n_{conf} , the number of the stochastic sources used in the approximation of the all-to-all quark propagator n_{src} , the intervals for fitting the resulting meson correlators I_{meson} , and the average value of the plaquette $\langle P \rangle$. In some cases, we were unable to identify a clear plateau in the effective masses and could not determine the singlet masses. In these cases, we do not report a fit interval. For the singlet mesons, the interval quoted here was used to fit the correlators after subtracting the excited state contributions in the connected pieces and after performing a numerical derivative.

Ensemble	Group	β	m_0	L	T	n_{conf}	n_{src}	$I_{\eta'}$	I_{π}	I_{σ}	$I_{\sigma^{\text{conn}}}$	I_{ρ}	$\langle P \rangle$
SU2B1L1M8	SU(2)	2.0	-0.947	20	32	1020	300	...	(10, 16)	(5, 8)	(7, 10)	(10, 16)	0.56734(2)
SU2B1L1M7	SU(2)	2.0	-0.94	14	24	1851	192	(8, 12)	(8, 12)	(9, 12)	0.56516(3)
SU2B1L1M6	SU(2)	2.0	-0.935	16	32	951	256	(7, 11)	(9, 16)	(9, 16)	0.563654(28)
SU2B1L1M5	SU(2)	2.0	-0.93	14	24	1481	256	(7, 12)	(8, 12)	(9, 12)	0.56245(3)
SU2B1L1M4	SU(2)	2.0	-0.925	14	24	1206	192	(6, 10)	(8, 12)	(9, 12)	0.56119(3)
SU2B1L1M3	SU(2)	2.0	-0.92	12	24	2401	192	(6, 9)	(7, 12)	...	(6, 11)	(8, 12)	0.559983(29)
SU2B1L1M2	SU(2)	2.0	-0.9	12	24	500	128	(6, 9)	(7, 12)	(8, 12)	0.55571(6)
SU2B1L1M1	SU(2)	2.0	-0.88	10	20	2582	128	(5, 8)	(8, 10)	(9, 10)	0.55225(4)
Sp4B3L1M8	Sp(4)	7.2	-0.799	32	40	451	224	...	(15, 20)	(5, 9)	(11, 19)	(15, 20)	0.590862(5)
Sp4B3L1M7	Sp(4)	7.2	-0.794	28	36	504	288	(7, 12)	(10, 18)	...	(11, 16)	(11, 18)	0.590452(7)
Sp4B3L1M6	Sp(4)	7.2	-0.79	24	36	500	320	(7, 12)	(12, 18)	(5, 8)	(10, 16)	(13, 18)	0.590127(9)
Sp4B3L1M5	Sp(4)	7.2	-0.78	24	36	508	384	(6, 12)	(12, 18)	...	(11, 15)	(13, 18)	0.589278(8)
Sp4B3L1M4	Sp(4)	7.2	-0.77	24	36	200	384	(6, 11)	(11, 18)	...	(10, 15)	(12, 18)	0.588460(12)
Sp4B3L1M3	Sp(4)	7.2	-0.76	16	36	200	384	...	(11, 18)	(5, 8)	(9, 14)	(12, 18)	0.587666(25)
Sp4B1L1M7	Sp(4)	6.9	-0.924	24	32	492	320	...	(9, 16)	(4, 7)	(7, 10)	(10, 16)	0.56317(2)
Sp4B1L1M6	Sp(4)	6.9	-0.92	24	32	503	484	...	(7, 16)	(4, 9)	(8, 12)	(8, 16)	0.562075(13)
Sp4B1L2M6	Sp(4)	6.9	-0.92	16	32	176	128	(6, 10)	(9, 16)	(4, 10)	(7, 10)	(9, 16)	0.56212(5)
Sp4B1L1M5	Sp(4)	6.9	-0.91	16	32	435	256	(6, 11)	(8, 16)	...	(7, 9)	(9, 16)	0.55935(3)
Sp4B1L2M5	Sp(4)	6.9	-0.91	14	24	513	256	(5, 10)	(8, 12)	(4, 7)	(9, 12)	(9, 12)	0.55941(3)
Sp4B1L1M4	Sp(4)	6.9	-0.9	16	32	547	512	(6, 10)	(9, 16)	...	(7, 10)	(10, 16)	0.556921(25)
Sp4B1L2M4	Sp(4)	6.9	-0.9	14	24	942	128	(7, 10)	(8, 12)	(4, 9)	(7, 9)	(9, 12)	0.556981(26)
Sp4B1L3M4	Sp(4)	6.9	-0.9	12	24	2904	128	(6, 10)	(8, 12)	(4, 8)	(8, 10)	(9, 12)	0.557009(18)
Sp4B1L2M3	Sp(4)	6.9	-0.89	14	24	461	128	(7, 10)	(8, 12)	(5, 9)	(8, 11)	(9, 12)	0.55468(4)
Sp4B1L3M3	Sp(4)	6.9	-0.89	12	24	1019	320	(6, 10)	(8, 12)	(3, 6)	(7, 11)	(9, 12)	0.55467(3)
Sp4B1L2M2	Sp(4)	6.9	-0.87	12	24	1457	128	(7, 11)	(8, 12)	(5, 8)	(8, 10)	(9, 12)	0.550497(27)
Sp4B1L2M3	Sp(4)	6.9	-0.87	10	20	976	128	(6, 9)	(8, 10)	...	(6, 10)	(8, 10)	0.55068(5)

probed by fermion-antifermion operators, even in the case of nondegenerate fermions. Furthermore, since fermions are moderately heavy, we find such operators are sufficient to study the ground states and for now do not consider others (such as $\pi\pi$ operators, glueballs, or even tetraquarks). We use the operators

$$O_1^{(\Gamma)}(n) = \bar{u}(n)\Gamma d(n),$$

$$O_{\pm}^{(\Gamma)}(n) = (\bar{u}(n)\Gamma u(n) \pm \bar{d}(n)\Gamma d(n))/\sqrt{2}, \quad (4)$$

where $n = (\vec{n}, t)$ denote lattice sites. For pseudoscalar mesons, $\Gamma = \gamma_5$, and we omit the superscript when its

TABLE II. List of all ensembles with nondegenerate fermion masses used in this work. We report the number of configurations n_{conf} , the number of the stochastic sources used in the approximation of the all-to-all quark propagator n_{src} , the intervals for fitting the resulting meson correlators I_{meson} , and the average value of the plaquette $\langle P \rangle$. In some cases, we were unable to identify a clear plateau in the effective masses and could not determine the singlet masses. In these cases, we do not report a fit interval. For the singlet mesons, the interval quoted here was used to fit the correlators after subtracting the excited state contributions in the connected pieces and after performing a numerical derivative.

Ensemble	β	m_0^1	m_0^2	L	T	n_{conf}	n_{src}	$I_{\eta'}$	I_{π^0}	$I_{\pi^{\pm}}$	I_{σ}	$I_{\sigma^{\text{conn}}}$	I_{ρ}	$\langle P \rangle$
Sp4B1L2M4ND1	6.9	-0.9	-0.89	14	24	300	64	(7, 10)	(7, 10)	(8, 14)	(4, 8)	(8, 14)	(8, 14)	0.55583(5)
Sp4B1L2M4ND2	6.9	-0.9	-0.88	14	24	191	128	(7, 10)	(7, 10)	(8, 14)	(4, 8)	(8, 14)	(8, 14)	0.55474(5)
Sp4B1L2M4ND3	6.9	-0.9	-0.87	14	24	400	128	(7, 10)	(7, 10)	(8, 14)	(5, 8)	(8, 14)	(8, 14)	0.55361(4)
Sp4B1L2M4ND4	6.9	-0.9	-0.85	14	24	300	64	(8, 14)	(5, 8)	(8, 14)	(8, 14)	0.55163(4)
Sp4B1L2M4ND5	6.9	-0.9	-0.8	14	24	400	128	(7, 10)	(7, 10)	(8, 14)	...	(8, 14)	(8, 14)	0.54735(4)
Sp4B1L2M4ND6	6.9	-0.9	-0.75	12	24	264	64	(7, 10)	(7, 10)	(8, 12)	...	(8, 12)	(8, 12)	0.54395(6)
Sp4B1L2M4ND7	6.9	-0.9	-0.7	12	24	249	128	(7, 10)	(7, 10)	(8, 12)	...	(8, 12)	(8, 12)	0.54104(6)

value is clear from the context. The pseudoscalar operators O_- and O_1 source the pion 5-plet, and the operator O_+ sources the pseudoscalar singlet, η' . The same pattern persists for the scalar mesons where $\Gamma = 1$, and we use the notation:

$$\begin{aligned} O_{\eta'}(n) &\equiv (\bar{u}(n)\gamma_5 u(n) + \bar{d}(n)\gamma_5 d(n))/\sqrt{2}, \\ O_{\sigma}(n) &\equiv (\bar{u}(n)u(n) + \bar{d}(n)d(n))/\sqrt{2}. \end{aligned} \quad (5)$$

$$\begin{aligned} \langle O_1(n)\bar{O}_1(m) \rangle &= -\text{diagram}, \\ 2\langle O_{\pm}(n)\bar{O}_{\pm}(m) \rangle &= -\text{diagram} - \text{diagram} \pm 2 \text{diagram} + \text{diagram} + \text{diagram} + \text{diagram}. \end{aligned} \quad (6)$$

It can be seen that the singlet mesons only differ from the nonsinglets by the additional disconnected diagrams. In the degenerate limit, they cancel exactly for the O_- operators. In order to determine the mesonic spectrum, we need to determine both the connected and disconnected pieces and then fit the zero momentum correlator,

$$C(t) \equiv \sum_{\vec{n}} \langle O(\vec{n}, t)\bar{O}(\vec{0}, 0) \rangle, \quad (7)$$

on a Euclidean time interval (t_{\min}, t_{\max}) , where the ground state dominates, and its energy—and thus the mass—can be extracted. The different components of $C(t)$ drop off exponentially with their energy $\propto \exp(-E_n t)$, and thus at sufficiently large t , only the ground state remains, as all other states are exponentially suppressed. However, we note that an additional constant term can arise, which is the case for both the η' and the σ meson. In the former case, this can arise due to an insufficient topological sampling of the path integral, and this constant vanishes in the continuum limit [234,235]. For the scalar singlet, σ , this constant arises due to the vacuum contributions, e.g., the fermion condensate, and persists in the continuum limit for vanishing momenta. At large times, the correlator $C(t)$ is then given by

$$\lim_{t \rightarrow \infty} C(t) = a(e^{-mt} + e^{-m(T-t)}) + \langle 0|O|0 \rangle^2, \quad (8)$$

where the second exponential term is due to the lattice periodicity. While in the case of the η' , this constant is small compared to the signal and only affects the correlator at large t , this is not the case for the σ meson. In the scalar case, this constant is several orders of magnitudes larger than the signal, and its removal is a significant challenge.

For vector mesons, $\Gamma = \gamma_i$, and all operators O_1 and O_{\pm} source states in the vector 10-plet [185]. In the nondegenerate case, the flavored multiplet is always probed by O_1 . For the vector mesons, both O_- and O_+ probe the same unflavored multiplet. In the case of the pseudoscalars and scalars, the O_- and O_+ probe distinct singlets. We note that the ensembles studied in this work have moderately heavy fermions—in all cases, the vector meson is lighter than twice the pNGB mass. After performing the required Wick contractions, we arrive at the following two-point correlation functions:

We choose to perform a numerical derivative as proposed in Ref. [236]. The resulting correlator is then antisymmetric with respect to the midpoint $T/2$,

$$\begin{aligned} \tilde{C}(t) &\equiv \frac{1}{2} (C(t-1) - C(t+1)) \xrightarrow{t \rightarrow \infty} a \sinh(mt) \\ &\times (e^{-mt} - e^{-m(T-t)}). \end{aligned} \quad (9)$$

In order to determine the Euclidean time interval for fitting, we use an effective mass $m_{\text{eff}}(t)$ defined by

$$\frac{\tilde{C}(t-1)}{\tilde{C}(t)} = \frac{e^{-m_{\text{eff}}(t) \cdot (T-t+1)} \pm e^{-m_{\text{eff}}(t) \cdot (t-1)}}{e^{-m_{\text{eff}}(t) \cdot (T-t)} \pm e^{-m_{\text{eff}}(t) \cdot t}}, \quad (10)$$

where the + is used for periodic correlators, and the - sign in case of antiperiodic correlators with respect to the lattice midpoint $T/2$. We determine (t_{\min}, t_{\max}) by visually inspecting the effective mass and identifying a plateau at large times t . We restrict ourselves to ensembles where the plateau persists over four or more time slices. We then perform a fit of a single exponential term to the correlator $\tilde{C}(t)$ for the mesons. In Appendix A, we compare this method to computing the additional constant $\langle 0|O|0 \rangle^2$ directly, without the use of a numerical derivative.

For the pseudoscalar sector in the nondegenerate $N_f = 1 + 1$ theory, both the π^0 and η' are pseudoscalar singlets, and the η' is not a ground state. Thus, we need to perform a variational analysis by computing the correlation matrix of the operators O_{π^0} and $O_{\eta'}$ and solve the resulting generalized eigenvalue problem (GEVP). In the minimal operator basis of (4) and (5), the cross-correlator are diagrammatically given by

$$2\langle O_+(n)\bar{O}_-(m)\rangle = -\left(\text{diagram 1} - \text{diagram 2}\right) + \left(\text{diagram 3} - \text{diagram 4}\right). \quad (11)$$

In the mass-degenerate limit, the cross-correlator vanishes, and the η' becomes the ground state of the pseudoscalar singlet sector, whereas the π^0 becomes part of the pNGB multiplet. Note the presence of connected diagrams in the cross-correlator. This implies that even in the limit of large fermion masses—which suppresses the disconnected pieces—the cross-correlator remains large for large mass differences, i.e., a system with heavy-light properties. Thus, sizeable mixing effects are expected to occur.

For a heavy-light system, a more diagonal basis is obtained by using the operators $O_A^{PS} = \bar{u}\gamma u$ and $O_B^{PS} = \bar{d}\gamma d$. The corresponding cross-correlator vanishes as the heavier fermion mass approaches infinity and is given by

$$\langle O_A^{PS}(n)\bar{O}_B^{PS}(m)\rangle = \text{diagram 5}. \quad (12)$$

B. Variance reduction techniques

In order to obtain the full singlet two-point functions, we need to measure both the connected and disconnected pieces in Eq. (6). The disconnected diagrams in particular are very noisy, and the signal is already lost at small to intermediate t where contaminations from excited states are non-negligible. A direct determination of the ground state mass at large t is thus not possible. We can circumvent this problem by removing the contributions of excited states in the singlet correlators manually. This is straightforward for the connected pieces. There, the signal for the connected pseudoscalar and vector mesons persists for all time slices t , and in the case of the connected piece of the scalar meson, we still have a signal up to large t . We fit the connected piece at large times (see Tables I and II for our choice of fit intervals) to a single exponential

$$C_{\text{conn}}^{1\text{ exp}}(t) = A_0(e^{-m_{\text{conn}}t} + e^{-m_{\text{conn}}(T-t)}), \quad (13)$$

and replace the full connected piece by the ground state correlator [237], where A_0 and m_{conn} are the fit parameters, such that

$$C_{\eta'}^{1\text{ exp}}(t) = C_{\pi,\text{conn}}^{1\text{ exp}}(t) + C_{\eta',\text{disc}}(t), \quad (14)$$

$$C_{\sigma}^{1\text{ exp}}(t) = C_{\sigma,\text{conn}}^{1\text{ exp}}(t) + C_{\sigma,\text{disc}}(t). \quad (15)$$

We find that the excited state contributions in the connected pieces are the dominant ones, and removing them shows a much earlier onset of a plateau in the effective masses. The

underlying assumption for these correlators is that the excited state contributions of full and connected pieces are indistinguishable within data quality as was noted in [209]. This is not guaranteed *a priori*. However, we find that the excited state contributions in the connected pieces are indeed the dominant ones. In Appendix B, we show that our results obtained by subtracting the connected excited state contributions through a fit at larger times produces the same results as using smeared operators for the connected pieces with more overlap with the ground state.

Note that this technique is not applicable to the non-degenerate case, as the η' is no longer a ground state and some relevant information is actually encoded in the excited states. Thus, we will not apply this technique there.

The evaluation of disconnected pieces requires all-to-all propagators. We use $Z_2 \times Z_2$ noisy sources with spin and even-odd dilution [238]. We typically use $\mathcal{O}(100)$ distinct noise vectors. The connected pieces are evaluated using stochastic wall sources. Uncertainties are estimated using the jackknife method.

IV. RESULTS

Here we report the main results of our numerical investigations on the mass spectrum of flavor-singlet pseudoscalar and scalar mesons, obtained using the techniques discussed in the previous section. We focus on the Sp(4) theory coupled to two fundamental dynamical fermions, but for degenerate fermions, we supplement it with the SU(2) theory with the same matter content. In the case of the pseudoscalar singlet, we further compare to the existing literature on lattice results for the SU(3) theory.

A. Pseudoscalar singlet in SU(2) and Sp(4) with $N_f = 2$

Our results for the mesons with degenerate fermions are tabulated in Table III. All the ensembles satisfy the condition $m_{\pi}L > 6$, suggested by the observations in Ref. [184] for Sp(4), and in Ref. [166] for SU(2), that the size of finite volume corrections to the low-lying spectrum for flavored mesons is of the order of 1–2% at $m_{\pi}L \simeq 6$ and becomes much smaller for the larger volumes, as it is exponentially suppressed with the volume. This observation is also confirmed by our measurements of m_{π} and m_{ρ} at different volumes in the Sp(4) theory with $\beta = 6.9$ by varying the bare fermion mass, m_0 . Finite volume corrections to $m_{\eta'}$ are compatible with the statistical uncertainties and expected to be less than 2%, which we estimated from the most precise results available, for

TABLE III. The light spectrum of SU(2) and Sp(4) with degenerate fermions: the lightest flavored pseudoscalar, π , and vector, ρ , and flavor-singlet pseudoscalar, η' , and scalar, σ , mesons, measured in different ensembles. All dimensionful quantities are given in lattice units and the omission of the lattice spacing $a = 1$ is understood. The missing entries for $m_{\eta'}$ and/or m_{σ} are due to the measurements not fulfilling the fitting criteria discussed in the main text.

	β	m_0	L	T	$m_{\pi}L$	m_{π}/m_{ρ}	m_{π}	m_{ρ}	$m_{\eta'}$	m_{σ}
SU(2)	2.0	-0.947	20	32	7.47(3)	0.690(7)	0.3735(13)	0.540(5)	...	0.53(4)
SU(2)	2.0	-0.94	14	24	6.40(2)	0.746(6)	0.4576(14)	0.612(4)	0.67(6)	...
SU(2)	2.0	-0.935	16	32	7.91(2)	0.767(5)	0.4946(14)	0.644(4)	0.60(3)	...
SU(2)	2.0	-0.93	14	24	7.491(19)	0.787(4)	0.5350(14)	0.679(3)	0.65(3)	...
SU(2)	2.0	-0.925	14	24	7.999(19)	0.806(4)	0.5713(14)	0.708(3)	0.634(16)	...
SU(2)	2.0	-0.92	12	24	7.323(10)	0.8210(19)	0.6102(8)	0.7432(14)	0.665(9)	...
SU(2)	2.0	-0.9	12	24	8.620(17)	0.862(3)	0.7183(14)	0.832(2)	0.770(16)	...
SU(2)	2.0	-0.88	10	20	8.120(11)	0.885(2)	0.8120(11)	0.9169(19)	0.842(5)	...
Sp(4)	7.2	-0.799	32	40	8.087(16)	0.668(4)	0.2527(5)	0.377(2)	...	0.36(5)
Sp(4)	7.2	-0.794	28	36	8.072(11)	0.710(2)	0.2882(4)	0.4055(11)	0.397(16)	...
Sp(4)	7.2	-0.79	24	36	7.505(19)	0.742(6)	0.3127(8)	0.421(3)	0.387(13)	0.56(6)
Sp(4)	7.2	-0.78	24	36	8.882(17)	0.793(4)	0.3700(7)	0.466(2)	0.418(7)	...
Sp(4)	7.2	-0.77	24	36	10.16(2)	0.829(5)	0.4236(10)	0.510(3)	0.456(8)	...
Sp(4)	7.2	-0.76	16	36	7.544(17)	0.850(4)	0.4715(10)	0.554(2)	...	0.64(12)
Sp(4)	6.9	-0.924	24	32	8.208(12)	0.663(2)	0.3420(5)	0.5157(17)	...	0.46(3)
Sp(4)	6.9	-0.92	24	32	9.356(12)	0.7036(17)	0.3898(5)	0.5540(12)	...	0.42(2)
Sp(4)	6.9	-0.92	16	32	6.22(2)	0.696(7)	0.3889(14)	0.558(5)	0.49(3)	0.45(6)
Sp(4)	6.9	-0.91	16	32	7.817(19)	0.769(5)	0.4885(12)	0.634(4)	0.560(14)	...
Sp(4)	6.9	-0.91	14	24	6.86(2)	0.766(6)	0.4902(16)	0.639(5)	0.541(9)	0.41(3)
Sp(4)	6.9	-0.9	16	32	9.006(13)	0.815(3)	0.5629(8)	0.690(2)	0.611(9)	...
Sp(4)	6.9	-0.9	14	24	7.897(14)	0.812(3)	0.5641(10)	0.694(2)	0.619(16)	0.57(4)
Sp(4)	6.9	-0.9	12	24	6.796(9)	0.809(2)	0.5663(8)	0.6994(18)	0.610(6)	0.55(2)
Sp(4)	6.9	-0.89	14	24	8.813(19)	0.843(4)	0.6295(13)	0.746(3)	0.69(2)	0.57(9)
Sp(4)	6.9	-0.89	12	24	7.581(15)	0.841(3)	0.6318(12)	0.751(3)	0.661(9)	0.62(7)
Sp(4)	6.9	-0.87	12	24	8.925(10)	0.878(2)	0.7437(9)	0.8468(17)	0.782(13)	0.80(15)
Sp(4)	6.9	-0.87	10	20	7.470(16)	0.871(3)	0.7470(16)	0.857(3)	0.764(9)	...

$m_0 = -0.9$, if $m_{\pi}L \gtrsim 6$. We therefore safely neglect finite volume corrections to $m_{\eta'}$ in the following.

In Fig. 1, we present our measurements of the ratios between the mass of the η' meson and that of the pseudoscalar nonsinglet π , as a function of m_{π}/m_{ρ} . For reference, we indicate the mass of the vector meson ρ by a solid line. In the Sp(4) theory, we find that the pseudoscalar singlet is consistently heavier than the nonsinglet, over the range of $0.7 \lesssim m_{\pi}/m_{\rho} \lesssim 0.9$, but lighter than the vector mesons. While in the lightest and finest ensembles, the hierarchy between the pseudoscalar singlet and vector mesons is not yet clearly resolved, the emerging trend is that $m_{\eta'}/m_{\pi}$ slowly increases as m_{π} decreases in this mass regime and approaches m_{ρ}/m_{π} for $m_{\pi}/m_{\rho} \lesssim 0.75$. We do not observe an appreciable difference in the mass ratios obtained with the two different values of β , within the quoted one-sigma error bars. We find a similar trend in the SU(2) theory, as shown in the right panel of Fig. 1. Since in this case only one fairly coarse lattice is considered, we cannot comment on the size of finite lattice spacing effects.

The smallness of lattice artifacts in the ratios of meson masses is somewhat surprising, as the lattice spacing for $\beta = 7.2$ is approximately 40% smaller than for $\beta = 6.9$ [184]. To assess this point, we present the meson masses in

units of the gradient flow scale w_0 , which defines a common scale in the continuum theory, and which we use also to compute the topological charge Q —see Appendix A. We borrow the definition and measurements of the gradient flow scale w_0 from Ref. [184] and refer the reader to that publication for details. The left panel of Fig. 2 shows that both the mass of the pseudoscalar singlet and the vector mesons receive significant corrections from the finite lattice spacing. By comparing with Fig. 1, we see that such corrections to $m_{\pi}w_0$ and $m_{\eta'}w_0$ happen to have the same sign and similar sizes, which cancel out in the mass ratios. We observe the same pattern for the mass ratio of m_{ρ} and $m_{\eta'}$, as depicted in the right panel of Fig. 2.

B. Pseudoscalar singlets in Sp(4) with $N_f = 1 + 1$

For nondegenerate fermions, the theory contains two flavor-singlet pseudoscalar mesons, the η' as well as the flavor-diagonal PNCB, π^0 . To understand the effects of (explicit) flavor-symmetry breaking on the low-lying spectrum, we first choose the ensemble for degenerate fermions with $\beta = 6.9$ and $m_0 = -0.9$ and vary the bare mass of one of the Dirac fermion, $m_0^{(2)} \geq m_0$, for which we effectively increase its mass, while keeping that of the other fixed,

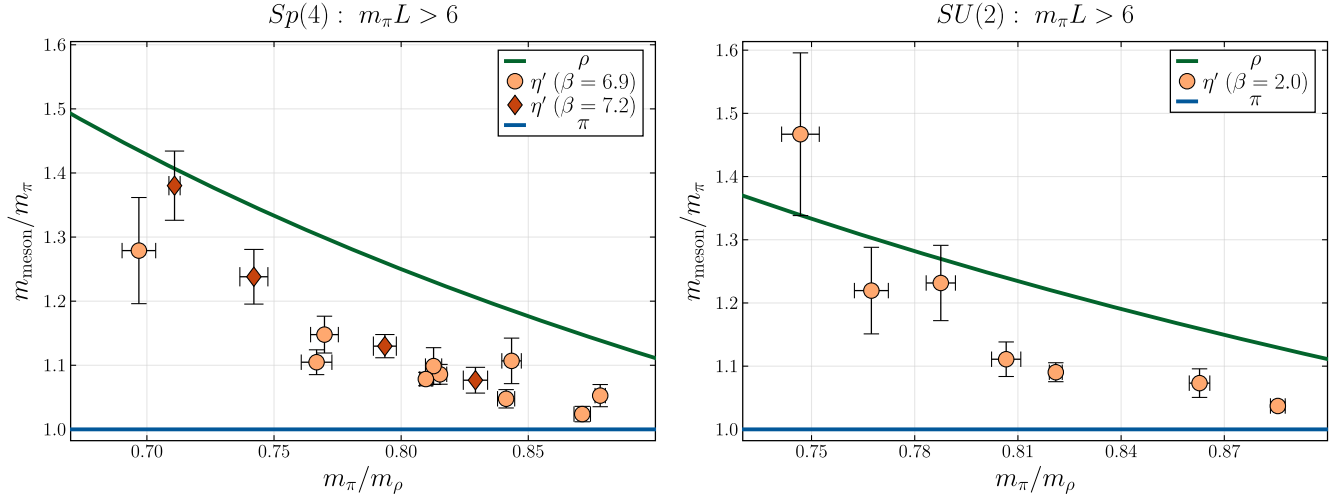


FIG. 1. Left panel: Mass ratios m_{meson}/m_π for pseudoscalar and vector mesons, including the flavor-singlet pseudoscalar η' , in the $Sp(4)$ gauge theory with $N_f = 2$ Dirac flavors of fermions in the fundamental representation measured at the two values of the inverse coupling $\beta = 6.9$ and 7.2 . Right panel: The same plot but in the $SU(2)$ gauge theory at $\beta = 2.0$. The green solid lines $m_\rho/m_\pi = 1/x$ are displayed for reference.

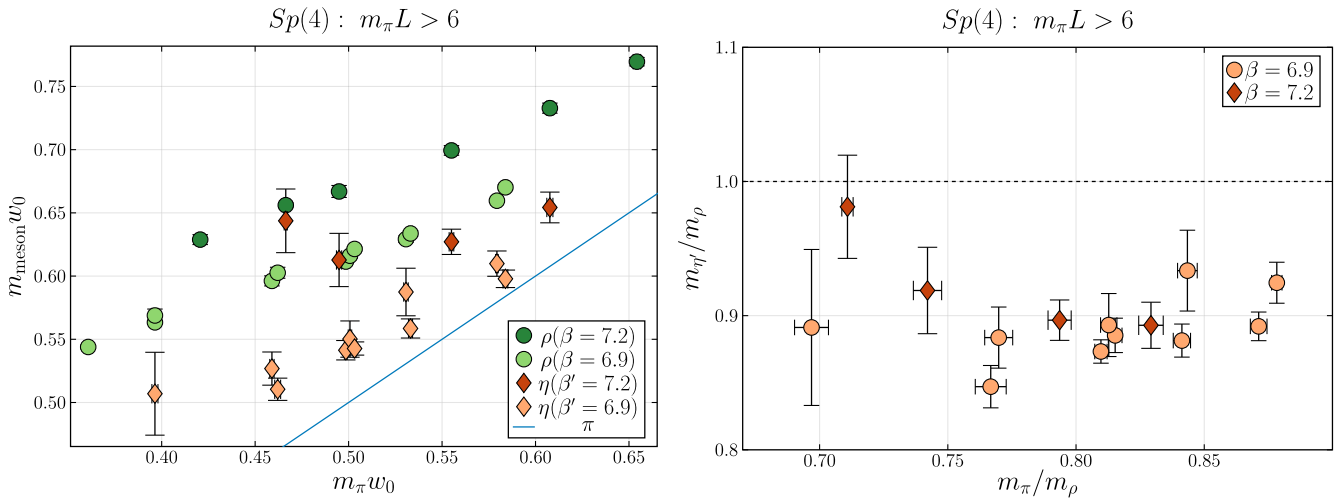


FIG. 2. Left panel: Same data as in the left panel of Fig. 1, but now masses are given in units of the gradient flow scale w_0 . The blue solid line $w_0 m_\pi = x$ is displayed for reference. Right panel: Mass ratio between of the vector mesons ρ and the scalar singlet η' .

$m_0^{(1)} = m_0$. We summarize the numerical results in Table IV. In the table, we also present the mass of the flavor-singlet PNGB obtained by computing only the connected diagrams after dropping the last three terms in Eq. (6), which we denote by $m_{\pi_c^0}$. Within the generally larger uncertainties, we find no statistically appreciable difference between m_{π^0} and $m_{\pi_c^0}$, which supports the connected-only approximation considered in Ref. [197].

In the left panel of Fig. 3, we show the meson masses, as a function of the flavoured pNGBs mass m_{π^\pm} . In the mass-degenerate limit, we recover the mass hierarchy of Sec. IV A, as expected. As we increase one of the fermion masses, we observe a clear separation between flavored mesons and the

unflavored π^0 as well as the unflavored vector mesons ρ^0 , with the former being heavier than the latter. At the same time, the pseudoscalar singlet η' , becomes heavier. This effect leads to an inversion of the mass hierarchy between the vector mesons ρ^\pm, ρ^0 , and the η' meson, and the η' becomes heavier than any other meson considered here.⁵

A couple of cautionary remarks should be added. First of all, we are in a moderately heavy mass regime, with

⁵This is qualitatively different from the preliminary results in [225], where the mixing between the pseudoscalar singlets was neglected, and the excited state subtraction of Sec. III B was incorrectly applied to the nondegenerate theory.

TABLE IV. Results for the light spectrum with nondegenerate fermions: the flavored pseudoscalar π^\pm and vector ρ^\pm , and the flavor-singlet pseudoscalar η' , π^0 , vector ρ^0 and scalar σ mesons. All dimensionful quantities are given in lattice units ($a = 1$). Missing entries for $m_{\eta'}$ or m_σ denote measurements that do not fulfill the fitting criteria discussed in the main text. We furthermore report the mass of the flavor-singlet pseudo-Goldstone $m_{\pi_c^0}$ in the connected-only approximation.

β	$m_0^{(1)}$	$m_0^{(2)}$	L	T	$m_{\pi_c^0}$	$m_{\pi_c^0}$	m_{π^\pm}	m_{ρ^0}	m_{ρ^\pm}	$m_{\eta'}$	m_σ
6.9	-0.9	-0.89	14	24	0.60(2)	0.597(2)	0.596(2)	0.723(3)	0.719(4)	0.65(4)	0.45(6)
6.9	-0.9	-0.88	14	24	0.63(3)	0.6261(18)	0.628(2)	0.749(2)	0.745(3)	0.69(4)	0.51(8)
6.9	-0.9	-0.87	14	24	0.664(17)	0.6510(14)	0.6606(17)	0.7731(19)	0.775(2)	0.77(3)	0.69(14)
6.9	-0.9	-0.85	14	24	...	0.6889(19)	0.709(2)	0.813(3)	0.813(4)	...	0.51(12)
6.9	-0.9	-0.8	14	24	0.75(2)	0.7563(16)	0.8277(18)	0.879(2)	0.922(3)	0.93(2)	...
6.9	-0.9	-0.75	12	24	0.79(3)	0.803(4)	0.921(4)	0.927(6)	1.005(5)	1.04(3)	...
6.9	-0.9	-0.7	12	24	0.83(3)	0.833(4)	0.996(3)	0.954(5)	1.073(5)	1.15(3)	...

$m_{\pi_c^0}/m_{\rho^0} \sim 0.85$. Secondly, some meson masses for heavy ensembles sit close to the lattice cutoff and thus could be affected by significant lattice artifacts.

For the heaviest fermion masses, the mass difference between the η' and the π^0 is approximately twice the mass difference between the π^0 and the π^\pm 's. This indicates that the mass differences are driven by the valence fermion masses.

In this regime, the singlet π^0 and the nonsinglet ρ^0 approach an approximate one-flavor theory—see, e.g., Ref. [170] for lattice results on the low-lying spectrum in the SU(2) gauge theory with one Dirac fermion.

In the right panel of Fig. 3, we plot the meson masses as a function of the quark mass ratio, defined through the partially conserved axial current (PCAC) relation. We

identify the average quark mass in the flavored pion π^\pm through the relation

$$\begin{aligned}
 m_{\text{avg}}^{\text{PCAC}} &= \lim_{t \rightarrow \infty} \frac{1}{2} \frac{\partial_t C_{\gamma_0 \gamma_5 \gamma_5}(t)}{C_{\gamma_5}(t)} \\
 &= \lim_{t \rightarrow \infty} \frac{1}{2} \frac{\partial_t \int d^3 \vec{x} \langle (\bar{u}(\vec{x}, t) \gamma_0 \gamma_5 d(\vec{x}, t))^\dagger \bar{u}(0) \gamma_5 d(0) \rangle}{\int d^3 \vec{x} \langle (\bar{u}(\vec{x}, t) \gamma_5 d(\vec{x}, t))^\dagger \bar{u}(0) \gamma_5 d(0) \rangle}.
 \end{aligned} \tag{16}$$

The unrenormalized PCAC quark mass ratio m_d/m_u for nondegenerate fermions is extracted by performing an additional measurement of the PCAC average mass at degeneracy. For a detailed discussion of the PCAC relation and different ways to calculate it, we refer to Ref. [239].

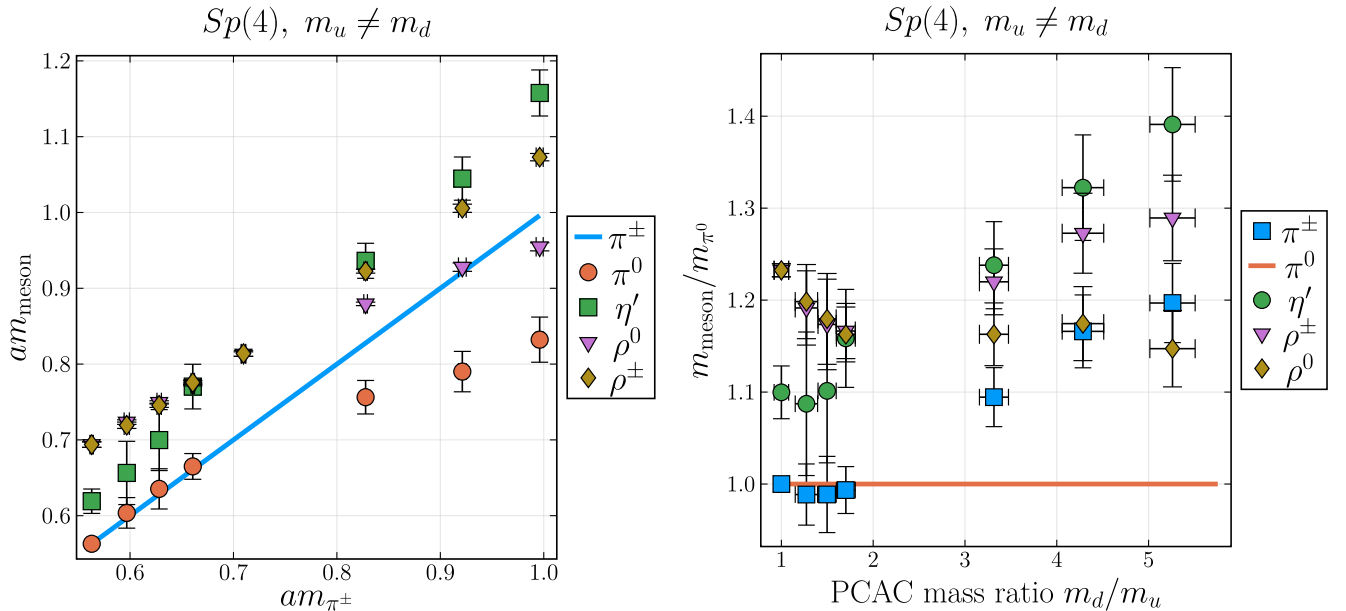


FIG. 3. Masses of the lightest nonsinglet mesons as well as the pseudoscalar singlet meson in the Sp(4) theory with nondegenerate Dirac fermions. We fix the lattice coupling and one of the bare fermion masses to $\beta = 6.9$ and $m_0^{(1)} = -0.9$, respectively, while varying the other bare fermion mass. In the left panel, we display our results as a function of the flavoured pion mass, while in the right panel, we show them as a function of ratio of the PCAC fermion masses in units of the π^0 mass.

C. Scalar singlet in Sp(4) with $N_f = 2$

In the case of the scalar singlet, σ , the signal is consistently worse than for the other states discussed so far. Furthermore, we see signs of finite spacing effects, shown in Fig. 4. For Sp(4) on the coarse $\beta = 6.9$ lattices, we observe a light σ state, of mass comparable to the mass of the π . This pattern persists over the entire mass range considered. On finer lattices, for $\beta = 7.2$, the mass of the σ increases and is heavier than the PGNBs and comparable to the vector meson, though with much larger statistical errors and still below the $\pi\pi$ threshold.

These results suggest the existence of larger finite-spacing effects that affect the mass of the scalar singlet. Yet, some caution should be used because, due to the large noise in our signal, the mass is extracted from much shorter times on the finer lattices and may therefore also be more severely affected by excited-state contamination and possibly other systematics. Nevertheless, even for the finer lattice, the σ state is lighter than its nonsinglet counterpart, suggesting that further studies are still needed. The scalar singlet might be a stable light meson at moderately heavy fermion masses and thus phenomenologically relevant.

D. Comparison to SU(3) with $N_f = 2$

In Fig. 5, we show a compilation of the available data published on the pseudoscalar singlet for the SU(3) theory with $N_f = 2$ (upper panels) as well a comparison of our results for Sp(4) and SU(2) to the available data for SU(3) (lower panels). In some cases, the measurement has been performed using different methods in the analysis, or

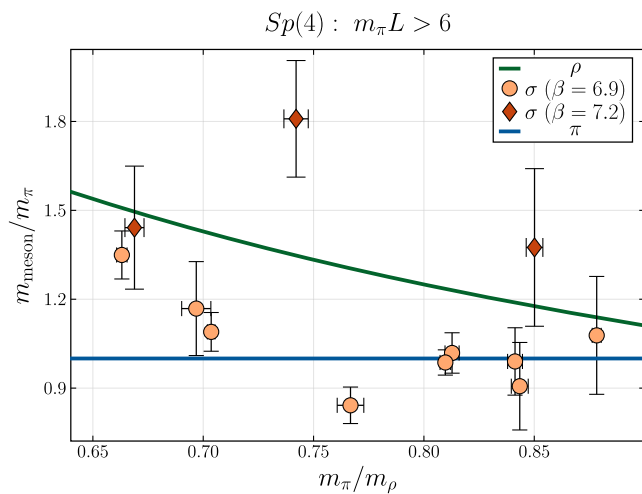


FIG. 4. Mass of the σ meson with degenerate fermions in the Sp(4) theory. We find signs of finite spacing effects even when considering ratios of hadron masses. On the coarser lattice, the scalar singlet appears to be quite light, in some cases, even lighter than the π . For the finer lattice, this changes drastically, and the scalar singlet σ is usually heavier than the vector meson ρ , though still below the two- π threshold. The green solid line $m_\rho/m_\pi = 1/x$ is displayed for reference.

different operators have been used to study the same mesons (e.g., the mass of the η' has been obtained from pure gluonic operators as well as the usual fermionic operators, or in the case of twisted mass fermions, the nonsinglet mesons include isospin breaking effects) and sets of results are available. In such cases, we have chosen the results that are closest to the standard determination of directly fitting the correlator of a pure fermionic operator. When this was not possible, we quote the largest and smallest values of $m_i \pm \Delta m_i$ of all measurements i and symmetrize the uncertainties. The data depicted in Fig. 5 has been taken from the UKQCD collaborations (denoted by UKQCD1 [202,203] and UKQCD2 [207]); the SESAM/T χ L collaboration [204,205]; the CP-PACS collaboration [206]; the RBC collaboration using domain-wall fermions [210]; the CLQCD collaboration using Wilson clover fermions on anisotropic lattices [211]; the ETMC collaboration (denoted by ETMC1 [208,209] and ETMC2 [212,213]); and from the analysis of η' -glueball mixing (denoted by Beijing [214]).

In all but the very lightest ensemble (and one obvious outlier at heavy fermion mass), the vector meson, ρ , is found to be heavier than the pseudoscalar singlet, η' . The authors of Ref. [213] point out that in the lightest ensemble, the ρ particle might be unusually light due to the small number of energy levels below the inelastic threshold in the determination of the $\pi\pi$ phase shift. It is lighter than their extrapolation to the physical point at which $m_\rho = 786(20)$ and even lighter than their extrapolation to the chiral limit. The mass dependence of the η' meson was found to be flat, and an extrapolation in Ref. [212] to the physical point gave $m_{\eta'} = 772(18)$ MeV. This is in contrast to SM QCD where the η' is significantly heavier—the current PDG lists $m_{\eta'}^{\text{PDG}} = 957.78(6)$ MeV [240], which is in agreement with recent SU(3), $N_f = 2 + 1$ lattice results of $m_{\eta'} = 929.9^{(47.5)}_{(21.0)}$ [241]. This suggests it is the contribution of the s quark that leads to the heavier mass. This can be understood in a quark model of the pseudoscalar singlet mesons based on approximate SU(3)_F flavor symmetry [242–244], which was applied to early lattice results in [203].

The bottom line of this brief survey is that in the regime of moderately large fermion masses, the pattern of ground state masses observed so far in SU(3) is quite similar, both qualitatively and quantitatively, to our findings in the Sp(4) case as can be seen in the lower panels of Fig. 5. The gauge group and modified chiral structure do not seem to have a very strong impact on mass of the η' .

E. Possible phenomenological implications

Our results provide evidence that the singlet sector, computed for moderately large fermion masses in the Sp(4) theory, is not dissimilar from what is observed in the SU(2) and SU(3) theories coupled to two fundamental fermions. In particular, both pseudoscalar and scalar singlets are light

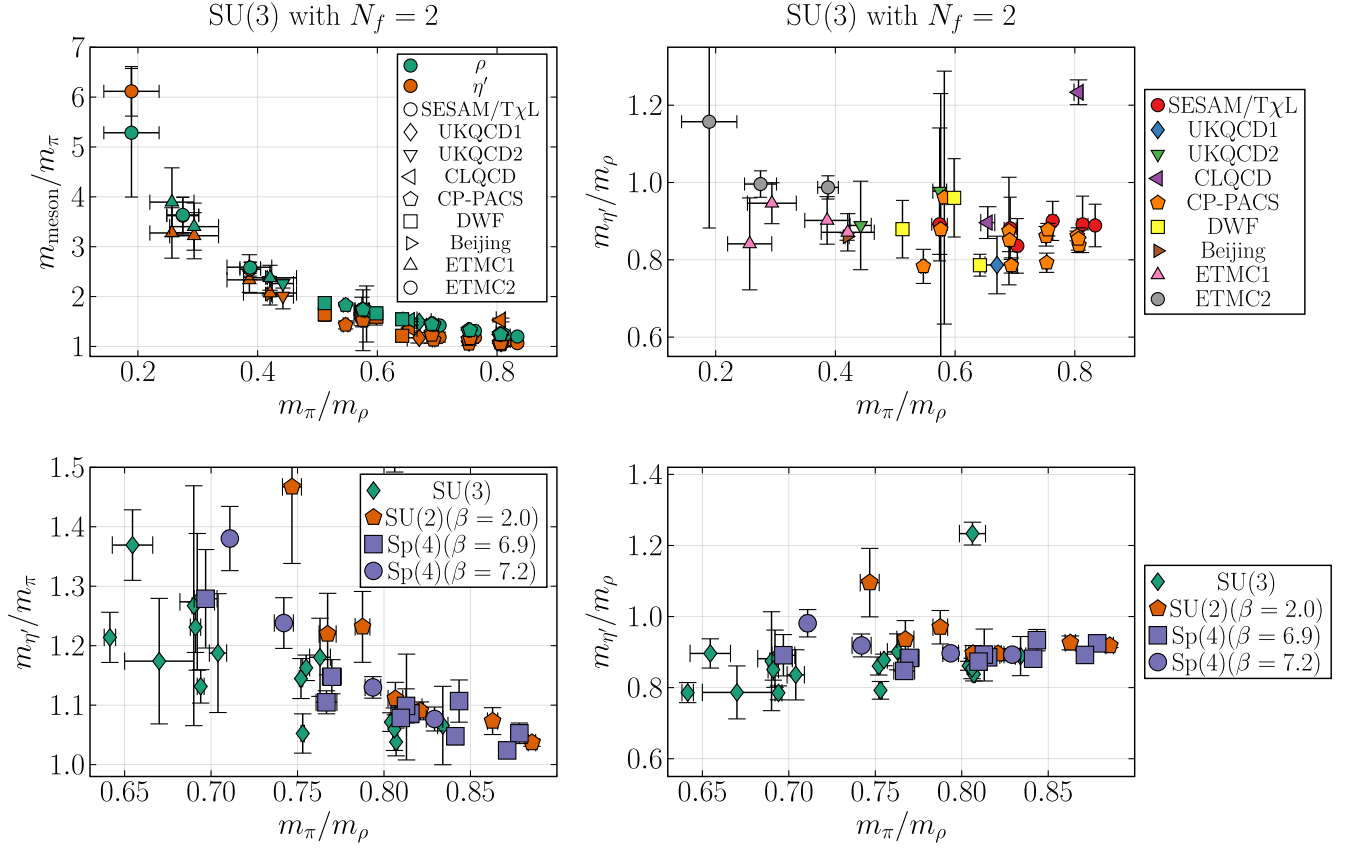


FIG. 5. Comparison to the available lattice data in SU(3) with two fundamental fermions. The upper panels depict all available lattice results in SU(3). In the upper left panel, the green markers denote the vector meson ρ and the orange ones the pseudoscalar singlet η' . The different marker shapes denote the different collaborations. We see that the η' is lighter than the vector mesons almost everywhere. In the upper right panel, we directly plot the ratio $m_{\eta'}/m_\rho$. In the lower panels, we compare the SU(3) results to our Sp(4) and SU(2) data. In the lower left panel, we show the ratio $m_{\eta'}/m_\pi$ as a function of m_π/m_ρ for values of $m_\pi/m_\rho \approx 0.7$ and larger. In the lower right plot, we compare the different results of the ratio $m_{\eta'}/m_\rho$.

enough to be stable against decay into Goldstone bosons, over a fermion-mass range within which also the flavored vector mesons would not decay. We now present a few examples of potential implications for phenomenological models for which these theories can be invoked to yield a short-distance completion.

Firstly, because the flavor singlets are not much heavier than the flavored mesons, if a model of this type were used as part of a hidden valley scenario, or a new dark sector, these states would then only decay via a mediator mechanism into standard model particle, but not strongly, and would be long lived. Their lifetime and branching fractions would be determined by the detailed structure of the coupling to the standard-model fields. They are unlikely to be long lived enough to play a significant role in a model explaining current dark matter density, yet they can easily appear as long-lived particles in experiments [245–248], and hence the existence of a new dark sector containing this theory is experimentally testable.

Other possible observable effects in this context could arise because the singlets can enhance interaction

cross-sections, as virtual particles, affecting processes even below production threshold. They can therefore play a relevant role for dark matter self-interactions [249]. Their effect could even affect form factors relevant to direct detection experiments [250]. Depending on details, they could also offer a possibility to create indirect detection signatures in cases of high dark matter densities. Finally, both singlets can serve, together or individually, as a Higgs portal, removing the need for an independent messenger.

In the alternative context of composite Higgs scenarios, in which the PNBs provide the longitudinal components of the W bosons and Z boson, as well giving rise to the experimentally observed Higgs boson, the pseudoscalar singlet can become a surprisingly strong limiting factor [251]. As its signature is possibly similar to that of the pseudoscalar Higgs in the minimal supersymmetric standard model, or in classes of two-Higgs doublet models, strong exclusion limits already exist, both for a pseudoscalar Higgs heavier and lighter than the standard model Higgs. To avoid these bounds requires one to open up substantially the mass gap between the scalar and

pseudoscalar singlets, but in our measurements, we always observe the opposite hierarchy.

V. SUMMARY

We have presented the results of the first dedicated lattice study of flavor singlet meson states in the Sp(4) theory coupled to two (Wilson-Dirac) fundamental dynamical fermions. We have computed the masses of the lightest pseudoscalar and scalar singlets in a portion of parameter space in which the fundamental fermion are moderately heavy. We have considered both the case of degenerate and of nondegenerate masses for the fermions. The continuum limit of this theory, in the range of parameters explored, is of interest because it provides the ultraviolet completion of several proposals for new physics extensions of the standard model, in the contexts of composite Higgs models and strongly interacting dark matter. In order to perform this study, we implemented in our analysis state-of-the-art techniques to account for the contribution of disconnected diagrams to correlation functions involving flavor singlets.

We observe that the qualitative (and to large extent even the quantitative) features of the mass spectrum we find in this Sp(4) theory are similar to those of SU(2) and SU(3) theories with the same field content, in comparable ranges of parameter space. More specifically, the mass range of the singlet states, in particular of the lightest pseudoscalar, is comparable to the masses of the lightest flavored mesons, at least for our choices of fermion masses. This remains true also in the mass-nondegenerate case.

Our findings suggest that the singlet sector cannot be neglected in phenomenological studies of models that have their dynamical, short-distance origin in this theory. However, notwithstanding the technical implementation of several techniques to enhance the signal-to-noise ratio in our measurements, and the comparatively large statistics provided by our numerical ensembles, we have also found that the observables are affected by large lattice artifacts, especially in the case of the scalar singlet. While we have noticed that taking certain ratios of masses reduces drastically the size of such effects, if phenomenological considerations require precision measurements for the mass spectrum, then this would provide strong incentive to further improve this study, in particular in order to better understand the approach to the continuum limit.

On more general and abstract theoretical ground, the similarity of our main results with the SU(N) cases strongly suggests that the altered chiral structure and gauge group has limited impact on the underlying dynamics. On the one hand, this might be expected in a gauge theory with small number of moderately heavy fermions. On the other hand, though, by extending this kind of analysis to different N and/or further gauge groups, we envision to be able to gain quantitative understanding the relevance of gauge dynamics for hadron dynamics beyond group-theoretical, and thus nondynamical, aspects.

The data generated for this manuscript can be downloaded from Ref. [252], and the software used to analyze and present it is similarly available from Ref. [253].

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APPENDIX A: CONSTANT CONTRIBUTIONS TO THE CORRELATORS

In Sec. III A, we noted the occurrence of constant terms in the propagators of both the pseudoscalar singlet η' meson and the scalar singlet σ meson. This makes it difficult to determine when the excited states in the meson correlator are sufficiently suppressed and a fit can be performed. As shown in Eqs. (6) and (8), we can circumvent this issue either by direct calculation of $\langle 0|O|0\rangle$ or by performing a numerical derivative. Once we determine the interval $[t_i, t_f]$ where only the ground state contributes, we can also fit the correlator to

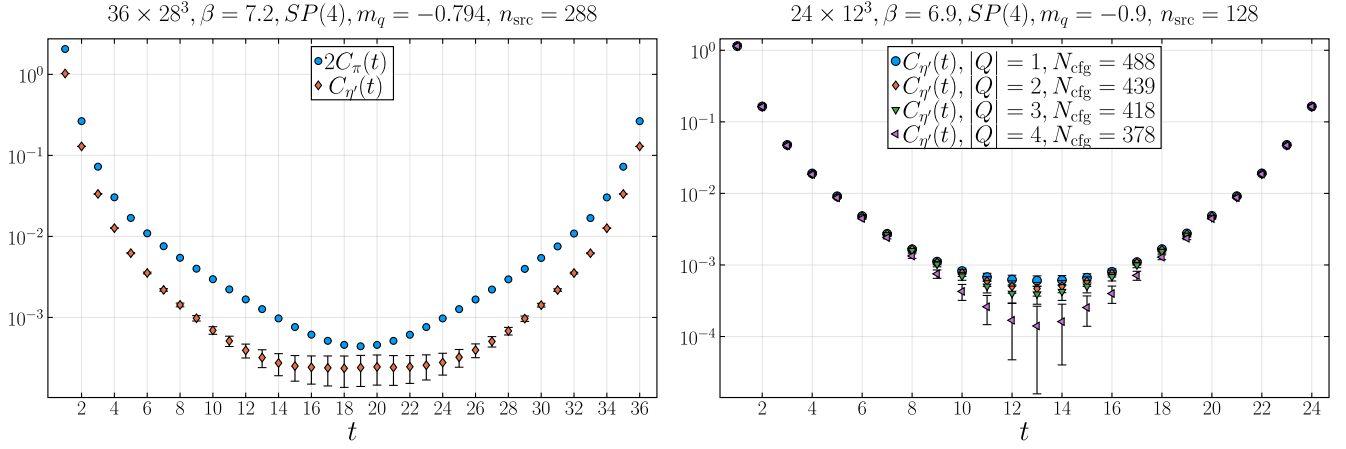


FIG. 6. Left: Correlator of the pseudoscalar nonsinglet π and the pseudoscalar singlet η' . For visual clarity, we multiplied the π correlator by a constant factor of 2. At large times, the singlet correlator shows a constant term, while this is absent for the nonsinglet case. Right: Correlators of the pseudoscalar singlet for fixed values of the topological charge Q . The constant term shows signs of a dependence on Q . While the constant is not significantly different for any two examples shown here, the constant appears to be increasing with $|Q|$.

an exponentially decaying term plus a constant. In Fig. 6, we give an example of the correlator for the flavor singlet, η' , and the flavored mesons, π . The flavor-singlet correlator shows a constant term at large Euclidean times, while such a contribution is absent for the π meson. This is expected to occur for the disconnected pieces in a finite volume and at finite statistics if the topological sampling is insufficient [212,234]. Then, the constant takes the form

$$\text{const} \propto \frac{1}{V} \left(\frac{Q^2}{V} - \chi_t - \frac{c_4}{2\chi_t V} \right) + \mathcal{O}(V^{-3}) + \mathcal{O}(e^{-m_\pi|x|}), \quad (\text{A1})$$

where V denotes the spatial volume of the lattice, χ_t is the topological susceptibility, and c_4 is a coefficient from a saddle-point expansion. Algorithms that provide an ergodic exploration of topological sectors in Yang-Mills theories and are compatible with our prescription for the boundary conditions have recently been introduced (see, e.g., [256–258]). However, they are generally computationally costly, and their adaptation to our model is outside the scope of this work. Hence, in our study, we explore other strategies, based on analyses that account for topological freezing. Therefore, we tried to test the relation in Eq. (A1) by taking our ensemble with the largest statistics (corresponding to the bare parameters $m_0 = -0.90$, $\beta = 6.9$ on a 24×12^3 lattice), measuring the topological charge Q using the same approach as in Ref. [184], and smoothening the gauge fields using the gradient flow. We then partition our full statistics into sets of configurations with equal topological charge⁶ and compute the correlator for the pseudoscalar

⁶In practice, the topological charge is not strictly an integer on a finite lattice in the employed approach as described, for instance, in [184] and references therein. We thus round Q to the closest integer.

singlet, η' , at fixed Q . We depict examples of the correlators for some values of Q with sufficient statistics in Fig. 6. The constant term arising is never statistically different for any pair of Q 's present in this ensemble. However, we see a slight trend toward a larger constant for larger $|Q|$ as expected from Eq. (A1).

In order to test the robustness of our subtraction choice, we report here the mass of the pseudoscalar singlet η' for various techniques. We remind the reader that the results reported in Sec. IV are based on correlators where the connected part is modeled by a single sum of exponentials as in Eq. (8), taking lattice periodicity into account and removing the constant by a numerical derivative. In Table V, we compare this to four alternative methods⁷: (i) direct calculation and subtraction of $\langle 0|O_{\eta'}|0\rangle$, (ii) ignoring the constant and restricting the fit to early time slices, (iii) performing a three-parameter fit of the decaying exponential plus a term modeling the constant,⁸ (iv) removing the constant using a numerical derivative but without any modeling of the connected part.

Whenever we obtain a signal without an explicit modeling of the connected pieces, our results agree within errors. The removal of excited state contamination [as used in methods (i), (ii), and (iii)] leads to masses that are generally slightly lighter. The same pattern has been observed in SU(3) [212]. We note that the removal of excited state

⁷We also applied an entirely different method designed for situations with large statistical noise [259]. Also, this approach gave results consistent with those shown in the main part of the paper for both singlets.

⁸This procedure gives the numerical value of the constant as a by-product. We subtract the constant from the correlator and *a posteriori* check that the resulting effective mass shows a plateau.

TABLE V. Determination of the masses of the pseudoscalar singlets using different techniques for removing the constant term in the correlator. We compare the method used in the main part of this work to: (i) Direct calculation and subtraction of $\langle 0|O_{\eta'}|0\rangle$; (ii) Ignoring the constant and restricting the fit to early time-slices; (iii) Performing a three-parameter fit of the decaying exponential plus a term modeling the constant; and (iv) Removing the constant using a numerical derivative but without any modeling of the connected part.

	β	m_0	L	T	$m_{\eta'}$	$m_{\eta'}^{(i)}$	$m_{\eta'}^{(ii)}$	$m_{\eta'}^{(iii)}$	$m_{\eta'}^{(iv)}$
SU(2)	2.0	-0.947	20	32
SU(2)	2.0	-0.94	14	24	0.67(6)	0.699(14)	0.572(14)	...	0.67(6)
SU(2)	2.0	-0.935	16	32	0.60(3)	0.67(3)	0.61(5)	0.60(3)	...
SU(2)	2.0	-0.93	14	24	0.65(3)	0.68(5)
SU(2)	2.0	-0.925	14	24	0.634(16)	0.63(8)
SU(2)	2.0	-0.92	12	24	0.665(9)	0.66(3)
SU(2)	2.0	-0.9	12	24	0.770(16)	0.79(8)
SU(2)	2.0	-0.88	10	20	0.842(5)	0.855(14)	0.855(14)
Sp(4)	7.2	-0.799	32	40	...	0.37(2)	0.37(2)	...	0.57(6)
Sp(4)	7.2	-0.794	28	36	0.397(16)	0.368(12)	0.368(12)	...	0.47(7)
Sp(4)	7.2	-0.79	24	36	0.387(13)	0.36(6)
Sp(4)	7.2	-0.78	24	36	0.418(7)	0.43(2)	0.45(2)	...	0.43(5)
Sp(4)	7.2	-0.77	24	36	0.456(8)	0.450(6)	0.450(6)	0.459(7)	...
Sp(4)	7.2	-0.76	16	36	...	0.511(13)	0.512(13)	...	0.59(3)
Sp(4)	6.9	-0.924	24	32	0.60(8)
Sp(4)	6.9	-0.92	24	32	...	0.51(4)	0.52(4)	0.486(16)	0.40(6)
Sp(4)	6.9	-0.92	16	32	0.49(3)	0.46(2)	0.46(2)	0.50(2)	0.45(13)
Sp(4)	6.9	-0.91	16	32	0.560(14)	0.59(4)	0.59(4)	0.560(13)	0.59(4)
Sp(4)	6.9	-0.91	14	24	0.541(9)	0.58(3)	0.58(3)
Sp(4)	6.9	-0.9	16	32	0.611(9)	0.63(3)
Sp(4)	6.9	-0.9	14	24	0.619(16)	0.614(12)	0.615(12)	0.620(9)	0.63(3)
Sp(4)	6.9	-0.9	12	24	0.610(6)	0.620(15)	0.620(15)	0.612(5)	...
Sp(4)	6.9	-0.89	14	24	0.69(2)	0.680(16)	0.681(16)	0.69(2)	0.72(4)
Sp(4)	6.9	-0.89	12	24	0.661(9)	0.660(5)	0.660(5)	0.660(10)	...
Sp(4)	6.9	-0.87	12	24	0.782(13)	0.80(4)	0.80(4)	...	0.80(2)
Sp(4)	6.9	-0.87	10	20	0.764(9)	0.763(6)	0.763(6)

contaminations should not be confused with the removal of the constant contribution to the correlator, as discussed earlier. The explicit calculation of the constant $\langle 0|O_{\eta'}|0\rangle$ in Eq. (8) does not quantitatively capture the constant in the correlator. The results are almost indistinguishable from not taking the constant into account. For some ensembles (e.g., Sp(4) with $\beta = 7.2$), these methods appear to underestimate the meson mass. This is a result of combining the modeling of the connected piece with an insufficient subtraction of the constant. Due to the absence of connected excited states in the correlator, the effective mass is increasing at small t , while for large t , the constant leads to a decrease of the effective masses. This can lead to the formation of an apparent plateau in the effective mass and thus to a possible underestimation of the meson mass. Overall, we conclude that methods (ii) and (iii) do not appear sufficiently reliable. Modeling the constant as an additional fit parameter did not lead to any significant improvements. In most cases, we cannot extract a reliable signal. In the few cases where this is possible, the constant term is quantitatively small, and this method agrees with the others while providing no improvement at the cost of an additional fit parameter.

We conclude that the method used throughout the main part of this work has proven to be the most reliable approach among the options considered here. Its results are always consistent with forgoing the explicit removal of subtracted states, and the removal of the additional constant through taking the derivative avoids any further estimations of the topological constant terms at the expense of a shorter plateau in the effective masses and thus, a smaller interval for fitting the correlator.

We find a different behavior for the scalar singlet. The constant term is not related to an insufficient sampling of all topological sectors but arises due to the vacuum quantum numbers of the scalar singlet. In addition, the modeling of the connected pieces is less important since the nonsinglet state appears generally heavier than the singlet states and the connected pieces show a stronger exponential decay. In this case, the direct estimation of the constant term $\langle 0|O_{\sigma}|0\rangle$ in Eq. (8) appears to be quantitatively reliable. Still, in some cases, the modeling of the connected pieces can extend the plateau in the effective mass to lower time slices t . Since the constant is several orders of magnitude larger than the actual signal of the σ state, a direct modeling of it as a fit parameter is infeasible, and the constant can also not be

TABLE VI. Results for the masses of the scalar singlet σ using our standard approach of a numerical derivative as well as (i) both a numerical derivative and a direct calculation of the vacuum term $\langle 0|O_\sigma|0\rangle$, (ii) only direct calculation of the vacuum term, and (iii) a numerical derivative without an explicit subtraction of excited states in the connected piece when possible.

	β	m_0	L	T	m_σ	$m_\sigma^{(i)}$	$m_\sigma^{(ii)}$	$m_\sigma^{(iii)}$
SU(2)	2.0	-0.947	20	32	0.53(4)	0.53(3)	0.58(5)	0.54(4)
SU(2)	2.0	-0.94	14	24	...	0.64(5)	0.61(4)	0.64(5)
SU(2)	2.0	-0.935	16	32	...	0.47(10)	0.55(8)	0.47(10)
SU(2)	2.0	-0.93	14	24	0.62(9)	...
SU(2)	2.0	-0.925	14	24
SU(2)	2.0	-0.92	12	24	...	0.71(7)	0.75(13)	0.72(7)
SU(2)	2.0	-0.9	12	24
SU(2)	2.0	-0.88	10	20
Sp(4)	7.2	-0.799	32	40	0.36(5)	0.35(8)	0.41(4)	0.38(8)
Sp(4)	7.2	-0.794	28	36	...	0.55(8)	...	0.55(8)
Sp(4)	7.2	-0.79	24	36	0.56(6)	0.56(6)	0.48(7)	0.65(12)
Sp(4)	7.2	-0.78	24	36	0.55(6)	...
Sp(4)	7.2	-0.77	24	36
Sp(4)	7.2	-0.76	16	36	0.64(12)	0.64(7)
Sp(4)	6.9	-0.924	24	32	0.46(3)	0.46(3)	0.45(3)	0.48(7)
Sp(4)	6.9	-0.92	24	32	0.42(2)	0.43(3)	0.45(3)	...
Sp(4)	6.9	-0.92	16	32	0.45(6)	0.40(8)	0.42(7)	0.37(11)
Sp(4)	6.9	-0.91	16	32	0.71(8)
Sp(4)	6.9	-0.91	14	24	0.41(3)	0.41(3)
Sp(4)	6.9	-0.9	16	32
Sp(4)	6.9	-0.9	14	24	0.57(4)	0.56(4)	0.48(5)	0.51(10)
Sp(4)	6.9	-0.9	12	24	0.55(2)	0.56(4)	...	0.57(3)
Sp(4)	6.9	-0.89	14	24	0.57(9)	0.56(9)	0.61(9)	0.59(9)
Sp(4)	6.9	-0.89	12	24	0.62(7)	...	0.64(4)	...
Sp(4)	6.9	-0.87	12	24	0.80(15)	0.76(11)	...	0.72(7)
Sp(4)	6.9	-0.87	10	20	...	0.70(6)

ignored in the analysis. In Table VI, we compare the approach used in the main part of this paper to (i) both a numerical derivative and a direct calculation and subsequent subtraction of the vacuum term $\langle 0|O_\sigma|0\rangle$, (ii) only direct subtraction of the vacuum terms as in [215], (iii) a numerical derivative without an explicit subtraction of excited states in the connected pieces and without a direct subtraction of $\langle 0|O_\sigma|0\rangle$.

APPENDIX B: COMPARISON BETWEEN EXCITED STATE SUBTRACTION AND SMEARED CONNECTED DIAGRAMS

In Sec. III B, we noted that the signal of the singlet mesons can be extended to smaller time separations, t , if we replace its connected contribution by approximating it with a single exponential term having the energy of the non-singlet meson. This removes all the excited state contaminations of the connected piece.

A similar effect can be obtained by using smearing techniques on the connected piece. This can increase the overlap of the source operator with the ground state of the nonsinglet and reduce the contribution of excited states. Recently, this approach has been implemented, tested, and shown to work in Sp(4) gauge theories [194]. These

developments allow us to compare our excited-state subtraction technique.⁹

In order to compare the two techniques, we need to apply smearing to only the connected piece. However, the use of smearing techniques leads to an overall change of normalization. Applying Wuppertal smearing [260] with N_1 steps at the source and N_2 steps at the sink leads to an asymptotic correlator of the form

$$C_{N_1, N_2}(t \rightarrow \infty) = \alpha_{N_1} \alpha_{N_2} e^{-m_{\text{conn}} t}, \quad (\text{B1})$$

where the normalization of unsmeared point sources is recovered for the choice of the parameters $\alpha_{N_1} = \alpha_{N_2} = \alpha_0$. We consider two sets of correlators with the smearing steps $(N_1, N_2) = (N, 0)$ and $(N_1, N_2) = (N, N)$, to restore the normalization as the point source. We define a new correlator

$$C_{\text{conn}}^{\text{smeared}}(t) \equiv \frac{C_{N,0}(t)^2}{C_{N,N}(t)}, \quad (\text{B2})$$

⁹We thank the authors of [194,254] for performing smeared measurements on a set of our configurations for comparison prior to publication.

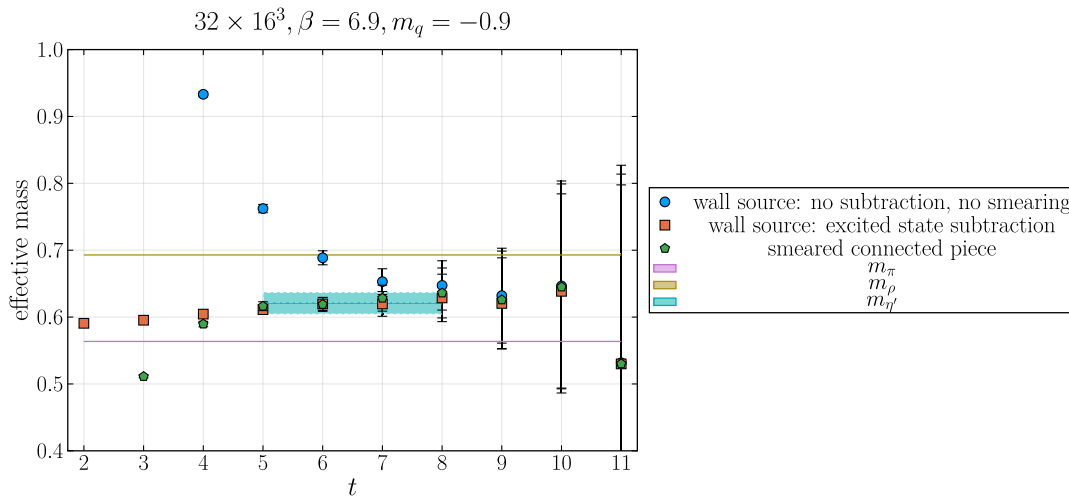


FIG. 7. Comparison between excited state subtraction (orange squares), obtained by modeling the connected part of the correlator as a single exponential term, with smeared operators (green pentagon), on a preliminary set of configurations, for a single ensemble. For reference, we also plot the correlator without excited state subtraction and without smearing (blue circles).

by squaring the connected correlator with N steps of source smearing and no sink smearing and divide that by the connected correlator with an equal amount of smearing steps at both the source and the sink. This correlator has the same large- t behavior and the same normalization as a nonsmeared one. From this, we then construct the full correlator of the singlet meson. In Fig. 7, we compare the

full singlet correlator obtained from Eq. (B2) using Wuppertal smearing with $N = 60$ smearing steps, to the correlator obtained using the single-exponential modeling and subtraction of the connected piece. We see that the subtracted correlator and the smeared correlator agree remarkably well in the interesting plateau region.

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