

Topology in the $SU(N_f)$ chiral symmetry restored phase of unquenched QCD and axion cosmology. II.

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We investigate the physical consequences of the survival of the effects of the $U(1)_A$ anomaly in the chiral symmetric phase of QCD, and show that the free energy density is a singular function of the quark mass m , in the chiral limit, and that the σ and $\bar{\pi}$ susceptibilities diverge in this limit at any $T \geq T_c$. We also show that the difference between the $\bar{\pi}$ and $\bar{\delta}$ susceptibilities diverges in the chiral limit at any $T \geq T_c$, a result which seems to be excluded by recent results of Tomiya *et al.* from numerical simulations of two-flavor QCD. We also discuss on the generalization of these results to the $N_f \geq 3$ model.

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I. INTRODUCTION

Quantum field theories with a topological term in the action [1] have proved to be particularly challenging to investigate. The strong CP problem in strong interactions, and the Haldane conjecture and the quantum Hall effect in condensed matter physics are representative of important open problems in theoretical physics closely related to the topological properties of the model.

In what concerns QCD, understanding the role of the θ parameter and its connection with the strong CP problem is a major challenge. On the other hand the aim to elucidate the existence of new low-mass, weakly interacting particles from a theoretical, phenomenological and experimental point of view, is intimately related to this issue. The light particle that has mostly gathered attention is the axion, predicted by Weinberg and Wilczek [2,3] in the Peccei and Quinn mechanism [4] to explain the absence of parity and temporal invariance violations induced by the QCD vacuum. The axion is also one of the more interesting candidates to make the dark matter of the universe, and the axion potential plays a fundamental role in the determination of the dynamics of the axion field. Moreover, the way in which the $U(1)_A$ anomaly manifests itself in the chiral symmetry restored phase of QCD at high temperature could be tested when probing the QCD phase transition in relativistic heavy ion collisions.

The topological properties of the QCD-vacuum are intrinsically nonperturbative, thus requiring a nonperturbative approach. The calculation of the topological susceptibility by means of simulations in lattice QCD is already a challenge, but calculating the complete potential requires a strategy to deal with the so-called sign problem, that is, the presence of a highly oscillating term in the path integral, which prevents the applicability of the importance sampling method [1]. But the QCD axion model relates the topological susceptibility χ_T at $\theta = 0$ with the axion mass m_a and decay constant f_a through the relation

$\chi_T = m_a^2 f_a^2$, and the axion mass is an essential ingredient in the calculation of the axion abundance in the Universe. Therefore a precise computation of the temperature dependence of the topological susceptibility in QCD becomes of primordial interest in this context. Indeed, several calculations of this quantity in unquenched QCD have been recently reported [5–7].

Unfortunately there are strong discrepancies among these three calculations. Bonati *et al.* [5] explore $N_f = 2 + 1$ QCD in a range of temperature going from T_c to around $4T_c$, and their results for the topological susceptibility differ strongly, both in size and in temperature dependence, from the dilute instanton gas prediction, giving rise to a shift of the axion dark matter window of almost one order of magnitude with respect to the instanton computation. Petreczky *et al.* [6] observe however very distinct temperature dependences of the topological susceptibility in the ranges above and below 250 MeV: while for temperatures above 250 MeV, the dependence is found to be consistent with the dilute instanton gas approximation, at lower temperatures the fall-off of topological susceptibility is milder. Borsanyi *et al.* [7] find, on the other hand, a topological susceptibility many orders of magnitude smaller than that of Ref. [5] in the cosmologically relevant temperature region. These discrepancies among the three calculations make more interesting, if possible, a theoretical approach to the issue.

The absence of the typical effects of the $U(1)_A$ anomaly in the chiral symmetry restored phase of QCD at high-temperature was suggested in [8,9], and investigated later on [10–24]. Indeed, years ago Cohen [8] showed, using the continuum formulation of two flavor QCD, and assuming the absence of the zero mode's contribution, that all the disconnected contributions to the two-point correlation functions in the $SU(2)_A$ symmetric phase at high-temperature vanish in the chiral limit. The main conclusion of this work was that the eight scalar and pseudoscalar mesons should have the same mass in the chiral limit, the

typical effects of the $U(1)_A$ anomaly being absent in this phase. Furthermore he argued in [9] that the analyticity of the free energy density in the quark mass m around $m = 0$, in the high temperature phase, imposes constraints on the spectral density of the Dirac operator around the origin which are enough to guarantee the previous results. Later on Aoki *et al.* [16] got constraints on the Dirac spectrum of overlap fermions, strong enough for all of the $U(1)_A$ breaking effects among correlation functions of scalar and pseudoscalar operators to vanish, and they concluded that there is no remnant of the $U(1)_A$ anomaly above the critical temperature of two flavor QCD , at least in these correlation functions. Their results were obtained under the assumptions that m -independent observables are analytic functions of the quarks mass m , at $m = 0$, and that the Dirac spectral density can be expanded in Taylor series near the origin, with a nonvanishing radius of convergence.

More recently we investigated by analytical methods in Ref. [22] the topological properties of QCD in the high temperature chiral symmetric phase, and we summarize here what was the starting hypothesis in [22], its physical motivation, and the main conclusion which follows from it. The starting hypothesis was to assume that the perturbative expansion of the free energy density in powers of the quark mass, m , has a nonvanishing convergence radius in the high temperature chiral symmetric phase of QCD . This is just what we expect on physical grounds if all correlation lengths remain finite in the chiral limit, and the spectrum of the model shows therefore a mass gap also in this limit. The main conclusion which followed from this hypothesis was that all the topological effects of the axial anomaly should disappear in this phase, the topological susceptibility and all θ -derivatives of the free energy density vanish, and the theory becomes θ independent at any $T > T_c$ in the infinite-volume limit.

Accordingly, the free energy density should be a singular function of the quark mass, in the chiral limit, if the topological effects of the $U(1)_A$ anomaly survive in the chiral symmetry restored phase of QCD at finite temperature, and the main purpose of this article is to investigate this issue. Our starting hypothesis will be now that the topological effects of the anomaly survive in the high temperature phase of QCD , and the model shows therefore a nontrivial θ -dependence in this phase. Under this assumption we will show here that indeed the free energy density is a singular function of the quark mass, m , in the chiral limit at any $T > T_c$, and that the correlation length and the σ and $\bar{\pi}$ susceptibilities diverge in this limit, as well as the difference between the $\bar{\pi}$ and $\bar{\delta}$ susceptibilities.

We will show first this result following the line of argumentation developed in [22], and thereafter exploiting the qualitative features of the phase diagram of QCD in the $Q = 0$ topological sector. Our main conclusion is that this scenario should be excluded, in the $N_f \geq 3$ case, by universality and renormalization group arguments, and in

the two flavor model, by recent results of numerical simulations of high temperature two-flavor QCD [23].¹

II. σ AND η SUSCEPTIBILITIES

The Euclidean continuum Lagrangian of N_f flavors QCD with a θ -term is

$$L = \sum_f L_F^f + \frac{1}{4} F_{\mu\nu}^a(x) F_{\mu\nu}^a(x) + i\theta \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x) \quad (1)$$

with L_F^f the fermion Lagrangian for the f -flavor, and

$$Q = \frac{g^2}{64\pi^2} \int d^4x \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x) \quad (2)$$

is the topological charge of the gauge configuration.

To avoid ultraviolet divergences we will assume along this paper a lattice regularization, the Ginsparg-Wilson (G-W) fermions [25], from which the overlap fermions [26] are an explicit realization, which shares with the continuum all essential ingredients and gives at the same time mathematical rigor to all developments. Indeed G-W fermions have a $U(1)_A$ anomalous symmetry [27], good chiral properties, a quantized topological charge, and allow us to establish and exact index theorem on the lattice [28].

The partition function of the model can be written as a sum over all topological sectors, Q , of the partition function in each topological sector times a θ -phase factor, as follows

$$Z(\theta) = \sum_Q Z_Q e^{i\theta Q} \quad (3)$$

where Q , which takes integer values, is bounded at finite volume by the number of degrees of freedom. At large spatial lattice volume V_x the partition function should behave as

$$Z(\theta) = e^{-V_x L_t E(\beta, m, \theta)} \quad (4)$$

where $E(\beta, m, \theta)$ is the free energy density, β the inverse gauge coupling, m the quark mass, and L_t the lattice temporal extent or inverse physical temperature T . Moreover the mean value of any intensive operator O , as for instance the scalar and pseudoscalar condensates, or any correlation function, in the $Q = 0$ topological sector, can be computed as

$$\langle O \rangle_{Q=0} = \frac{\int d\theta \langle O \rangle_\theta Z(\theta, m)}{\int d\theta Z(\theta, m)} \quad (5)$$

with $\langle O \rangle_\theta$ the mean value of O computed with the integration measure (1).

¹We should notice however that the results of Ref. [23] for the two-flavor case do not agree with those of Ref. [18], and any further clarification on this point would be therefore welcome.

We are also assuming along this paper that the topological effects of the $U(1)_A$ anomaly survive in the high temperature phase of QCD , or in other words, that the free energy density (4) shows a non trivial θ -dependence also in the high temperature chiral symmetric phase. Then, since the free energy density, as a function of θ , has its absolute minimum at $\theta = 0$ for non-vanishing quark masses, the following relation holds in the infinite lattice volume limit

$$\langle O \rangle_{Q=0} = \langle O \rangle_{\theta=0}. \quad (6)$$

We want to remark that, as discussed in [22], in spite of the fact that the $Q = 0$ topological sector is free from the $U(1)_A$ global anomaly, and spontaneously breaks the $U(N_f)_A$ axial symmetry at $T = 0$, Eq. (6) is compatible with a massive flavor-singlet pseudoscalar meson in the chiral limit. We will also make use of Eq. (6) along this paper.

Let us consider, for simplicity, the two-flavor model with degenerate up and down quark masses. In the high temperature phase the $SU(2)_A$ symmetry is fulfilled in the ground state for massless quarks, and therefore the mean value of the flavor singlet scalar condensate $\langle S \rangle$, as well as of any order parameter for this symmetry, vanishes in the chiral limit. Moreover the infinite lattice volume limit and the chiral limit should commute, provided the order parameter remains bounded. In addition Eq. (6) implies that the $SU(2)_A$ symmetry is also fulfilled in the $Q = 0$ topological sector. However, the $U(1)_A$ symmetry should be spontaneously broken in this sector, giving account in this way for the $U(1)_A$ anomaly.² In fact, the σ and η correlation functions, which take in the $Q = 0$ sector the same value as in QCD at $\theta = 0$ (6), should be different in the chiral limit, and the difference of these correlation functions is an order parameter for the $U(1)_A$ symmetry of the $Q = 0$ sector.

Therefore we can characterize the ground states of the $Q = 0$ sector, in the chiral limit, by an angle α .

Let us assume that the correlation length, and hence the σ susceptibility, $\chi_\sigma(m)$, are finite in the chiral limit. In such a case the flavor singlet scalar condensate behaves as

$$\langle S \rangle_{\theta=0, m \rightarrow 0} \approx \chi_\sigma(0)m \quad (7)$$

but since Eq. (6) tells us that $\langle S \rangle_{Q=0} = \langle S \rangle_{\theta=0}$, Eq. (7) holds also in the $Q = 0$ sector,

$$\langle S \rangle_{Q=0, m \rightarrow 0} \approx \chi_\sigma(0)m. \quad (8)$$

The $Q = 0$ sector is on the other hand free from the $U(1)_A$ global anomaly, hence the following relation between the flavor singlet scalar condensate $\langle S \rangle_{Q=0}$, and the η and $\bar{\pi}$ susceptibilities, $\chi_\eta(m)_{Q=0}$, $\chi_{\bar{\pi}}(m)_{Q=0}$, holds in this sector³

$$\chi_{\bar{\pi}}(m)_{Q=0} = \chi_\eta(m)_{Q=0} = \frac{\langle S \rangle_{Q=0}}{m}. \quad (9)$$

Equations (8) and (9) tell us that the flavor singlet scalar and pseudoscalar susceptibilities, in the $Q = 0$ sector, take the same value, $\chi_\sigma(0)$, in the chiral limit, and this is a rather unexpected result because $\chi_\sigma(0)_{Q=0} - \chi_\eta(0)_{Q=0}$ is an order parameter for the spontaneously broken $U(1)_A$ symmetry.

A loophole to this paradoxical result would be a divergent flavor singlet scalar susceptibility, $\chi_\sigma(m)$, in the chiral limit. However it could also be that, for some accidental reason, the quark mass term selects an α -ground state, in the chiral limit, in which $\chi_\sigma(0)_{Q=0} = \chi_\eta(0)_{Q=0}$. We will therefore continue exploring the physical consequences of assuming the correlation length, and $\chi_\sigma(m)$, are finite in the chiral limit.

The flavor singlet scalar $\langle S(x)S(0) \rangle_{Q=0}$ and pseudoscalar $\langle P(x)P(0) \rangle_{Q=0}$ correlation functions transform under $U(1)_A$ rotations of angle α as

$$\begin{aligned} \langle S(x)S(0) \rangle_{Q=0}^\alpha &= \cos^2 \alpha \langle S(x)S(0) \rangle_{Q=0}^{\alpha=0} + \sin^2 \alpha \langle P(x)P(0) \rangle_{Q=0}^{\alpha=0} + \sin \alpha \cos \alpha (\langle S(x)P(0) \rangle_{Q=0}^{\alpha=0} + \langle P(x)S(0) \rangle_{Q=0}^{\alpha=0}) \\ \langle P(x)P(0) \rangle_{Q=0}^\alpha &= \sin^2 \alpha \langle S(x)S(0) \rangle_{Q=0}^{\alpha=0} + \cos^2 \alpha \langle P(x)P(0) \rangle_{Q=0}^{\alpha=0} - \sin \alpha \cos \alpha (\langle S(x)P(0) \rangle_{Q=0}^{\alpha=0} + \langle P(x)S(0) \rangle_{Q=0}^{\alpha=0}) \end{aligned} \quad (10)$$

and therefore the flavor singlet scalar and pseudoscalar susceptibilities, in the $Q = 0$ sector, in the chiral limit, take the value $\chi_\sigma(0)$ not only in the ground state selected by the quark mass term, but also in all the other α -states, provided that parity is not spontaneously broken.⁴

Moreover a simple calculation, based on an anomalous $U(1)_A$ transformation in the chiral limit, gives the following relation for the θ -dependence of the flavor singlet scalar correlation function at vanishing quark mass

²The Goldstone theorem however can be fulfilled without a Nambu-Goldstone boson [22].

³Notice that notwithstanding the σ and $\bar{\pi}$ susceptibilities in the $Q = 0$ sector are equal to the corresponding quantities in QCD at $\theta = 0$ in the thermodynamic limit, this is not true for the η susceptibility, as discussed in Ref. [22].

⁴Because $SU(2)_A$ symmetry is fulfilled in the $Q = 0$ sector in the chiral limit, the flavor singlet scalar and pseudoscalar condensates vanish in the α -ground state selected by the quark-mass term, and therefore also in all other α -states. Hence the disconnected contributions to the connected correlation functions are always canceled.

$$\begin{aligned} \langle S(x)S(0) \rangle_{\theta}^{m=0} &= \cos^2\left(\frac{\theta}{2}\right) \langle S(x)S(0) \rangle_{\theta=0}^{m=0} \\ &+ \sin^2\left(\frac{\theta}{2}\right) \langle P(x)P(0) \rangle_{\theta=0}^{m=0} \end{aligned} \quad (11)$$

By performing the integral over the θ -angle in Eq. (11), as stated by Eq. (5), we get

$$\langle S(x)S(0) \rangle_{Q=0}^{m=0} = \frac{1}{2} \langle S(x)S(0) \rangle_{\theta=0}^{m=0} + \frac{1}{2} \langle P(x)P(0) \rangle_{\theta=0}^{m=0} \quad (12)$$

and therefore a similar relation for the susceptibilities holds

$$\chi_{\sigma}(0)_{Q=0} = \frac{\chi_{\sigma}(0) + \chi_{\eta}(0)}{2}. \quad (13)$$

The flavor singlet scalar susceptibility of the $Q = 0$ sector in the chiral limit is the average of this quantity over all α -ground states [29], but we have previously shown that it takes the same value, $\chi_{\sigma}(0)$, in all α -ground states. The compatibility of this result with Eq. (13) requires therefore the η and σ susceptibilities to be equal, in contradiction with the assumption that the topological effects of the $U(1)_A$ anomaly survive in the high temperature phase.

We conclude that the assumption on the finitude of the correlation length and σ -susceptibility in the chiral limit is wrong, this susceptibility diverges, and the free energy density is therefore singular at $m = 0$.

Under the standard assumption that the critical behavior of the model is well described by a power law for the flavor singlet scalar condensate

$$\langle S \rangle_{\theta=0, m \rightarrow 0} \approx C(T) m^{\frac{1}{\delta}} \quad (14)$$

we get that the flavor singlet scalar susceptibility χ_{σ} diverges at any $T \geq T_c$ in the chiral limit as⁵

$$\chi_{\sigma}(m) \approx C(T) \frac{1}{\delta} m^{\frac{1-\delta}{\delta}}, \quad (15)$$

and since the $SU(2)_A$ symmetry is not anomalous, the pion susceptibility verifies the relation

$$\chi_{\pi}(m) = \frac{\langle S \rangle}{m}, \quad (16)$$

⁵The critical exponent δ should be that of the three-dimensional $O(4)$ vector universality class, $\delta = 4.789(6)$, at $T = T_c$. Universality arguments suggest it would be T -independent, but we do not exclude a temperature dependence of δ corresponding to a critical line with continuously varying critical exponents.

and diverges also in the chiral limit as

$$\chi_{\pi}(m) \approx C(T) m^{\frac{1-\delta}{\delta}}. \quad (17)$$

Moreover the vector meson $\bar{\delta}$ susceptibility, $\chi_{\bar{\delta}}$, which is bounded by the scalar susceptibility, χ_{σ} , verifies the following inequality

$$\chi_{\pi}(m) - \chi_{\bar{\delta}}(m) \geq \chi_{\pi}(m) - \chi_{\sigma}(m) \approx C(T) \frac{\delta - 1}{\delta} m^{\frac{1-\delta}{\delta}} \quad (18)$$

which shows explicitly that $\chi_{\pi}(m) - \chi_{\bar{\delta}}(m)$ diverges in the chiral limit.

This result seems to be ruled out by the results of a numerical simulation of two-flavor QCD by Tomiya *et al.* reported in Ref. [23], where they find a value of $\chi_{\pi}(m) - \chi_{\bar{\delta}}(m)$ in the chiral limit, and in a temperature range $T \sim 190\text{--}220$ MeV slightly above the critical temperature T_c , that not only does not diverge but is compatible with zero. However, previous results by Dick *et al.* [18] on larger lattices, but using overlap fermions only in the valence sector, seem to predict a divergent $\chi_{\pi}(m) - \chi_{\bar{\delta}}(m)$ in the chiral limit, in agreement with Eq. (18).

III. PHASE DIAGRAM OF QCD IN THE $Q=0$ TOPOLOGICAL SECTOR

The nonanalyticity of the free energy density at $m = 0$ can also be shown by an alternative or complementary way. The $SU(2)_A$ symmetry is fulfilled in QCD at any $T > T_c$, and therefore the up and down scalar condensates $\langle S_u \rangle$, $\langle S_d \rangle$ vanish in the chiral limit $m_u = m_d = 0$. However if we consider QCD with two nondegenerate quark flavors, and take the limit $m_u \rightarrow 0$ keeping m_d fixed, or vice versa, the condensate $\langle S_u \rangle$, or $\langle S_d \rangle$, takes a nonvanishing mean value due to the fact that the $U(1)_u$ symmetry at $m_u = 0$, or the $U(1)_d$ symmetry at $m_d = 0$, which would enforce the condensate to be zero, is anomalous. But since Eq. (6) can be applied to these condensates, this result tell us that the $Q = 0$ topological sector, which is not anomalous, spontaneously breaks the $U(1)_u$ axial symmetry at $m_u = 0$, $m_d \neq 0$, and the $U(1)_d$ symmetry at $m_d = 0$, $m_u \neq 0$. The phase diagram of QCD in the $Q = 0$ topological sector, in the (m_u, m_d) plane, shows therefore two first order phase transition lines, which coincide with the coordinate axes, finishing at the end point $m_u = m_d = 0$, which is a critical point for any $T > T_c$.

Equation (6) tell us that the critical equation of state of QCD at $\theta = 0$ should be the same as the one of the $Q = 0$ topological sector, which should show a divergent correlation length at any $T > T_c$. We expect therefore a continuous finite temperature chiral transition, and a divergent correlation length for any $T \geq T_c$, and because the symmetry breaking pattern is, in the two flavor model, $SU(2)_L \times SU(2)_R \rightarrow SU(2)_V$, the critical equation of state should be that of the three-dimensional $O(4)$ vector

universality class [30], which shows a critical exponent $\delta = 4.789(6)$ [31] ($\delta = 3$ in the mean field or Landau approach).

For $N_f \geq 3$ a similar argument on the phase diagram of the $Q = 0$ sector applies, but the scenario that emerges in this case is also not plausible because no stable fixed points are expected in the corresponding Landau-Ginzburg-Wilson Φ^4 theory compatible with the given symmetry-breaking pattern [32].

IV. CONCLUSIONS AND DISCUSSION

The aim to elucidate the existence of new low-mass weakly interacting particles from a theoretical, phenomenological, and experimental point of view, is intimately related to the role of the θ parameter in QCD . Indeed the axion is one of the more interesting candidates to make the dark matter of the universe, and the QCD axion model relates the topological susceptibility χ_T at $\theta = 0$ with the axion mass m_a and decay constant f_a through the relation $\chi_T = m_a^2 f_a^2$, the axion mass being an essential ingredient in the calculation of the axion abundance in the Universe. Moreover, the way in which the $U(1)_A$ anomaly manifests itself in the chiral symmetry restored phase of QCD at high temperature could be tested when probing the QCD phase transition in relativistic heavy ion collisions.

With these motivations we started recently an investigation of the topological properties of QCD in the high temperature chiral symmetric phase in Ref. [22]. The starting hypothesis in [22] was to assume that the perturbative expansion of the free energy density in powers of the quark mass, m , has a nonvanishing convergence radius in the high temperature chiral symmetric phase of QCD , which is just what we expect if all correlation lengths remain finite in the chiral limit, and the spectrum of the model shows therefore a mass gap also in this limit. The main conclusion in [22] was that all the topological effects of the axial anomaly should disappear in this phase, the topological susceptibility and all θ -derivatives of the free energy density vanish, and the theory becomes θ independent at any $T > T_c$ in the infinite-volume limit. Accordingly, the free energy

density should be a singular function of the quark mass, in the chiral limit, if the topological effects of the $U(1)_A$ anomaly survive in the chiral symmetry restored phase of QCD at finite temperature.

Ongoing with this research line, the main purpose of this article has been to further investigate this issue. To this end our starting hypothesis has been now to assume that the topological effects of the anomaly survive in the high temperature phase of QCD , and the model shows therefore a nontrivial θ -dependence in this phase. Under this assumption we have shown that indeed, the free energy density is a singular function of the quark mass, m , in the chiral limit at any $T > T_c$, and that the correlation length and the σ and $\bar{\pi}$ susceptibilities diverge in this limit. Under the same assumption we have also shown that the difference between the $\bar{\pi}$ and $\bar{\delta}$ susceptibilities diverges in the chiral limit at any $T \geq T_c$, a result which seems to be excluded by recent results of Tomiya *et al.* [23] from numerical simulations of two-flavor QCD , thus suggesting the topological effects of the $U(1)_A$ anomaly are absent in the chiral symmetric phase of two-flavor QCD . However, previous results by Dick *et al.* [18] on larger lattices, but using overlap fermions only in the valence sector, seem to predict a divergent $\chi_{\bar{\pi}}(m) - \chi_{\bar{\delta}}(m)$ in the chiral limit, in agreement with Eq. (18), and any further clarification on this point would be therefore welcome.

We have also discussed that the previous results for the two-flavor model apply also to $N_f \geq 3$. However, universality and renormalization-group arguments, based on the most general Landau-Ginzburg-Wilson Φ^4 theory compatible with the given symmetry-breaking pattern, make this scenario not plausible too because no stable fixed points are expected in the corresponding Landau-Ginzburg-Wilson Φ^4 theory for $N_f \geq 3$ [32].

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