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Quark mass dependence of two-flavor QCD

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Abstract

I explore the rich phase diagram of two-flavor QCD as a function of the quark masses. The theory involves three parameters, including one that is CP violating. As the masses vary, regions of both first and second order transitions are expected. For non-degenerate quarks, non-perturbative effects cease to be universal, leaving individual quark mass ratios with a renormalization scheme dependence. This raises complications in matching lattice results with perturbative schemes and demonstrates the tautology of attacking the strong CP problem via a vanishing up quark mass.

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I. INTRODUCTION

The standard theory of the strong interactions is based on quarks interacting through non-Abelian gauge fields. This system is remarkable in its paucity of parameters. Once the overall scale is set, perhaps by working in units where the proton mass is unity, the only remaining parameters are the quark masses. In general these are complex numbers, although field redefinitions allow removing all phases but one, usually called the strong CP parameter Theta. For a recent review, see Ref. [1]. Thus the number of physical parameters for QCD is one more than the number of quark species. As is well known, if Theta is non-trivial, the theory violates CP symmetry. As CP appears to be a good symmetry of hadronic physics, the strong CP puzzle asks the question why should this parameter be so small experimentally.

In this paper I restrict myself to two-flavor QCD and explore the qualitative behavior as the most general mass terms are varied. Using effective potential techniques, I find a rich phase diagram with regions of both first and second order phase transitions. I find that there can be interesting long distance physics even when no individual quark mass vanishes. I also delve more deeply into the old argument [2] for a fundamental ambiguity in defining a vanishing quark mass. These effects are inherently non-perturbative and lead to unsettled issues for matching lattice with perturbative results.

Of course, with QCD being an interacting quantum field theory, nothing has been proven rigorously. To proceed I assume that QCD exists as a field theory and confines in the usual way. In addition I will work in the conventional picture of spontaneous breaking of approximate chiral symmetry as the explanation for the lightness of the pions. I also assume the generation of the singlet pseudoscalar meson mass is tied to the anomaly. For simplicity I work with the two-flavor theory with only the *u* and *d* quarks, assuming their masses are light enough that conventional chiral expansions make sense. The generalization to more flavors is straightforward, although there are some rather fascinating further consequences [3].

I begin in Section II with a simple argument on how the various quark masses indirectly influence each other. The obscurity of these effects in a mass independent regularization scheme has raised some controversy, which I address in Section III. Section IV turns to the most general mass term for the two-flavor theory. Here I discuss some of the conventions needed for formulating this question. Section V relates the mass parameters to the strong CP problem and discusses the issues with pursuing a vanishing lightest quark mass. Section VI uses an effective potential argument to develop the qualitative phase diagram as a function of the independent mass parameters. Finally, the basic ideas are summarized in section VII.

II. SPIN-FLIP QUARK SCATTERING

I begin with a reminder of some basic properties expected for massless two-flavor QCD. While the classical theory is conformally invariant, it is commonly believed that in the quantized theory confinement and dimensional transmutation generate a non-trivial mass scale Λ_{qcd} . This scale is scheme dependent, but that will not enter the qualitative discussion here. In particular, the theory should contain massive stable nucleons. On the other hand, spontaneous chiral-symmetry breaking is expected to give rise to three massless pions as Goldstone bosons. In addition, the two-flavor analog of the eta prime meson should acquire a mass from the anomaly.

In this picture, the eta prime and neutral pion involve distinct combinations of quark-antiquark bound states. In the simple quark model the neutral pseudoscalars involve the combinations

$$\pi_0 \sim \overline{u} \gamma_5 u - \overline{d} \gamma_5 d \tag{1}$$

$$\eta' \sim \overline{u} \gamma_5 u + \overline{d} \gamma_5 d + \text{glue.}$$
⁽²⁾

Here I include a gluonic contribution from mixing between the η' and glueball states. When the quarks are degenerate, isospin forbids such mixing for the pion.

Projecting out helicity states for the quarks, $q_{R,L} = (1 \pm \gamma_5)q/2$, the pseudoscalars are combinations of left with right states, *i.e.* $\overline{q}_L q_R - \overline{q}_R q_L$. Thus, as shown schematically in Fig. 1, meson exchange will contribute to a hypothetical quark-quark spin-flip scattering experiment. More precisely, the four point function $\langle \overline{u}_R u_L \overline{d}_R d_L \rangle$ should not vanish. (Scalar meson exchange will also contribute to this process, but this is not important for the qualitative argument below.) Of course I assume that some sort of gauge fixing has been done to eliminate a trivial vanishing of this function from an integral over gauges.

It is important that the π_0 and η' are not degenerate. This is due to the anomaly and the fact that the η' is not a Goldstone boson. At a more abstract level this $\pi_0 - \eta'$ splitting is ascribed to topological structures in the gauge field, but such details are not necessary for the discussion here. Because the mesons are not degenerate, their contributions to the above diagram cannot cancel. The conclusion of this simple argument is that helicity-flip quark-quark scattering is not suppressed as the mass goes to zero.



FIG. 1: Both pion and eta prime exchange can contribute to spin flip scattering between up and down quarks.



FIG. 2: Through physical meson exchange, a down quark mass can induce an effective mass for the up quark. The gluon exchanges can compensate for the pseudoscalar nature of the meson fields.

Now consider turning on a small *d* quark mass while leaving the up quark massless. Formally this mass allows one to connect the in-going and out-going down-quark lines in Fig. 1 and thereby induce a mixing between the left and right handed up quark. Such a process is sketched in Fig. 2. Here I allow for additional gluon exchanges to compensate for turning the pseudoscalar field into a traditional mass term.

So the presence of a non-zero *d* quark mass will induce an effective mass for the *u* quark, even if the latter initially vanishes. As a consequence, non-perturbative effects will renormalize m_u/m_d . If this ratio is zero at some scale, it cannot remain so for all scales. Only in the isospin limit are quark mass ratios renormalization group invariant. As lattice simulations include all perturbative and non-perturbative effects, this phenomenon is automatically included in such an approach.

Confinement plays a crucial role in what is effectively an ambiguity in defining quark masses. Because quarks cannot travel long distances in isolation, their masses cannot be directly inferred from long distance propagators. This is tied directly with the phase diagram discussed in Section 6, where it is shown that no discernable physical structure is seen when single quark mass vanishes.

This cross talk between the masses of different quark species is a relatively straightforward

consequence of the chiral anomaly and has been discussed several times in the past, usually in the context of gauge field topology and the index theorem [2, 4–6]. Despite the simplicity of the above argument, the conclusion is frequently met with skepticism from the perturbative community. In perturbation theory, spin flip processes are suppressed as the quark masses go to zero. The above discussion shows that this lore need not apply when anomalous processes come into play. In particular, mass renormalization can not be flavor blind and the concept of mass independent regularization is problematic. Since the quark masses influence each other, there are inherent ambiguities defining $m_u = 0$. This has consequences for the strong CP problem, discussed further below. Furthermore, since these effects involve quark mass differences, a traditional perturbative regulator such as \overline{MS} is not complete when $m_u \neq m_d$. Because of this, the practice of matching lattice calculations to \overline{MS} is problematic, a point that is sometimes ignored [7, 8]. (Ref. [7] also suffers from an uncontrolled extrapolation in the number of quark species [9].)

III. SPECIFIC CRITIQUES

Given the simplicity of the argument in the previous section, it may seem surprising that it often receives severe criticism. The first complaint sometimes made is that one should work directly with bare quark masses. This ignores the fact that the bare quark masses all vanish under renormalization. The renormalization group equation for a quark mass reads

$$a\frac{dm_i}{da} = \gamma(g)m_i = \gamma_0 g^2 + O(g^4) \tag{3}$$

where the leading coefficient is well known, $\gamma_0 = \frac{8}{(4\pi)^2}$. As asymptotic freedom drives the bare coupling to zero, the bare masses behave as

$$m \sim g^{\gamma_0/\beta_0}(1+O(g^2)) \to 0$$
 (4)

where β_0 (explicitly given later) is the first term in the beta function controlling the vanishing of the bare coupling in the continuum limit. Since all bare quark masses are formally zero, one must address these questions in terms of a renormalization scheme at a finite cutoff.

The second objection often made is that in a mass independent regularization scheme, mass ratios are automatically constant. Such an approach asks that the renormalization group function $\gamma(g)$ in Eq. (3) be chosen to be independent of the quark species and mass. This immediately implies the constancy of all quark mass ratios. As only the first term in the perturbative expansion

of $\gamma(g)$ is universal, a mass independent scheme is indeed an allowed procedure. However, such a scheme obscures the off-diagonal m_d effect on m_u discussed above. In particular, by forcing constancy of bare mass ratios, one will find that the ratios of physical particle masses will vary as a function of cutoff. This will be in a manner that cancels the flow from the process in Section II. The fact that physical particle mass ratios are not just a function of quark mass ratios is shown explicitly in Section 6, where it is shown that in the chiral limit the combination $1 - m_{\pi_0}^2/m_{\pi_{\pm}}^2$ is proportional to $\frac{(m_d - m_u)^2}{(m_d + m_u)\Lambda_{qcd}}$.

From a non-perturbative point of view, having physical mass ratios vary with cutoff seems rather peculiar; indeed, the particle masses are physical quantities that would be natural to hold fixed. And, even though a mass independent approach is theoretically possible, there is no guarantee that any given ratio $\frac{m_i}{m_j}$ will be universal between schemes. Finally, the lattice approach itself is usually implemented with physical particle masses as input. As such it is not a mass independent regulator, making a perturbative matching to lattice results rather subtle.

A third frequent complaint against the argument in Section II is that one should simply do the matching at some high energy, say 100 GeV, where "instanton" effects are exponentially suppressed and irrelevant. This point of view has several problems. First, the lattice simulations are not done at miniscule scales and non-perturbative effects are present and substantial. Furthermore, the exponential suppression of topological effects is in the inverse coupling, which runs logarithmically with the scale. As such, the non-perturbative suppression is a power law in the scale and straightforward to estimate.

Recall the renormalization group prediction for how the eta prime mass depends on the coupling in the continuum limit

r

$$n_{\eta'} \propto \frac{1}{a} e^{-1/(2\beta_0 g^2)} g^{-\beta_1/\beta_0^2}.$$
 (5)

Here $\beta_0 = \frac{11-2n_f/3}{(4\pi)^2}$, $\beta_1 = \frac{102-12n_f}{(4\pi)^4}$, n_f is the number of quark flavors, and *a* is the cutoff scale, *i.e.* the lattice spacing with such a renormalization scheme. While this formula indeed shows the exponential suppression in $1/g^2$, this is cancelled by the inverse cutoff factor in just such a way that the mass of this physical particle remains finite. The ambiguity in the quark mass splitting is controlled by the mass splitting $m_{\eta'} - m_{\pi_0}$ as well as being proportional to $m_d - m_u$. Considering $m_d = 5$ MeV at a scale of $\mu = 2$ GeV, a rough estimate of the order of the *u* quark mass shift is

$$\Delta m_u(\mu) \sim \left(\frac{m_{\eta'} - m_{\pi_0}}{\Lambda_{qcd}}\right) \ (m_d - m_u) = O(1 \text{ MeV}),\tag{6}$$

a number comparable to typical phenomenological estimates. Of course the result depends on

scale, but that dependence is only logarithmic and given by Eq. (4). Additional flavors will reduce the size of this effect; with the strange quark present, it should be proportional to $m_d m_s$.

It is important to note that for a modest number of flavors the exponent controlling the coupling constant suppression in Eq. 5 differs substantially from the classical instanton action

$$\frac{8\pi^2}{(11-2n_f/3)g^2} << \frac{8\pi^2}{g^2}.$$
(7)

This difference arises because one should consider topological excitations above the quantum, not the classical, vacuum. Zero modes of the Dirac operator are still responsible for the bulk of the eta prime mass, but naive semi-classical arguments strongly underestimate their effect.

IV. GENERAL MASSES IN TWO-FLAVOR QCD

Given the confusion over the meaning of quark masses, it is useful to explore the behavior of two-flavor QCD as these quantities are varied. Here I review how the theory depends on the three non-trivial mass parameters. These includes the possibility of explicit CP violation. The full theory has a rather rich phase diagram, including both first and second order phase transitions, some occurring when none of the quark masses vanish.

For the following the quark fields ψ carry implicit isospin, color, and flavor indices. I assume that the theory in the massless limit has the flavored chiral symmetry under

$$\begin{split} \psi &\longrightarrow e^{i\gamma_5\tau_\alpha\phi_\alpha/2}\psi\\ \overline{\psi} &\longrightarrow \overline{\psi}e^{i\gamma_5\tau_\alpha\phi_\alpha/2}. \end{split}$$
(8)

Here τ_{α} represents the Pauli matrices generating isospin rotations. The angles ϕ_{α} are arbitrary rotation parameters. This, of course, is the chiral symmetry that is spontaneously broken to give the massless Goldstone pions.

I wish to construct the most general possible two-flavor mass term to add to the massless Lagrangian. Such should be a dimension 3 quadratic form in the fermion fields and should transform as a singlet under Lorentz transformations. For simplicity, I only consider quantities that are charge neutral as well. This leaves four candidate fields, giving the generalized form for consideration

$$m_1 \overline{\psi} \psi + m_2 \overline{\psi} \tau_3 \psi + i m_3 \overline{\psi} \gamma_5 \psi + i m_4 \overline{\psi} \gamma_5 \tau_3 \psi. \tag{9}$$

The first two terms are naturally interpreted as giving the average quark mass and the quark mass difference, respectively. The remaining two terms are less conventional. The m_3 term is connected

with the CP violating parameter of the theory. The final m_4 term has been used in conjunction with the Wilson discretization of lattice fermions, where it is referred to as a "twisted mass" [10, 11]. Its utility in that context is the ability to reduce lattice discretization errors, but that is not the subject of this note.

These four terms are not independent. Indeed, consider the above flavored chiral rotation in the τ_3 direction, $\psi \rightarrow e^{i\theta \tau_3 \gamma_5} \psi$. Under this the terms transform as

$$\overline{\psi}\psi \longrightarrow \cos(\theta)\overline{\psi}\psi + \sin(\theta)i\overline{\psi}\gamma_5\tau_3\psi$$

$$\overline{\psi}\tau_3\psi \longrightarrow \cos(\theta)\overline{\psi}\tau_3\psi + \sin(\theta)i\overline{\psi}\gamma_5\psi$$

$$i\overline{\psi}\tau_3\gamma_5\psi \longrightarrow \cos(\theta)i\overline{\psi}\tau_3\gamma_5\psi - \sin(\theta)\overline{\psi}\psi$$

$$i\overline{\psi}\gamma_5\psi \longrightarrow \cos(\theta)i\overline{\psi}\gamma_5\psi - \sin(\theta)\overline{\psi}\tau_3\psi$$
(10)

Such a rotation mixes m_1 with m_4 and m_2 with m_3 . Using this freedom, one can select any one of the m_i to vanish and a second to be positive.

The most common choice is to set $m_4 = 0$ and use m_1 as controlling the average quark mass. Then m_2 gives the quark mass difference, and CP violation appears in m_3 . This, however, is only a convention. The alternative "twisted mass" scheme [10, 11], makes the choice $m_1 = 0$. This uses $m_4 > 0$ for the average quark mass, and m_3 becomes the up-down mass difference. In this case m_2 becomes the CP violating term. It is amusing to note that an up down quark mass difference in this formulation involves the naively CP odd $i\overline{\psi}\gamma_5\psi$. The strong CP problem has been rotated into the smallness of the $\overline{\psi}\tau_3\psi$ term, which with the usual conventions is the mass difference. But because of the flavored chiral symmetry, both sets of conventions are physically equivalent.

For the following I make the arbitrary choice $m_4 = 0$, although one should remember that this is only a convention and I could have chosen any of the four parameters in Eq. (9) to vanish. With this choice two-flavor QCD, after scale setting, depends on three mass parameters

$$m_1 \overline{\psi} \psi + m_2 \overline{\psi} \tau_3 \psi + i m_3 \overline{\psi} \gamma_5 \psi. \tag{11}$$

It is the possible presence of m_3 that represents the strong CP problem. As all the parameters are independent and transform differently under the symmetries of the problem, there is no connection between the strong CP problem and m_1 or m_2 .

As is well known, the chiral anomaly is responsible for the singlet rotation

$$\begin{split} \psi &\longrightarrow e^{i\gamma_5 \phi/2} \psi \\ \overline{\psi} &\longrightarrow \overline{\psi} e^{i\gamma_5 \phi/2} \end{split} \tag{12}$$

not being a valid symmetry, despite the fact that γ_5 naively anti-commutes with the massless Dirac operator. The anomaly is quite nicely summarized via Fujikawa's [12] approach where after the above rotation the fermion measure in the path integral picks up a factor of

$$\det(e^{i\gamma_5\phi}) = \exp(i\phi\operatorname{Tr}\gamma_5). \tag{13}$$

Using the Dirac operator D itself as a regulator, define

$$\operatorname{Tr} \gamma_5 = \lim_{\Lambda \to \infty} \gamma_5 e^{D^2/\Lambda^2}.$$
 (14)

In any give gauge configuration only the zero eigenmodes of D contribute, and by the index theorem this is connected to the winding number of the gauge configuration. The conclusion is that the above rotation changes the fermion measure by an amount depending non-trivially on the gauge field configuration.

Note that this anomalous rotation allows one to remove any topological term from the gauge part of the action. Naively this would have been yet another parameter for the theory, but by including all three mass terms for the fermions, this can be absorbed. For the following I consider that any topological term has thus been rotated away. After this one is left with the three mass parameters above, all of which are independent and relevant to physics.

These parameters are a complete set for two-flavor QCD; however, this choice differs somewhat from what is often discussed. Formally one defines the more conventional variables as

$$m_{u} = m_{1} + m_{2} + im_{3}$$

$$m_{d} = m_{1} - m_{2} + im_{3}$$

$$e^{i\Theta} = \frac{m_{1}^{2} - m_{2}^{2} - m_{3}^{2} + 2im_{1}m_{3}}{\sqrt{m_{1}^{4} + m_{2}^{4} + m_{3}^{4} + 2m_{1}^{2}m_{3}^{2} + 2m_{2}^{2}m_{3}^{2} - 2m_{1}^{2}m_{2}^{2}}}.$$
(15)

Particularly for Θ , this is a rather complicated change of variables. For non-degenerate quarks in the context of the phase diagram discussed below, the variables $\{m_1, m_2, m_3\}$ are more natural.

V. THE STRONG CP PROBLEM

The strong interactions preserve CP to high accuracy. Thus only two of the three possible mass parameters seem to be needed. With the above conventions, it is natural to ask why is m_3 so small?

It is the concept of unification that brings this question to the fore. The weak interactions of course do violate CP. Thus, if the electroweak and the strong interactions separate at some

high scale, why doesn't some remnant of this breaking survive in the strong sector? How is CP recovered for the nuclear force?

Several "solutions" to this puzzle have been proposed. Perhaps the simplest is that there is no unification and the strong interactions should be considered on their own with the electroweak effects being only a small perturbation. A second approach is to add an additional "axion" field to make the CP phase a dynamical field that relaxes to zero [13, 14]. The coupling of this additional field is not determined a priori, and thus it need only be small enough to have avoided detection in past experiments.

Another often proposed solution involves having the lightest quark mass vanish, making its phase irrelevant. Several years ago this was criticized because the definition of an isolated quark mass is inherently ambiguous due to confinement [2]. As this conclusion remains controversial, I return to this topic and reexpress the problem in terms of the above mass terms. I hope this language will clarify why relating a vanishing up quark mass to the strong CP problem is a tautology.

Why is a vanishing up quark mass not a sensible approach? From the above, one can define the up quark mass as a complex number

$$m_u \equiv m_1 + m_2 + im_3 \tag{16}$$

But the quantities m_1 , m_2 , and m_3 are independent parameters with different symmetry properties. With our conventions, m_1 represents an isosinglet mass contribution, m_2 is isovector in nature, and m_3 is CP violating. And, as extensively discussed earlier, the combination $m_1 + m_2 = 0$ is scale and scheme dependent. The strong CP problem only requires small m_3 . So while it may be true formally that

$$m_1 + m_2 + im_3 = 0 \Rightarrow m_3 = 0,$$
 (17)

this would depend on scale and one might well regard this as "not even wrong."

VI. PHASE DIAGRAM FOR GENERAL QUARK MASSES

As a function of the three mass parameters, QCD has a rather intricate phase diagram. From simple chiral Lagrangian arguments this diagram can be qualitatively mapped out. Ref. [15] studied this system in the $m_2 = 0$ case; a first order transition is expected along the m_3 axes at $m_1 = 0$. In conventional notation, this corresponds to the strong CP parameter Θ taking the value π . That paper, however, incorrectly speculated on the structure for non-degenerate quarks. In Ref. [16] the



FIG. 3: The m_2 and m_3 terms warp the Mexican hat potential into two separate minima. The direction of the warping is determined by the relative size of these parameters.

picture was generalized to several degenerate flavors and the first order transition at $\Theta = \pi$ was shown to be generic for all $n_f > 1$. Ref. [17] studied the phase diagram for $m_3 = 0$ and showed how the isospin breaking m_2 term splits the chiral transition into two second-order transitions separated by a phase with spontaneous CP violation. These second order transitions occur where none of the quarks are massless.

The full phase diagram in terms of all mass parameters can be deduced from a linear sigma model [18] analysis, generalizing Ref. [15]. For this, define the composite fields

$$\sigma = \overline{\psi}\psi \qquad \qquad \eta' = i\overline{\psi}\gamma_5\psi \vec{\pi} = i\overline{\psi}\gamma_5\vec{\tau}\psi \qquad \qquad \vec{a}_0 = \overline{\psi}\vec{\tau}\psi.$$
(18)

In terms of these, a natural starting effective potential is

$$V = \lambda (\sigma^{2} + \vec{\pi}^{2} - v^{2})^{2} - m_{1}\sigma - m_{2}a_{03} - m_{3}\eta' + \alpha (\eta'^{2} + \vec{a}_{0}^{2}) - \beta (\eta'\sigma + \vec{a}_{0} \cdot \vec{\pi})^{2}.$$
(19)

Here α and β are "low energy constants" that bring in a chirally symmetric coupling of $(\sigma, \vec{\pi})$ with (η', \vec{a}_0) . As discussed in Ref. [15], α gives mass to the η' and \vec{a} mesons while β splits their masses. The sign of the β term is suggested so that $m_{\eta'} < m_{a_0}$. The effect of the anomaly is manifest in these terms.



FIG. 4: When $m_3 = 0$, the warping of the effective potential is downward in the π_0 direction. The sign of m_1 can not pick one of the minima uniquely, giving the possibility of the π_0 field spontaneously acquiring an expectation value.

The potential in Eq. (19) is a somewhat arbitrary model. It is natural to ask if the results of this section are robust under variations of this form. The crucial feature of the potential is the non-trivial minima associated with chiral symmetry breaking. Something similar to the α term is needed to give the η' a non-vanishing mass. The β term is somewhat arbitrary; Ref. [15] discusses how things would change qualitatively if it sign was reversed. The other implicit assumption is that the masses are small enough that they don't dramatically alter the underlying structure of the potential. With these caveats, the final phase diagram should be qualitatively correct for any similar potential.

This potential builds on the famous "Mexican hat" or "wine bottle" potential, in which the Goldstone pions are associated with the flat directions running around at constant $\sigma^2 + \vec{\pi}^2 = v^2$. The m_2 and m_3 terms do not directly affect the σ and π fields, but induce an expectation value for a_{03} and η' , respectively. This in turn results in the α and β terms inducing a warping of the Mexican hat into two separate minima, as sketched in Fig. 3. The direction of this warping is determined by the relative size of m_2 and m_3 ; m_2 (m_3) warps downward in π_0 (σ) direction. Turning on m_1 , this selects one of the two minima as favored. Which one depends on the sign of m_1 . This selection gives rise to a generic first order transition at $m_1 = 0$.

In addition to this transition, there is an interesting structure in the m_1, m_2 plane when m_3 vanishes. In this situation the quadratic warping is downward in the π_0 direction, as sketched in



FIG. 5: In the m_1, m_2 plane, $m_{\pi_0}^2$ can pass through zero, giving rise to pion condensation at an Ising-like transition. Figure taken from [15].

Fig. 4. For large $|m_1|$ only σ will have an expectation, with sign determined by the sign of m_1 . The pion will be massive, but the quark mass difference will give a neutral pion mass below that of the charged pions. As m_1 decreases in magnitude at fixed m_2 , eventually the neutral pion becomes massless and condenses. This is sketched in Fig. 5. An order parameter for the transition is the expectation value of the π_0 field, with the transition being in the class of the four dimensional Ising model.

In this simple model the ratio of the neutral to charged pion masses can be estimated from a quadratic expansion about the minimum of the potential. For $m_3 = 0$ and m_1 above the transition line, this gives

$$\frac{m_{\pi_0}^2}{m_{\pi_+}^2} = 1 - \frac{\beta v m_2^2}{2\alpha^2 m_1} + O(m^2).$$
⁽²⁰⁾

The second order transition is located where this vanishes, and thus occurs for m_1 proportional to m_2^2 . Note that this equation shows that a constant quark mass ratio does not correspond to a constant meson mass ratio and vice versa. This is the ambiguity discussed in Section II. This model should not be trusted when the quark masses become of order Λ_{qcd} , but the Vafa-Witten theorem [19] shows that the transition can only occur in a region where the two flavors have opposite signs for their masses, i.e. $|m_1| < |m_2|$.

Note that this transition occurs when both m_u and m_d are non-vanishing but of opposite sign. At the transition the correlation length diverges. This is a simple example of how it is possible to have significant long distance physics without small Dirac eigenvalues. Complimentarily, there is no structure at points where only one of the quark masses vanishes. In this situation there is no long distance physics despite the possible existence of small Dirac eigenvalues. This is connected with the difficulty in defining a vanishing quark mass as discussed in Section II.

Putting this all together gives the final phase diagram sketched in Fig. 6. There are two intersecting first-order surfaces, one at $\{m_1 = 0, m_3 \neq 0\}$ and the second at $\{m_1 < m_2, m_3 = 0\}$. The latter ends at second-order curves that touch the lines of vanishing quark mass only at the origin.



FIG. 6: The full phase diagram for two-flavor QCD as a function of the three mass parameters. It consists of two intersecting first-order surfaces with second-order edges along curves satisfying $m_3 = 0$, $|m_1| < |m_2|$. There is no structure along the $m_u = 0$ line except when both quark masses vanish.

The transition at the origin itself is, of course, that of the four dimensional O(4) sigma model. The octets defined by the signs of the three mass terms are characterized by the signs of the expectation values for the conjugate fields σ , π_0 , η' . The flavored chiral symmetry of Eq. (10) combined with permutation symmetry for the two flavors shows that the eight corresponding regions divide into two sets of four with equivalent physics, the sets differing in the sign of CP violating effects.

The first-order surfaces both occur where the formal parameter Θ takes the value π . However, note that with non-degenerate quarks there is also a finite $\Theta = \pi$ region with m_2 near m_1 where there is no transition. The absence of any physical singularity at $m_u = 0$ when $m_d \neq 0$ lies at the heart of the problem of defining a vanishing quark mass.

VII. SUMMARY

Non-perturbative effects in QCD couple the renormalization group flow for the masses of different fermion species. This effect is absent in perturbation theory, but is automatically included in lattice gauge simulations. This coupling means that quark mass ratios are generally not constants but depend on renormalization scale. This is true for vanishing as well as non-vanishing quark masses. One practical consequence is that it is inappropriate to match lattice and perturbative masses.

Taking into account the possibility of CP violation, the general two-flavor theory depends on 3 mass parameters. A simple effective Lagrangian approach reveals an intricate phase diagram containing both first and second order transitions as the mass parameters are varied. This diagram displays no structure at $m_u = 0$ when $m_d \neq 0$, suggesting that $m_u = 0$ is not an appropriate solution to the strong CP problem.

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