Spontaneous CP-violation in the strong interaction at $\theta = \pi$  

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(Dated: September 26, 2008)

Spontaneous CP-violation in the strong interaction is analyzed at $\theta = \pi$ within the framework of the two-flavor NJL model. It is found that the occurrence of spontaneous CP-violation at $\theta = \pi$ depends on the strength of the 't Hooft determinant interaction, which describes the effect of instanton interactions. The dependence of the phase structure, and in particular of the CP-violating phase, on the quark masses, temperature, baryon and isospin chemical potential is examined in detail. When available a comparison to earlier results from chiral perturbation theory is made. From our results we conclude that spontaneous CP-violation in the strong interaction is an inherently low-energy phenomenon. In all cases we find agreement with the Vafa-Witten theorem, also at nonzero density and temperature. Meson masses and mixing in the CP-violating phase display some unusual features as a function of instanton interaction strength. A modification of the condition for charged pion condensation at nonzero isospin chemical potential and a novel phase of charged $a_0$ mesons are discussed.

PACS numbers: 12.39.-x,11.30.Er,11.30.Rd

I. INTRODUCTION

The possibility of CP-violation in the strong interaction has been studied extensively. The QCD Lagrangian naturally incorporates a $\theta$-term $\mathcal{L}_\theta = \frac{a}{\sqrt{2\pi}} \tilde{F} \tilde{F}$, which can lead to CP-violation due to instanton contributions. Only for $\theta = 0 \mod \pi$ the Lagrangian is CP-conserving. In nature the value of $\theta$ is extremely close to zero, as has been concluded from pseudoscalar mass ratios and the neutron electric dipole moment [1, 2, 3]. This suggests that $\theta = 0$, but the lack of a satisfactory explanation of why this should be the case is commonly referred to as the strong CP problem.

At $\theta = 0$ no explicit CP-violation is present in the Lagrangian, but in addition, the well-known Vafa-Witten theorem states that spontaneous parity violation in QCD at $\theta = 0$ does not arise [4]. This rules out the possibility that $\langle \tilde{F} \tilde{F} \rangle \neq 0$ at $\theta = 0$ and implies that the QCD ground state for nonzero $\theta$ must have higher energy than at $\theta = 0$. The situation is different at $\theta = \pi$, when the Lagrangian is also explicitly CP-conserving. In this case spontaneous CP-violation could arise, as was first pointed out by Dashen [5]. There are then two degenerate CP-violating vacua, which differ by a CP transformation from each other.

This possibility of spontaneous CP-violation is one of the reasons why people have studied the $\theta$-dependence of the strong interactions. However, to study this in full QCD is very difficult due to the nonperturbative nature of the $\theta$-term. Even in lattice QCD, studies are limited to small $\theta$, because of the problem of how to deal with complex phases. Therefore, the $\theta$-dependence of the strong interaction and Dashen’s phenomenon have been studied extensively using low energy effective theories, such as chiral perturbation theory [6, 7, 8, 9, 10, 11, 12, 13], or by using specific models, such as the NJL model [14]. In a quark model, like the NJL model, the effects of instantons and the $\theta$-term are incorporated via an effective interaction, the ‘t Hooft determinant interaction [15, 16]. In chiral perturbation theory these effects can be included in a similar way via a log determinant interaction [6, 7]. Here we shall denote the strength of the latter interaction by $a$. Whether or not the theory exhibits spontaneous CP-violation at $\theta = \pi$ depends on $a$ and on the values of the quark masses. Two limiting cases were discussed in the literature, Ref. [6], which considers lowest-order chiral perturbation theory, states that when $a/N$ is nonzero but much smaller than the quark masses, the theory always exhibits spontaneous CP-violation at $\theta = \pi$, independent of the values of the quark masses and number of flavors $N$. The opposite case [1, 7, 8], i.e. when the masses of the quarks are much smaller than $a/N$, leads to different results. In this case it does depend on the values of the quark masses. In the two-flavor case for $a/N \to \infty$ (which means no $\eta$ meson is included), spontaneous CP-violation only occurs for degenerate quark masses (in that case actually for all finite values of $a/N$). For finite $a/N \gg m_\pi m_d$ spontaneous CP-violation also occurs for nondegenerate quark masses in a finite interval of $m_d/m_u$ around 1, as was shown in Ref. [8]. In the three-flavor case, a region exists in the $(m_u, m_d)$-plane where the theory spontaneously violates CP invariance [11], as shown in Fig. 1. The asymptotes depend on the value of the strange quark mass.

In first-order chiral perturbation theory there are only a few parameters, namely the quark masses, the pion
decay constant and the strength of the determinant interaction. It is therefore interesting to study CP-violation in a somewhat richer situation, such as chiral perturbation theory beyond leading order, which has been studied in Ref. [8] for $a/N \to \infty$. Here we will make a comprehensive study of the $\theta$-dependence and especially spontaneous CP-violation at $\theta = \pi$ within the framework of the two-flavor NJL model in the mean-field approximation. We will study the dependence on the effective instanton interaction strength (denoted by $c$ in this case), not only in the two limiting cases, but for all possible values. We find that there is a critical value of the interaction strength above which spontaneous CP violations occurs and which depends linearly on the quark masses, as expected from axial anomaly considerations.

As will be discussed, the two-flavor NJL model allows for spontaneous CP-violation also for nondegenerate quark masses. We find a region in the $(m_u, m_d)$-plane very similar to the three-flavor lowest-order chiral perturbation theory result shown in Fig. 1. However, for the two-flavor NJL model the asymptotes are determined by the strength of the instanton induced interaction.

We will also study the influence of nonzero temperature and baryon and isospin chemical potential. It has been suggested that in those cases the Vafa-Witten theorem may no longer apply (see for instance Ref. [17] for some explicit arguments, but also Ref. [18] for counterarguments). But even if it does apply, spontaneous CP-violation at finite temperature or baryon chemical potential (through meta-stable states) has been considered in the literature [19, 20, 21, 22] and possible experimental signatures in heavy ion collisions have been put forward [23, 24, 25, 26]. This would also be relevant in the early universe, when possibly $\theta$ was nonzero and later relaxed to zero, for example via a Peccei-Quinn-like mechanism [27, 28, 29]. We therefore wish to check the Vafa-Witten theorem and the possible presence of CP-violating local minima in the NJL model at finite temperature and density.

Spontaneous CP-violation at $\theta = \pi$ within the two-flavor NJL model including temperature dependence has been considered before in Ref. [14], but only for a very limited range of quark masses: $|m_u \pm m_d| < 6$ MeV and without chemical potentials.

In Ref. [13] the phase diagram as a function of $\theta$ and isospin chemical potential has been investigated within first-order chiral perturbation theory for two flavors and effectvely $a/N \to \infty$ (due to the absence of the $\eta$ meson). We will compare this to our results at nonzero isospin chemical potential, where a modification of the pattern of charged pion condensation is observed at $\theta = \pi$.

This article is organized as follows. First the NJL model is briefly introduced to set the notation, then we discuss the effect of chiral transformations on the theory, which is relevant for the calculation of the effective potential and for a comparison to earlier results from the literature. We continue with a discussion of the $\theta$-dependence of the ground-state, including temperature effects and nonzero baryon and isospin chemical potential. Also we discuss the $c$-dependence of the meson masses and mixing in the CP-violating phase. We end with conclusions and a further discussion of the results.
II. THE NJL MODEL

The Nambu-Jona-Lasinio (NJL) model, introduced in Refs. [30, 31], is a low energy effective theory that contains four-point interactions between the quarks. In this article the following form of the NJL-model is used

$$\mathcal{L} = \bar{\psi} (i \gamma^\mu \partial_\mu + \gamma_0 \mu) \psi - \mathcal{L}_M + \mathcal{L}_{\bar{q}q} + \mathcal{L}_{\text{det}},$$

(1)

where the mass term of the Lagrangian is

$$\mathcal{L}_M = \bar{\psi} M_0 \psi,$$

(2)

and $\mu = (\mu_u, \mu_d)$ denotes the chemical potential. Furthermore,

$$\mathcal{L}_{\bar{q}q} = G_1 \left[ (\bar{\psi} \lambda_a \psi)^2 + (\bar{\psi} \lambda_a i \gamma_5 \psi)^2 \right],$$

(3)

is the attractive part of the $\bar{q}q$ channel of the Fierz transformed color current-current interaction [32] and

$$\mathcal{L}_{\text{det}} = G_2 e^{i \theta} \text{det} (\bar{\psi}_R \psi_L) + \text{h.c.},$$

(4)

is the 't Hooft determinant interaction which depends on the QCD vacuum angle $\theta$. Often $G_1$ and $G_2$ are taken equal, which at $\theta = 0$ means the low energy spectrum consists of $\sigma$ and $\pi$ fields only. We will restrict to the two flavor case, using $\lambda_a$ with $a = 0, \ldots, 3$ as generators of U(2). We will not take into account diquark interactions, and therefore do not consider color superconductivity that is expected to arise at high baryon chemical potential and low temperatures. We choose an appropriate basis of quark fields, such that the mass-matrix $M_0$ is diagonal, i.e.,

$$\begin{pmatrix} m_u & 0 \\ 0 & m_d \end{pmatrix}.$$  

(5)

The symmetry structure of the NJL model is very similar to that of QCD. In the absence of quark masses and the instanton interaction there is a global SU(3)$_c \times$U(2)$_R \times$U(2)$_L$-symmetry. The instanton interaction breaks it to SU(3)$_c \times$SU(2)$_R \times$SU(2)$_L \times$U(1)$_B$. For nonzero, but equal quark masses this symmetry is reduced to SU(3)$_c \times$SU(2)$_V \times$U(1)$_B$. For unequal quark masses and chemical potentials one is left with SU(3)$_c \times$U(1)$_B \times$U(1)$_I$, where $B$ and $I$ stand respectively for baryon number and isospin.

III. CHIRAL TRANSFORMATIONS AND NEGATIVE QUARK MASS

It is well known that a theory with $\theta = \pi$ can be related to a theory with a negative quark mass. Since this sometimes leads to confusion concerning the terminology used for the meson spectrum, we will elaborate on this relation in this section.

A. QCD

We start with the QCD partition function including the $\theta$ term:

$$Z = \int \mathcal{D} \psi' \mathcal{D} \bar{\psi}' \mathcal{D} A e^{i \int d^4x \left[ \mathcal{L}_{\text{QCD}} + \mathcal{L}_\theta \right]},$$

(6)

where

$$\mathcal{L}_{\text{QCD}} = \bar{\psi} (i \partial_\mu - m) \psi - \frac{1}{4} \text{Tr} F^{\mu \nu} F_{\mu \nu},$$

$$\mathcal{L}_\theta = \frac{\theta g^2}{32 \pi^2} \text{Tr} F^{\mu \nu} F_{\mu \nu}.$$

(7)

The fermion measure of gauge theories is not invariant under chiral transformations [33], which can be used to remove $\mathcal{L}_\theta$. Since the mass term is not invariant under chiral transformations, a $\theta$ dependence then appears in the mass term. One obtains

$$Z = \int \mathcal{D} \psi' \mathcal{D} \bar{\psi}' \mathcal{D} A e^{i \int d^4x \mathcal{L}'_{\text{QCD}}},$$

(8)
where the $\theta$-dependence resides in the mass term. Although the physical results one obtains using the transformed expression will be equivalent, one has to be careful when evaluating vacuum expectation values. We define vacuum expectation values of an operator $\mathcal{O} = \mathcal{O}(\bar{\psi}, \psi)$ in terms of the original fields (the one of the Lagrangian) and in terms of the transformed or “primed” fields as follows:

$$
\langle \mathcal{O} \rangle_\theta = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A \mathcal{O}(\bar{\psi}, \psi) e^{i\int d^4x [\mathcal{L}_{\text{QCD}} + \mathcal{L}_\theta]},
$$

$$
\langle \mathcal{O}' \rangle_\theta = \int \mathcal{D}\psi' \mathcal{D}\bar{\psi}' \mathcal{D}A' \mathcal{O}'(\bar{\psi}', \psi') e^{i\int d^4x' \mathcal{L}'_{\text{QCD}}}. 
$$

(9)

Clearly, the condensates $\langle \mathcal{O} \rangle_\theta$ and $\langle \mathcal{O}' \rangle_\theta$ differ for $\theta \neq 0$ and are related by a $\theta$-dependent transformation. For instance,

$$
\langle \bar{\psi}\psi \rangle_\theta = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A \bar{\psi}\psi e^{i\int d^4x [\mathcal{L}_{\text{QCD}} + \mathcal{L}_\theta]} \neq \int \mathcal{D}\psi' \mathcal{D}\bar{\psi}' \mathcal{D}A' \bar{\psi}'\psi' e^{i\int d^4x' \mathcal{L}'_{\text{QCD}}} = \langle \bar{\psi}'\psi' \rangle_\theta.
$$

(10)

When discussing a vacuum expectation value like $\langle \bar{\psi}\psi \rangle_\theta$ it has to be accompanied by a statement about which Lagrangian one is using.

In what follows we will select the chiral transformation that only affects the up quark:

$$
u_L = e^{-i\theta/2}u'_L, 
\nu_R = e^{i\theta/2}u'_R.
$$

(11)

This removes $\mathcal{L}_\theta$ from the Lagrangian and the up-quark mass term changes according to

$$
\tilde{u}m_u \nu = \tilde{u}' [m_u \cos \theta + m_u i\gamma_5 \sin \theta] \nu'.
$$

(12)

For $\theta = \pi$ a negative up-quark mass results. In addition,

$$
\langle \tilde{u}\nu \rangle_\theta = \langle \tilde{u}'\nu' \rangle_\theta \cos \theta + \langle \tilde{u}'i\gamma_5\nu' \rangle_\theta \sin \theta.
$$

(13)

Below we will use the following notation for the meson condensates:

$$
\langle \sigma \rangle = \langle \bar{\psi}\lambda_0\psi \rangle, 
\langle \eta \rangle = \langle \bar{\psi}\lambda_0i\gamma_5\psi \rangle, 
\langle \pi \rangle = \langle \bar{\psi}\lambda_i\gamma_5\psi \rangle.
$$

(14)

These condensates transform according to:

$$
\langle \sigma \rangle = \frac{1}{2} (\cos \theta + 1) \langle \sigma' \rangle + \frac{1}{2} (\cos \theta - 1) \langle a_0' \rangle + \frac{1}{2} \sin \theta \langle \eta' \rangle + \frac{1}{2} \sin \theta \langle \pi' \rangle,
$$

$$
\langle a_0^\pm \rangle = \cos \frac{\theta}{2} \langle a_0^\mp \rangle + \sin \frac{\theta}{2} \langle \pi^\pm \rangle,
$$

$$
\langle a_0^\pi \rangle = \frac{1}{2} (\cos \theta - 1) \langle \sigma' \rangle + \frac{1}{2} (\cos \theta + 1) \langle a_0' \rangle + \frac{1}{2} \sin \theta \langle \eta' \rangle + \frac{1}{2} \sin \theta \langle \pi' \rangle,
$$

$$
\langle \eta \rangle = \frac{1}{2} (\cos \theta + 1) \langle \eta' \rangle + \frac{1}{2} (\cos \theta - 1) \langle \pi^0 \rangle - \frac{1}{2} \sin \theta \langle \sigma' \rangle - \frac{1}{2} \sin \theta \langle a_0' \rangle,
$$

$$
\langle \pi^\pm \rangle = \cos \frac{\theta}{2} \langle \pi^\mp \rangle - \sin \frac{\theta}{2} \langle a_0^\pm \rangle,
$$

$$
\langle \pi^0 \rangle = \frac{1}{2} (\cos \theta - 1) \langle \eta' \rangle + \frac{1}{2} (\cos \theta + 1) \langle \pi^0 \rangle - \frac{1}{2} \sin \theta \langle \sigma' \rangle - \frac{1}{2} \sin \theta \langle a_0^0 \rangle.
$$

(15)

Therefore, one has to be careful assigning the names $\pi^0$ and $\eta$ to the condensates after doing a chiral transformation. For example, Ref. [14] discusses a $\langle \pi^0 \rangle$-condensate using a Lagrangian without $\theta$ term, but with negative up or down quark mass. This corresponds to an $\langle \eta \rangle$-condensate using a Lagrangian with positive quark masses and a $\theta$-term with $\theta = \pi$. We emphasize that these transformations are just a matter of consistently naming mesons and vev’s, but this is nevertheless important for the comparison of quantities from different calculations.
B. NJL-model

As the NJL-model is not a gauge-theory, the fermion measure is invariant under chiral transformations. But now the Lagrangian contains two terms that are not invariant under chiral transformations, the mass-term and the determinant interaction. The latter is \( \theta \)-dependent. Like for QCD, this \( \theta \)-dependence can be put in the up-quark mass term using a chiral transformation. So the analysis for the NJL-model is similar to the analysis for QCD, but instead of a noninvariant measure we have a noninvariant effective interaction.

The calculation of the ground-state of the NJL-model is more conveniently done with the \( \theta \)-dependence in the up-quark mass term, i.e. we use

\[
\mathcal{L}_M' = \bar{u}R m_\alpha e^{-i\theta} u_L' + \bar{d}R m_\alpha d_L' + \text{h.c.},
\]

\[
\mathcal{L}_\text{det}' = G_2 \det \left( \bar{\psi}_R' \psi_L' \right) + \text{h.c.}
\]

Therefore, below we will calculate the effective potential using the transformed (primed) fields, but discuss the ground state phase structure solely in terms of the condensates in terms of the original fields. Only in the latter case the SU(2)\(_V\) symmetry among the three pions (and among the \( a_0 \)-mesons) is manifest when we consider degenerate quark masses for instance.

Because we want to investigate the effects of instantons on the vacuum, we are interested in the dependence on the strength of the determinant interaction, which is the effective instanton interaction. Frank et al. \[34\] have investigated the effects of this interaction at \( \theta = 0 \), in particular flavor-mixing effects, on the QCD phase diagram, by choosing the following expressions for \( G_1 \) and \( G_2 \) (where our \( c \) is their \( \alpha \))

\[
G_1 = (1 - c)G_0, \quad G_2 = cG_0.
\]

In this way, the strength of the instanton interaction is controlled by the parameter \( c \), while the value for the quark condensate at \( \theta = 0 \) (which is determined by the combination \( G_1 + G_2 \)) is kept fixed. As mentioned, for \( G_1 = G_2 \), or equivalently \( c = \frac{1}{2} \), only the \( \sigma \) and \( \pi \) mesons are present. For our numerical studies we will use the following values for the parameters unless stated otherwise: \( m_u = m_d = 6 \text{ MeV} \) in case of degenerate quark masses, a three-dimensional momentum cut-off \( \Lambda = 590 \text{ MeV}/c \) and \( G_0 \Lambda^2 = 2.435 \). This corresponds \[34\] to a pion mass of 140.2 MeV, a pion decay constant of 92.6 MeV and finally, a quark condensate \( \langle \bar{u}u \rangle = \langle \bar{d}d \rangle = (-241.5 \text{ MeV})^3 \). These values are in reasonable agreement with experimental determinations.

IV. CALCULATION OF THE GROUND-STATE

To obtain the ground-state of the theory, we introduce 8 real condensates as follows

\[
\alpha_0' = -2(G_1 + G_2) \langle \sigma' \rangle,
\]

\[
\alpha' = -2(G_1 - G_2) \langle \alpha_0' \rangle,
\]

\[
\beta_0' = -2(G_1 - G_2) \langle \eta' \rangle,
\]

\[
\beta' = -2(G_1 + G_2) \langle \pi' \rangle.
\]

All quantities in this section refer to the primed fields, but for notational convenience we will drop the primes from now on in this section only. Results presented in the subsequent sections will refer exclusively to the unprimed quantities.

It will be assumed that all condensates are space-time independent. A Hubbard-Stratonovich transformation eliminates the four-point quark interactions, such that the Lagrangian becomes quadratic in the quark fields and the integration over these fields is straightforward to perform. One obtains the following expression for the thermal effective potential \( \mathcal{V} \) in the mean-field approximation \[33\]

\[
\mathcal{V} = \frac{\alpha_0^2 + \beta_0^2}{4(G_1 + G_2)} + \frac{\alpha^2 + \beta^2}{4(G_1 - G_2)} - T \sum_{p_0 = (2n+1)\pi T} \int \frac{d^3p}{(2\pi)^3} \log \det K
\]

where \( K \) is a matrix in flavor and Dirac space,

\[
K = 1_f \otimes (i\gamma_0\rho_0 + \gamma_i\rho_i) - \mu \otimes \gamma_0 - M
\]
is the inverse quark propagator, and

$$M = m_u (\cos \theta \lambda_u \otimes \mathbb{1}_d + \sin \theta \lambda_u \otimes i 7_5) + m_d \lambda_d \otimes \mathbb{1}_d + \alpha_0 \lambda_u \otimes \mathbb{1}_d + \beta_u \lambda_u \otimes i 7_5, \quad (21)$$

with $\lambda_u = (\lambda_1 + \lambda_3)/2$ and $\lambda_d = (\lambda_1 - \lambda_3)/2$.

The values of the condensates are found by minimizing the effective potential with respect to these condensates. By exploiting $U(1)$ flavor symmetry one only has to study the condensates $\alpha_0, \alpha_1, \alpha_3, \beta_0, \beta_1, \beta_3$. In Ref. [33] the $\beta_0$ and $\beta_3$ condensates have been ignored based on the Vafa-Witten theorem. As we wish to check the validity of this theorem at finite temperature and density in our model calculation, we do take these condensates into account.

In order to calculate the effective potential, it is convenient to multiply $K$ with $\mathbb{1}_f \otimes \gamma_0$ which leaves the determinant invariant and yields a new matrix $\tilde{K}$ with $i p_0$‘s on the diagonal. The determinant of $\tilde{K}$ can be calculated as $\det \tilde{K} = \prod_{i=1}^{8} (\lambda_i - i p_0)$, where $\lambda_i$ are the eigenvalues of $\tilde{K}$ with $p_0 = 0$. After performing the sum over the Matsubara frequencies, we obtain

$$T \sum_{p_0=(2n+1)\pi T} \log \det \tilde{K} = \sum_{i=1}^{8} \left[ \frac{\lambda_i}{2} + T \log \left( 1 + \frac{1}{e^{\lambda_i/T} + 1} \right) \right]. \quad (22)$$

Finally we need to integrate over the three-momenta $p$ up to the ultraviolet cutoff $\Lambda$ to determine the effective potential.

Minimizing $V$ implies solving the equations

$$\frac{\partial V}{\partial x_i} = 0, \quad (23)$$

where $x = \{ \alpha_0, \alpha_1, \alpha_3, \beta_0, \beta_1, \beta_3 \}$. The derivatives of the effective potential can be calculated from the expression

$$T \sum_{p_0=(2n+1)\pi T} \log \det \tilde{K} = \frac{1}{2} \sum_{i=1}^{8} b_{ij} \left( 1 - \frac{2}{e^{\lambda_i/T} + 1} \right) \text{sgn} (\lambda_i), \quad (24)$$

where $b_{ij} = \left( U^\dagger \partial \tilde{K}(p_0 = 0)/\partial x_j U \right)_{ii}$. Here $U$ is a unitary matrix which contains in the $i$-th column the normalized eigenvector of $\tilde{K}$ with eigenvalue $\lambda_i$. Again, one has to integrate over $p$ to obtain the complete derivative. Since this calculation does not use the finite distance method, the derivatives can be determined very accurately. Also, it is very efficient as one needs the eigenvalues of $\tilde{K}$ anyway in order to calculate the effective potential.

When a solution to Eq. (23) has been found, it has to be checked whether the solution is indeed a minimum and not a maximum or saddle-point. This is checked by verifying that the Hessian of the solution only has positive eigenvalues. If more than one minimum is found, the one with the lowest value is chosen. Also the continuity of the effective potential is checked.

The speed of the calculation mainly depends on how fast the eigenvalues of $\tilde{K}$ can be calculated. To speed up the evaluation of the calculation of the eigenvalues, one can make use of the fact that the determinant of $\tilde{K}$ is invariant under the interchanging of rows and columns. This can be used to bring $\tilde{K}$ to a block-diagonal form of two $4 \times 4$-matrices. This reduces the computing time to determine the eigenvalues with a factor of four as the time to numerically calculate the eigenvalues scales cubically with the dimension of the matrix.

Another way of improving the speed of the calculation is to choose $\vec{p}$ to lie along the $z$-direction, exploiting the fact that $\det \tilde{K}$ does not depend on the direction of $\vec{p}$.

One final remark we have to make regarding Eq. (19) is the fact that in order for the effective potential to have a minimum at finite values for the condensates, the coupling $G_2$ has to satisfy $-G_1 \leq G_2 \leq G_1$, and correspondingly, $-\frac{1}{2} \leq c \leq \frac{1}{2}$. From Eq. (4) we can see that a negative value for $G_2$ corresponds to shifting $\theta \rightarrow \theta + \pi$, implying that the minimum of the theory will be at $\theta = \pi$, in violation of the Vafa-Witten theorem at zero temperature and density. Therefore, we will restrict to $0 \leq c \leq \frac{1}{2}$. The case $c = \frac{1}{2}$ is special, because then only the $\sigma'$ and $\pi'$ fields are present in the theory, which means at $\theta = 0$ the $\sigma$ and $\pi$ mesons and at $\theta = \pi$ the $\eta$ and $a_0$ mesons.

V. THE GROUND-STATE OF THE NJL MODEL

This section deals with our results for the ground-state of the NJL model. First we discuss the $\theta$-dependence of the condensates and the effective potential. It turns out that for nonzero $c$, two different situations can be
distinguished: below a certain critical \( c \) value (\( c_{\text{crit}} \)) no spontaneous CP violation takes place at \( \theta = \pi \), whereas for \( c \) larger than this critical value it does take place. The value of this \( c_{\text{crit}} \) depends on the values of the quark masses. In Fig. 2 we show the phase diagram at \( \theta = \pi \) in the \( (c, m)-\)plane for degenerate quark masses \( m_u = m_d = m \), two phases can be distinguished,

1. \( \langle \sigma \rangle \neq 0 \), the ordinary chiral condensate.

2. \( \langle \sigma \rangle \neq 0, \langle \eta \rangle \neq 0 \), the CP-violating phase.

The phase transition corresponds to \( c_{\text{crit}} \) and is of second order. A linear relation exists between the quark mass and \( c_{\text{crit}} \).

**A. The \( \theta \)-dependence of the vacuum**

When the determinant interaction is turned off, there is no \( \theta \)-dependence. In terms of the unprimed fields, only the \( \langle \sigma \rangle \) condensate is nonzero.

In Fig. 3 we show the \( \theta \)-dependence of the various condensates for the case \( c = 0.005 \), which for our choice \( m_u = m_d = 6 \) MeV is below \( c_{\text{crit}} \approx 0.008 \). As can be seen, no spontaneous CP violation occurs, since \( \langle \eta \rangle = 0 \) at \( \theta = \pi \). Explicit CP violation for other values of \( \theta \) does occur, as expected. In this figure the condensates are normalized with respect to \( \langle \sigma \rangle \) at \( \theta = 0 \). Both \( \langle \pi \rangle \) and \( \langle a_0 \rangle \) are zero for all \( \theta \) and this remains true for \( c \) above \( c_{\text{crit}} \) for degenerate quark masses.

Fig. 4 shows the case of \( c = 0.2 \). Spontaneous CP violation is clearly visible, as \( \langle \eta \rangle \) is nonzero at \( \theta = \pi \). As can be seen two degenerate vacua then exist, with opposite signs for \( \langle \eta \rangle \). These two degenerate vacua differ by a CP transformation. This is known as Dashen’s phenomenon \([5]\) and is also apparent from the \( \theta \)-dependence of the effective potential. In Fig. 5 we show the effective potential as a function of \( \theta \) normalized to its value at \( \theta = 0 \), for the two cases \( c = 0.005 \) and \( c = 0.2 \). In both cases, the minimum of the effective potential is at \( \theta = 0 \), in agreement with the Vafa-Witten theorem. Furthermore, it can be seen that the case with spontaneous CP-violation has a cusp at \( \theta = \pi \), and therefore a left and a right derivative which differ by a sign. Due to the axial anomaly, the \( \theta \)-derivative of the effective potential is proportional to \( \langle \eta \rangle \). This explains the occurrence of two values for the \( \eta \) condensate.

**B. Phase structure at \( \theta = \pi \)**

In this section we concentrate further on the case \( \theta = \pi \). We will start with a discussion of the mass-dependence of the ground-state. From Ref. \([11]\) we know that in three-flavor chiral perturbation theory a region exists in the
FIG. 3: The $\theta$-dependence of the normalized condensates, with $c = 0.005 < c_{\text{crit}}$.

FIG. 4: The $\theta$-dependence of the normalized condensates, with $c = 0.2 > c_{\text{crit}}$.

$(m_u, m_d)$-plane where CP is spontaneously violated, cf. Fig. [1] In that case the shape of the CP violating region depends on the strange quark mass. In the present case it depends on the choice of $c$.

In Fig. [3] we show the phase diagram of the NJL model at $\theta = \pi$ with $c = 0.4$ in the $(m_u, m_d)$-plane. Four phases can be distinguished

1. $\langle \sigma \rangle < 0$, $\langle a_0^0 \rangle < 0$
2. $\langle \sigma \rangle < 0$, $\langle a_0^0 \rangle > 0$
3. $\langle \sigma \rangle < 0$, $\langle a_0^0 \rangle < 0$, $\langle \eta \rangle \neq 0$, $\langle \pi^0 \rangle \neq 0$
4. $\langle \sigma \rangle < 0$, $\langle a_0^0 \rangle > 0$, $\langle \eta \rangle \neq 0$, $\langle \pi^0 \rangle \neq 0$

In phases [3] and [4] two degenerate vacua exist with opposite signs for both $\langle \eta \rangle$ and $\langle \pi^0 \rangle$. The phase transitions
FIG. 5: The $\theta$-dependence of the normalized effective potential at $c = 0.005$ and $c = 0.2$.

FIG. 6: The $(m_u, m_d)$ phase diagram of the NJL at $\theta = \pi$ with $c = 0.4$. The dashed lines denote second order phase transitions and the dotted line a crossover.

between the CP-conserving phases 1 and 2 to the CP-violating phases 3 and 4 are second order. The phases 1 and 2 only differ in the sign for the $\langle a_0^0 \rangle$-condensate, the same holds for the phases 3 and 4. The phase transition between the phases 3 and 4 is a crossover, as is the case for the phase transition between phase 1 and 2 for large $m_u$ and $m_d$. Exactly at the crossover, $\langle a_0^0 \rangle$ vanishes and in the CP-violating region the same applies to $\langle \pi^0 \rangle$, but not to $\langle \eta \rangle$. The fact that $a_0^0$-condensation (and $\pi^0$-condensation in the CP-violating region) occurs when the masses are not equal simply reflects the explicit breaking of SU(2)$_V$ which occurs for nondegenerate quark masses.

The shape of the CP-violating region is determined by the asymptotes, which are proportional to $c$. We conclude that in contrast to two-flavor lowest-order chiral perturbation theory (the case of $m_s \to \infty$ in Ref. [11], such that the asymptotes are moved to $m_u = m_d = \infty$), the NJL model does have a spontaneous CP-violating phase for two nondegenerate quark flavors. This is in accordance with the chiral perturbation theory analysis of Ref. [9] in
the large $N_c$ limit and for finite $a/N \gg m_u, m_d$.

**VI. FINITE TEMPERATURE AND BARYON CHEMICAL POTENTIAL**

In this section we turn to the changes in the phase structure at nonzero temperature and density. Ref. [14] states that the CP-violating phase at $\theta = \pi$ does not exist at high temperatures, i.e. a critical temperature exists above which the CP-violating condensates are zero. Ref. [14] only considered the case $c = 0.5$. Here we generalize their results to other $c$ values. In Fig. 7 the $(T, c)$ phase diagram is shown for degenerate quark masses. The following three phases arise

1. $\langle \sigma \rangle \neq 0$, the ordinary chiral condensate.
2. $\langle \sigma \rangle \neq 0$, $\langle \eta \rangle \neq 0$, the CP-violating phase.
3. $\langle \sigma \rangle \approx 0$, the (almost) chiral symmetry restored phase.

The phase structure at $T = 0$ can be understood from Fig. 6 for degenerate quark masses the two phases are encountered on its diagonal. The phase transition occurs at that particular value of $m_u = m_d$ for which $c = 0.4$ is the critical $c$. The phase transition between phases 1 and 2 is of second order for all temperatures. For nondegenerate quark masses these two phases would be phases 1 and 2 or 2 and 4 of Fig. 6 depending on whether $m_u$ is larger or smaller than $m_d$, respectively. In that case two second order phase transitions are present.

Above a certain temperature one observes in Fig. 7 an approximate restoration of chiral symmetry (phase 3). Note that the chiral symmetry is not fully restored due to the quark masses. The phase transition between phases 1 and 3 is a crossover, like it is at $\theta = 0$. The crossover line is defined by the inflection points $\partial^2 \langle \sigma \rangle / \partial T^2 = 0$.

At high temperature also the CP-violating phase disappears. This is consistent with the fact that at high temperature instanton effects become exponentially suppressed [37]. The CP-violating phase is after all realized due to the instanton induced interaction. The maximum value of the critical temperature as function of $c$ is 219 MeV.

We have verified that also for nonzero temperature the minimum of the effective potential is at $\theta = 0$, which means the Vafa-Witten theorem continues to hold in the NJL model at nonzero temperature. The same applies to baryon and isospin chemical potential. We also have checked whether there are any local minima in the effective potential at nonzero temperature and density, but we found none.
Now we will briefly consider nonzero baryon chemical potential \( \mu_B = \mu_u + \mu_d \), where \( \mu_{u,d} \) denote the \( u,d \) quark chemical potentials. The \((\mu_B, c)\) phase diagram is displayed in Fig. 8 for a restricted range of \( \mu_B \) values. The same phases occur as in the \((T, c)\) phase diagram, but now the phase transition to the (almost) chiral symmetry restored phase is of first order, like for \( \theta = 0 \). Furthermore, the first-order phase transition has a small \( c \) dependence. As always, the phase transition from phase 1 to phase 2 is of second order.

VII. NONZERO ISOSPIN CHEMICAL POTENTIAL

In quark matter systems equilibrium and neutrality conditions can require that \( \mu_u \neq \mu_d \). Son and Stephanov [38] observed that charged pion condensation can occur for nonzero isospin chemical potential \( \mu_I = \mu_u - \mu_d \). At \( \theta = 0 \) this second order phase transition between the ordinary phase of broken chiral symmetry \((\langle \sigma \rangle \neq 0)\) to the pion condensed phase (which also breaks chiral symmetry) occurs when \( \mu_I \) equals the vacuum pion mass. In this subsection we address this issue at \( \theta = \pi \).

In Fig. 9 we show the phase diagram of the NJL model in the \((\mu_I, c)\)-plane, for \( m_u = m_d = 6 \) MeV. The solid line indicates a first-order phase transition, the dashed lines indicate second-order phase transitions. The four phases are characterized as follows

1. \( \langle \sigma \rangle \neq 0 \)
2. \( \langle \sigma \rangle \neq 0, \langle \pi^\pm \rangle \neq 0 \)
3. \( \langle \sigma \rangle \neq 0, \langle \eta \rangle \neq 0 \)
4. \( \langle a_0^\pm \rangle \neq 0 \)

![FIG. 9: The \((\mu_I, c)\) phase diagram of the NJL model at \( \theta = \pi \).](image)

Phase 4 is a novel phase characteristic of \( \theta = \pi \). This phase also has a small nonzero \( \langle \sigma \rangle \)-condensate (not indicated), due to the explicit breaking by the quark masses.

For \( c < c_{\text{crit}} \) a nonzero \( \langle \pi^\pm \rangle \)-condensate exists above a certain \( \mu_I \) value. Like at \( \theta = 0 \) the second order phase transition turns out to be at \( \mu_I = m_\pi \), where \( m_\pi \) is the vacuum pion mass. In addition, there is a second phase transition, a first-order phase transition, at larger \( \mu_I \), where charged pion condensation makes way for charged \( a_0 \) condensation. For \( c > c_{\text{crit}} \) no nonzero \( \langle \pi^\pm \rangle \)-condensate exists, only nonzero \( \langle a_0^\pm \rangle \). The phase transition between phases 3 and 4 is of first-order. The question arises what determines the value of \( \mu_I \) at this phase transition to charged meson condensation? To answer this question, the meson masses need to be calculated.
A. The $c$-dependence of the meson masses and mixing

As said, at $\theta = 0$ charged pion condensation occurs when $\mu_I$ is larger or equal to the vacuum ($\mu_I = 0$) pion mass. For the NJL model this has been studied extensively in Refs. [35, 39, 40, 41]. This condition is independent of $c$. To see what happens in the $\theta = \pi$ case, we calculate the $c$-dependence of the meson masses, with $\mu_I = 0$. The results are shown in Fig. 10 and in Fig. 11 the $c$-dependence of the mixing is shown. Clearly, at $\theta = \pi$ the situation quite different from $\theta = 0$.

![Figure 10](image1.png)

**FIG. 10:** The $c$-dependence of the meson masses at $\theta = \pi$. The masses are calculated in the RPA.

![Figure 11](image2.png)

**FIG. 11:** The $c$-dependence of the mixing-angle of the mesons at $\theta = \pi$. The mixing is calculated in the RPA.

At $c = 0$ (no instanton interactions) the $\eta$ and $\pi$ masses are equal and also the $\sigma$ and $a_0$ masses. This follows from the symmetry of the Lagrangian at $c = 0$, which has a $U(2)_L \otimes U(2)_R$-symmetry that is spontaneously broken.
by the chiral condensate (ignoring the explicit breaking by the quark masses) to \( U(2)_V \). This means there are four (pseudo-)Goldstone bosons, with the same (small) masses: the \( \eta \) and \( \pi \) mesons. The instanton interactions remove the degeneracy for \( c \neq 0 \).

When \( c > c_{\text{crit}} \), i.e. when \( \langle \eta \rangle \neq 0 \), a complication arises: the mass eigenstates are not CP or P eigenstates any longer. The occurrence of the \( \eta \) condensate results in mixing of the \( \sigma \)-particle with its parity partner, the \( \eta \)-particle. Similarly, the pions mix with their parity partners, the \( a_0 \)'s. The mixing is to be expected because when the ground-state is not CP-conserving, there is no need for the excitations, i.e. the mesons, to be CP eigenstates or states of definite parity in case of charged mesons.

The mass eigenstates, denoted with a tilde, are defined in the following way

\[
\begin{align*}
|\tilde{\sigma}\rangle &= \cos \theta_\eta |\sigma\rangle + \sin \theta_\eta |\eta\rangle, \\
|\tilde{\eta}\rangle &= \cos \theta_\eta |\eta\rangle - \sin \theta_\eta |\sigma\rangle, \\
|\tilde{a}_0\rangle &= \cos \theta_\pi |a_0\rangle + \sin \theta_\pi |\pi\rangle, \\
|\tilde{\pi}\rangle &= \cos \theta_\pi |\pi\rangle - \sin \theta_\pi |a_0\rangle,
\end{align*}
\]

where \( \theta_\eta \) and \( \theta_\pi \) are the mixing angles. The states on the r.h.s. are the usual states of definite parity.

The calculation of the mixing and the resulting masses is similar to the mixing of \( \eta_0 \) and \( \eta_8 \) in the three-flavor NJL-model, which was discussed in great detail in Ref. [42] using the random phase approximation (RPA), the approach we will also employ here. As a side remark, we mention that we have also calculated the curvature of the effective potential at the minimum which should approximately be proportional to the masses, giving indeed very similar results\(^1\).

When \( c < c_{\text{crit}} \), no mixing takes place and the tilde fields are equal to their counterparts without tilde. When \( c > c_{\text{crit}} \), mixing occurs. The mixing between \( \eta \) and \( \sigma \) increases rapidly as \( c \) increases, reaching a maximum at \( c = 0.09 \), where \( \tilde{\sigma} \) is almost completely \( \eta \) and vice versa. For larger \( c \) the mixing however decreases rapidly again, so that when \( c = \frac{1}{2} \), \( \tilde{\sigma} \) (\( \tilde{\eta} \)) is again equal to \( \sigma \) (\( \eta \)).

The mixing between \( a_0 \) and the pions behaves differently, here the mixing angle increases rapidly to become \( 90^\circ \) at \( c = \frac{1}{2} \), i.e. \( \tilde{\pi} \) becomes \( a_0 \) and vice versa.

Now we turn to the behavior of the tilde-meson masses, which also display unusual features as function of \( c \). When \( c < c_{\text{crit}} \), the \( \tilde{\pi} \) masses are constant, and equal to the ordinary pion masses. Furthermore, the \( \tilde{\eta} \) mass decreases with increasing \( c \). This is peculiar to \( \theta = \pi \), because at \( \theta = 0 \) the \( \eta \) mass increases with increasing \( c \). The \( \tilde{\eta} \) mass has its lowest, nonzero value at \( c_{\text{crit}} \). This is in contrast to three-flavor lowest order chiral perturbation theory [11], where the \( \eta \) mass (in Ref. [11] actually the \( \pi^0 \) mass using the primed theory) vanishes at the phase transition. Finally, also the masses of the \( a_0 \)'s and \( \sigma \) decrease slightly with increasing \( c \).

When \( c > c_{\text{crit}} \), the \( \epsilon \)-dependence of the masses changes dramatically. The \( \tilde{\pi} \) mass now decreases monotonically with increasing \( c \), whereas the \( a_0 \) and \( \tilde{\sigma} \) mass both increase monotonically to infinity towards \( c = \frac{1}{2} \). The latter can be understood, because when \( c = \frac{1}{2} \), \( G_1 \) equals \( G_2 \), which as mentioned means for \( \theta = \pi \) that there are no \( \pi \) and \( \sigma \) mesons in the spectrum.

Another striking feature is that the \( \tilde{\eta} \) mass rises until it almost reaches the \( \tilde{\sigma} \) mass, after which it remains approximately constant. The behavior of the \( \tilde{\sigma} \) mass is opposite, first it is almost constant and when it becomes almost equal to the \( m_\eta \) mass it increases to infinity. The masses of \( \tilde{\sigma} \) and \( \tilde{\eta} \) cannot cross when there are interactions that mix the two states, which is similar to level repulsion in quantum mechanics. The point where both masses are almost equal corresponds to a mass that is twice the constituent quark mass. This forms the threshold to decay into two quarks, which makes one of the two mesons unstable when \( c > c_{\text{crit}} \).

Now we turn again to the original question concerning the charged meson condensation phase transition. From the calculation of the masses of the tilde-mesons, we infer that the condition for charged meson condensation at \( \theta = \pi \) is \( \mu_\ell \geq m_\pi(c) \). For \( c < c_{\text{crit}} \), the phase transition takes place when \( \mu_\ell \) equals \( m_\pi(m_\pi) \), as it does at \( \theta = 0 \). For \( c > c_{\text{crit}} \) it takes place at the mass of \( \tilde{\pi} \), which is now a mixed state of \( \pi \) and \( a_0 \). At \( c = \frac{1}{2} \) this means at the mass of the \( a_0 \). The latter observation is in agreement with a result of Ref. [13], where the \((\mu_\ell, \theta)\) phase diagram of degenerate two-flavor chiral perturbation theory is investigated to lowest order at effectively \( c = \frac{1}{2} \) (due to the absence of the \( \eta \) meson). There it is observed that charged pion condensation occurs when \( \mu_\ell \) is equal to the \( \theta \)-dependent pion mass \( m_\pi(\theta) \). In Ref. [13] all \( \theta \)-dependence resides in the mass matrix, with both quarks having

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\(^1\) This method was also used in Ref. [39] to calculate the pion mass in order to check the condition \( \mu_\ell \geq m_\pi \) for charged pion condensation. A discrepancy of approximately 25% was obtained.
a \( \theta \)-dependent mass. Hence, their \( \theta \)-dependent pion field corresponds to what we call \( \pi' \), which at \( \theta = \pi \) is the \( a_0 \) field in the original, unprimed theory, leading to an agreement with our finding.

The second phase transition for \( c < c_{\text{crit}} \) from the charged pion condensed phase to the charged \( a_0 \) condensed phase does not correspond to \( \mu_I \) being equal to a meson mass calculated at \( \mu_I = 0 \). Although we have not found a condition in terms of the calculated masses, \( \mu_I \) at this first-order phase transition follows a line that is the smooth continuation of the \( \tilde{\pi} \) mass in the region \( c > c_{\text{crit}} \) to infinity at \( c = 0 \). A calculation of the meson masses at nonzero \( \mu_I \), such as performed in Ref. [11], might resolve this open issue.

VIII. CONCLUSION AND DISCUSSION

The \( \theta \)-dependence of the ground-state of the two-flavor NJL model is investigated in the mean-field approximation. The main focus is on the case \( \theta = \pi \), when spontaneous CP-violation is possible. The \( \theta \)-dependence of the theory is found to strongly depend on the strength of the \( 't \) Hooft determinant interaction. When the strength of this interaction, which is governed by the parameter \( c \), is small or zero, no spontaneous CP-violation takes place at \( \theta = \pi \). The low-energy physics is then almost the same as at \( \theta = 0 \). At larger \( c \) however, spontaneous CP-violation does take place at \( \theta = \pi \). So the phenomenon of spontaneous CP-violation is governed by the \( 't \) Hooft determinant interaction, which describes the effect of instantons in the effective theory. The question whether \( c \) is sufficiently large for CP-violation to occur at \( \theta = \pi \) depends on the quark masses. In other words, spontaneous CP-violation requires instantons, but its actual realization depends on the size of their contribution w.r.t. the quark masses. This is also expected to be the case in QCD, where it can be phrased in terms of the low-energy theorem identity \( \sum_q 2m_q \langle q \gamma_5 q \rangle = -N_f (g^2 F^2) / 8\pi^2 \) (cf. e.g. Ref. [12]), which relates \( \langle q \rangle \) to the first derivative of the effective potential w.r.t. \( \theta \). Depending on \( m_q \) the coupling constant \( g \) needs to be sufficiently large for spontaneous CP-violation to take place. Or in other words, the energy needs to be sufficiently low. The latter observation is in agreement with the disappearance of the CP-violation at temperatures above a certain critical temperature or density. Therefore, we conclude that spontaneous CP-violation in the strong interaction is an inherently low-energy phenomenon.

We have checked that the Vafa-Witten theorem holds in the NJL model also at finite temperature and density and found that no local minima arise, indicating the absence of meta-stable CP-violating states in the NJL model. We have confirmed several previous results that were obtained in two-flavor chiral perturbation theory. We found (in accordance with the results of Ref. [2]) that two-flavor lowest-order chiral perturbation theory with \( a/N \to \infty \) is in general not rich enough to yield results that one might expect to hold in QCD too. It leads for instance to the conclusion that only for \( m_u = m_d \) spontaneous CP-violation occurs, without a critical strength of the instanton induced interaction. In contrast, the phase diagram of the two-flavor NJL model is very similar to that of three-flavor chiral perturbation theory [11], where spontaneous CP-violation arises for specific ranges of quark masses.

We also found that the presence of a nonzero \( \eta \)-condensate has a strong effect on the \( c \)-dependence of the meson masses and gives rise to mixing among the states of definite parity, as expected when CP invariance is not a symmetry anymore. As a result, the pions mix with their parity partners, the \( a_0 \)'s, and the \( \eta \) meson mixes with its parity partner, the \( \sigma \) meson. Unlike the mixing discussed as a function of \( \theta \) which is just a matter of consistently naming the states in order to be able to compare to results obtained with negative quark masses and which does not affect physical results, the mixing as function of \( c \) does change the physics. For instance, the condition for charged pion condensation at nonzero isospin chemical potential becomes modified. At \( \theta = \pi \) for \( c < c_{\text{crit}} \), a second-order phase transition takes place when \( \mu_I \) equals \( m_\pi \), just as at \( \theta = 0 \) found by Son and Stephanov. However, we find that for \( c > c_{\text{crit}} \) it becomes a first-order phase transition to a novel phase of charged \( a_0 \) condensation that takes place at the mass of \( \tilde{\pi} \), which is a mixed state of \( \pi \) and \( a_0 \). At \( c = \frac{1}{2} \) it is entirely \( a_0 \). Charged \( a_0 \) condensation also arises for \( c < c_{\text{crit}} \) and \( \mu_I > m_\pi \), but it appears there is no condition in terms of vacuum meson masses for this second phase transition.

We expect the presented two-flavor NJL model results to remain valid in the case of three flavors and when going beyond the mean-field approximation, but this remains to be studied. It would be very interesting if the results could in the future be compared to lattice QCD results on the low-energy physics at \( \theta = \pi \).
Acknowledgments

We would like to thank Harmen Warringa for kindly sharing with us his code to calculate the effective potential. We also thank the members of the theory group at the VU, in particular Wilco den Dunnen and Erik Wessels, for fruitful discussions.

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