Spontaneous Violation of *CP* Symmetry in the Strong Interactions

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Some time ago Dashen [Phys. Rev. D **3**, 1879 (1971)] pointed out that spontaneous *CP* violation can occur in the strong interactions. I show how a simple effective Lagrangian exposes the remarkably large domain of quark mass parameters for which this occurs. I close with some warnings for lattice simulations.

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The SU(3) non-Abelian gauge theory of the strong interactions is quite remarkable in that, once an arbitrary overall scale is fixed, the only parameters are the quark masses. Using only a few pseudoscalar meson masses to fix these parameters, the non-Abelian gauge theory describing quark confining dynamics is unique. It has been known for some time [1] that, as these parameters are varied from their physical values, exotic phenomena can occur, including spontaneous breakdown of *CP* symmetry. Here I consider the theory with three flavors of quark and map out in detail the regions of parameter space where this breaking occurs.

While the spontaneous breaking considered here occurs only in unphysical regions of parameter space, there are several reasons the phenomenon may be of wider interest. Indeed, *CP* is broken in the real world, and thus some mechanism along these lines may be useful for going beyond the strong interactions. Also, the analysis demonstrates that when the other quarks are massive, nothing special happens at vanishing up-quark mass. This raises the question of whether a nondegenerate massless quark is a physical concept and is the main subject of a separate recent paper [2]. These observations also raise questions for practical lattice calculations of hadronic physics, where current algorithms ignore any phases in the fermion determinant and are unable to explore this phenomenon.

The possibility of a spontaneous *CP* violation is most easily demonstrated in terms of an effective chiral Lagrangian. I begin with a brief review of this model with three quarks, namely, the up, down, and strange quarks. This lays the groundwork for discussion of the *CP* violating phase. I then briefly discuss how heavier states, most particularly the η' meson, enter without qualitatively changing the picture. Finally, I make some concluding remarks on possible impacts of the *CP* violating structures for lattice gauge simulations. An unpublished preliminary version of these arguments appears as part of Ref. [3]. The occurrence of this phenomenon with three degenerate quarks is presented in Ref. [4]. A discussion of the *CP* violating phenomenon in terms of the analytic structure of the partition function is in Ref. [5].

I consider the three flavor theory with its approximate SU(3) symmetry. Using three flavors simplifies the discussion, although the *CP* violating phase can also be demonstrated for the two flavor theory following the discussion in Ref. [6]. I work with the familiar octet of light pseudoscalar meson fields π_α with $\alpha = 1, \ldots, 8$. In a standard way (see, for example, Ref. [7]) I consider an effective field theory defined in terms of the SU(3) valued group element

$$\Sigma = \exp(i\pi_\alpha \lambda_\alpha / f_\pi) \in \mathrm{SU}(3). \tag{1}$$

Here the λ_α are the usual Gell-Mann matrices, and f_π has a phenomenological value of about 93 MeV. I follow the normalization convention that $\mathrm{Tr}\lambda_\alpha\lambda_\beta = 2\delta_{\alpha\beta}$. In the chiral limit of vanishing quark masses, the interactions of the eight massless Goldstone bosons are modeled with the effective Lagrangian density

$$L_0 = \frac{f_\pi^2}{4}\mathrm{Tr}(\partial_\mu \Sigma^\dagger \partial_\mu \Sigma). \tag{2}$$

The nonlinear constraint of Σ onto the group SU(3) makes this theory nonrenormalizable. It is to be understood only as the starting point for an expansion of particle interactions in powers of their masses and momenta. Expanding Eq. (2) to second order in the meson fields gives the conventional kinetic terms for our eight mesons.

This theory is invariant under parity and charge conjugation, manifested by

$$P : \Sigma \to \Sigma^{-1} \qquad CP : \Sigma \to \Sigma^*, \tag{3}$$

where the operation $*$ refers to complex conjugation. The eight meson fields are pseudoscalars. The neutral pion and the eta meson are both even under charge conjugation.

With massless quarks, the underlying quark-gluon theory has a chiral symmetry under

$$\psi_L \to \psi_L g_L \qquad \psi_R \to \psi_R g_R. \tag{4}$$

Here (g_L, g_R) is in $[SU(3) \times SU(3)]$ and $\psi_{L,R}$ represent the chiral components of the quark fields, with flavor indices understood. This symmetry is expected to break spontaneously to a vector SU(3) via a vacuum expectation value for $\overline{\psi}_L \psi_R$. This motivates the sigma model through the identification

$$\langle 0|\overline{\psi}_L \psi_R|0\rangle \leftrightarrow v\Sigma. \tag{5}$$

The quantity v characterizes the strength of the spontaneous breaking. The effective field transforms under the chiral symmetry as

$$\Sigma \to g_L^\dagger \Sigma g_R. \tag{6}$$

Equation (2) represents the simplest nontrivial expression invariant under this symmetry.

Quark masses break the chiral symmetry explicitly. These are introduced through a three by three mass matrix M appearing in an added potential term

$$L = L_0 - v\mathrm{ReTr}(\Sigma M). \tag{7}$$

Here v is the same dimensionful factor appearing in Eq. (5). The chiral symmetry of our starting theory shows the physical equivalence of a given mass matrix M with a rotated matrix $g_R^\dagger M g_L$. Using this freedom to put the mass matrix into a standard form, I take it as diagonal with increasing eigenvalues

$$M = \begin{pmatrix} m_u & 0 & 0 \\ 0 & m_d & 0 \\ 0 & 0 & m_s \end{pmatrix} \tag{8}$$

representing the up, down, and strange quark masses.

In general the mass matrix can still be complex. The chiral symmetry allows one to move phases between the masses, but the determinant of M is invariant. Under charge conjugation the mass term would be invariant only if $M = M^*$. If $|M|$ is not real, then its phase is the famous CP violating parameter usually associated with topological structure in the gauge fields. Here I take all quark masses as real. Since I am looking for spontaneous symmetry breaking, I consider the case where there is no explicit CP violation.

Expanding the mass term quadratically in the meson fields generates the effective mass matrix for the eight mesons

$$\mathcal{M}_{\alpha\beta} \propto \mathrm{ReTr}\lambda_\alpha \lambda_\beta M. \tag{9}$$

The isospin-breaking up-down mass difference plays a crucial role in the later discussion. This gives this matrix an off diagonal piece mixing the π_0 and the η,

$$\mathcal{M}_{3,8} \propto m_u - m_d. \tag{10}$$

The eigenvalues of $\mathcal{M}$ give the standard mass relations

$$\begin{aligned} m_{\pi_+}^2 = m_{\pi_-}^2 \propto m_u + m_d, \qquad m_{K_+}^2 = m_{K_-}^2 \propto m_u + m_s, \qquad m_{K_0}^2 = m_{\overline{K}_0}^2 \propto m_d + m_s, \\ m_{\pi_0}^2 \propto \tfrac{2}{3}\left(m_u + m_d + m_s - \sqrt{m_u^2 + m_d^2 + m_s^2 - m_u m_d - m_u m_s - m_d m_s}\right), \\ m_\eta^2 \propto \tfrac{2}{3}\left(m_u + m_d + m_s + \sqrt{m_u^2 + m_d^2 + m_s^2 - m_u m_d - m_u m_s - m_d m_s}\right). \end{aligned} \tag{11}$$

Here I label the mesons with their conventional names. From these relations, ratios of meson masses give estimates for the ratios of the quark masses [7–9].

So far all this is standard. Now I vary the quark masses and look for interesting phenomena. In particular, I want to find spontaneous breaking of the CP symmetry. Normally the Σ field fluctuates around the identity in SU(3). However, for some values of the quark masses this ceases to be true. When the vacuum expectation of Σ deviates from the identity, some of the meson fields acquire expectation values. As they are pseudoscalars, this necessarily involves a breakdown of parity, as noted by Dashen [1].

To explore this possibility, concentrate on the lightest meson from Eq. (11), the π_0. From Eq. (11) one can calculate the product of the π_0 and η masses

$$m_{\pi_0}^2 m_\eta^2 \propto m_u m_d + m_u m_s + m_d m_s. \tag{12}$$

The π_0 mass vanishes whenever

$$m_u = \frac{-m_s m_d}{m_s + m_d}. \tag{13}$$

For increasingly negative up-quark masses, the expansion around vanishing pseudoscalar meson fields fails. The vacuum is no longer approximated by fluctuations of Σ around the unit matrix; instead it fluctuates about an SU(3) matrix of form

$$\Sigma = \begin{pmatrix} e^{i\phi_1} & 0 & 0 \\ 0 & e^{i\phi_2} & 0 \\ 0 & 0 & e^{-i\phi_1 - i\phi_2} \end{pmatrix}, \tag{14}$$

where the phases satisfy

$$m_u \sin(\phi_1) = m_d \sin(\phi_2) = -m_s \sin(\phi_1 + \phi_2). \tag{15}$$

There are two minimum action solutions, differing by flipping the signs of these angles. The transition is a continuous one, with Σ going smoothly to the identity on approaching the boundary in Eq. (13). The magnitude of these angles controls the magnitude of the resulting CP violation.

In the new vacuum the neutral pseudoscalar meson fields acquire expectation values. As they are CP odd, this symmetry is spontaneously broken. This has various experimental consequences; for example, eta decay into two pions becomes allowed since a virtual third pion can be absorbed by the vacuum. Figure 1 sketches the inferred phase diagram as a function of the up- and down-quark masses.

Chiral rotations ensure a symmetry under the flipping of the signs of both quark masses. This produces a distinct CP conserving phase. When the magnitudes of both the up- and down-quark masses exceed the strange quark mass, two additional CP conserving phases are found. The figure indicates the values of Σ around which the vacua fluctuate for the four respective CP conserving phases.

The asymptotes of the boundaries of the CP violating region are determined by the strange quark mass. If the strange quark mass is taken to a large value, then this scale will instead be controlled by the strong interaction scale.

At first sight the appearance of the CP violating phase at negative up-quark mass may seem surprising. Naively in perturbation theory the sign of a fermion mass can be rotated away by a redefinition $\psi \to \gamma_5 \psi$. However, this rotation is anomalous, making the sign of the quark mass observable. A more general complex phase in the mass would also have physical consequences, i.e., explicit CP violation. With real quark masses the underlying

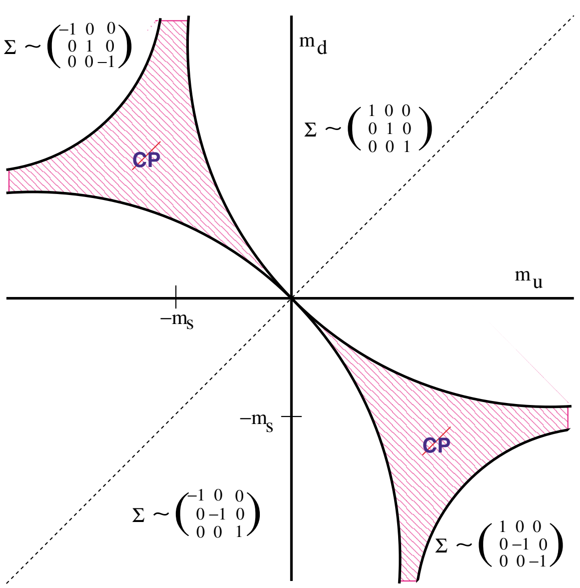

FIG. 1 (color online). The schematic phase diagram of quark-gluon dynamics as a function of the two lightest quark masses. The shaded regions exhibit spontaneous CP breaking. On the diagonal line with $m_u = m_d$ there are three degenerate pions due to isospin symmetry. The neutral pion mass vanishes on the boundary of the CP violating phase. The asymptotes of the boundaries are given by the strange quark mass. In the CP conserving phases, the vacuum fluctuates about the indicated values for Σ.

Lagrangian is CP invariant, but the above discussion shows that there exists a large region where the ground state spontaneously breaks this symmetry.

Vafa and Witten [10] argued on rather general conditions that CP could not be spontaneously broken in the strong interactions. However, their argument makes positivity assumptions on the path integral measure. When a quark mass is negative, the fermion determinant need not be positive for all gauge configurations; in this case their assumptions fail. Azcoiti and Galante [11] have also criticized the generality of the Vafa and Witten result.

The possible existence of this phase was anticipated some time ago on the lattice by Aoki [12]. For the one flavor case he found this parity breaking phase with Wilson lattice gauge fermions. He went on to discuss also two flavors, finding both flavor and parity symmetry breaking. The latter case is now regarded as a lattice artifact. The chiral breaking terms in the Wilson action open up the CP violating phase for a finite region along $m_u = m_d$ line. For a review of these issues, see Ref. [13].

In conventional discussions of CP noninvariance in the strong interactions [14] appears a complex phase $e^{i\theta}$ appearing on tunneling between topologically distinct gauge field configurations. The famous U(1) anomaly formally allows moving this phase into the determinant of the quark mass matrix. Rotating all phases into the up-quark mass shows that the spontaneous breaking of CP is occurring at an angle $\theta = \pi$. Note that when the down-quark mass is positive, the CP violating phase does not appear for up-quark masses greater than a negative minimum value. There exists a finite gap with $\theta = \pi$ without this symmetry breaking. The chiral model predicts a smooth behavior in all physical processes as the up-quark mass passes through zero.

An interesting special case occurs when the up and down quarks have the same magnitude but opposite sign for their masses, i.e., $m_u = -m_d$. In this situation it is illuminating to rotate the minus sign into the phase of the strange quark. Then the up and down quarks are degenerate, and an exact vector SU(2) flavor symmetry is restored. The spectrum will show three degenerate pions.

The above discussion was entirely in terms of the pseudoscalar mesons that become Goldstone bosons in the chiral limit. One might wonder how higher states can influence this phase structure. Of particular concern is the η' meson associated with the anomalous U(1) symmetry present in the classical quark-gluon Lagrangian. Nonperturbative processes, including topologically nontrivial gauge field configurations, are well known to generate a mass for this particle. I now argue that, while this state can shift masses due to mixing with the lighter mesons, it does not make a qualitative difference in the existence of a phase with spontaneous CP violation.

The easiest way to introduce the η' into the effective theory is to promote the group element Σ to an element of U(3) via an overall phase factor. Thus I generalize Eq. (1) to

$$\Sigma = \exp(i\pi_\alpha\lambda_\alpha/f_\pi + i\sqrt{2/3}\eta'/f_\pi) \in \mathrm{U}(3). \qquad (16)$$

The factor $\sqrt{2/3}$ gives the η' field the same normalization as the π fields. Our starting kinetic Lagrangian in Eq. (2) would have this particle also be massless. One way to fix this deficiency is to mimic the anomaly with a term proportional to the determinant of Σ,

$$L_0 = \frac{f_\pi^2}{4}\mathrm{Tr}(\partial_\mu\Sigma^\dagger\partial_\mu\Sigma) - C|\Sigma|. \qquad (17)$$

The parameter C parametrizes the strength of the anomaly in the U(1) factor.

On including the mass term exactly as before, additional mixing occurs between the η', the π_0, and the η. The corresponding mixing matrix takes the form

$$\begin{pmatrix} m_u + m_d & \frac{m_u - m_d}{\sqrt{3}} & \sqrt{\frac{2}{3}}(m_u - m_d) \\ \frac{m_u - m_d}{\sqrt{3}} & \frac{m_u + m_d + 4m_s}{3} & \frac{\sqrt{2}(m_u + m_d - 2m_s)}{3} \\ \sqrt{\frac{2}{3}}(m_u - m_d) & \frac{\sqrt{2}(m_u + m_d - 2m_s)}{3} & \frac{2}{3}m_a \end{pmatrix}, \qquad (18)$$

where m_a characterizes the contribution of the nonperturbative physics to the η' mass. This should have a value of the order of the strong interaction scale; in particular, it should be large compared to at least the up- and down-quark masses. The two by two matrix in the upper left of this expression is exactly what is diagonalized to find the neutral pion and eta masses in Eq. (11).

The boundary of the CP violating phase occurs where the determinant of this matrix vanishes. This modifies Eq. (12) to

$$\begin{aligned} m_{\pi_0}^2 m_\eta^2 m_{\eta'}^2 \propto\ & m_a(m_u m_d + m_u m_s + m_d m_s) \\ & - m_u(m_d - m_s)^2 - m_d(m_u - m_s)^2 \\ & - m_s(m_u - m_d)^2. \end{aligned} \qquad (19)$$

The boundary shifts slightly from the earlier result but still passes through the origin, leaving Fig. 1 qualitatively unchanged.

While I have been exploring rather unphysical regions in parameter space, these observations do raise some wider issues. For practical lattice calculations of hadronic physics, current simulations are done at relatively heavy values for the quark masses. This is because the known fermion algorithms tend to converge rather slowly at light quark masses. Extrapolations by several tens of MeV are needed to reach physical quark masses, and these extrapolations tend to be made in the context of chiral perturbation theory. While certainly not a proof of a problem, the presence of a CP violating phase quite near the physical values for the quark masses suggests strong variations in the vacuum state with rather small changes in the up-quark mass; indeed, less than a 10 MeV change in the traditionally determined up-quark mass can drastically change the low energy spectrum. Most simulations consider degenerate quarks, and chiral extrapolations so far have been quite successful. But some quantities, namely, certain baryonic properties [15], do seem to require rather strong variations as the chiral limit is approached. These effects and the strong dependence on the up-quark mass may be related.

Another worrying issue is the validity of current simulation algorithms with nondegenerate quarks. With an even number of degenerate flavors the fermion determinant is positive and can contribute to a measure for Monte Carlo simulations. With light nondegenerate quarks the positivity of this determinant is not guaranteed. Indeed, the CP violation can occur only when the fermions contribute large phases to the path integral. Current algorithms for dealing with nondegenerate quarks [16] take a root of the determinant with multiple flavors. In this process any possible phases are ignored. Such an algorithm is incapable of seeing the CP violating phenomena discussed here. This point may not be too serious in practice since the up and down quarks are nearly degenerate and the strange quark is fairly heavy. Again this is not a proof, but these issues should serve as a warning that things might not work as well as desired.

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