Mesoscopic QCD and the $\theta$-Vacua

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The partition function of QCD is analyzed for an arbitrary number of flavors, $N_f$, and arbitrary quark masses including the contributions from all topological sectors in the Leutwyler–Smilga regime. For given $N_f$ and arbitrary vacuum angle, $\theta$, the partition function can be reduced to $N_f - 2$ angular integrations of single Bessel functions. For two and three flavors, the $\theta$ dependence of the QCD vacuum is studied in detail. For $N_f = 2$ and 3, the chiral condensate decreases monotonically as $\theta$ increases from zero to $\pi$ and the chiral condensate develops a cusp at $\theta = \pi$ for degenerate quark masses in the macroscopic limit. We find a discontinuity at $\theta = \pi$ in the first derivative of the energy density with respect to $\theta$ for degenerate quark masses. This corresponds to the first–order phase transition in which CP is spontaneously broken, known as Dashen’s phenomena.

I. INTRODUCTION

For $N_f$ flavors of massless quarks, the Lagrangian of quantum chromodynamics (QCD) is invariant under the global symmetry group $SU(N_f)_R \times SU(N_f)_L \times U(1)_A$ at the classical level. At the quantum level, however, the $SU(N_f)_R \times SU(N_f)_L$ symmetry is spontaneously broken to the diagonal subgroup of vector transformations, $SU(N_f)_{R+L} = SU(N_f)_V$, by an expectation value for the quark-antiquark condensate. The $U(1)_A$ symmetry is explicitly broken to $Z(N_f)_A$ by a non-vanishing topological susceptibility. For scales well below $\Lambda$, the typical hadronic mass scale, the effects of the explicit breaking of the $U(1)_A$ symmetry can be essentially ignored and the dynamics of the theory are dominated by the $N_f^2 - 1$ Goldstone bosons that arise from the spontaneous breaking of the chiral symmetry. For small, nonzero quark masses, these excitations become pseudo–Goldstone bosons.

In addition to the quark masses, the QCD Lagrangian depends on another parameter, $\theta$, the so-called vacuum angle. Though this parameter explicitly violates the discrete CP symmetry for all

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non-integer multiples of $\pi$, experimental results for the value of the neutron dipole moment constrain $\theta$ to be zero within a deviation of less than $10^{-9}$ \cite{2,3}. The reason why $\theta = 0$, however, is still poorly understood, and there is considerable theoretical interest in the physics of QCD at $\theta \neq 0$. The most well-known example is the Veneziano–Witten formula which in the large-$N_c$ limit relates the mass of the $\eta'$ meson to the second derivative of the pure Yang–Mills vacuum energy with respect to $\theta$ \cite{4,5}. Another phenomenologically motivated example is the work of Refs. \cite{6,7} in which it is argued that metastable states in which $\theta$ is effectively nonzero may be created in ultrarelativistic heavy ion collisions.

Physics at $\theta \neq 0$ is inherently nonperturbative and one must rely either on effective theories or perform lattice gauge theory simulations \cite{10}. The latter approach is prohibitively difficult at present because at nonzero values of $\theta$ the action is complex and standard importance sampling methods that are usually employed are no longer applicable. This difficulty is similar to that for nonzero values of the baryonic chemical potential, but there has been recent progress in solving the complex action problem in simpler models \cite{11,12}. While many observables associated with the quark masses have been studied extensively in lattice gauge theory computations, properties of the QCD vacuum associated with $\theta$ such as the topological susceptibility have only recently been given extensive attention by the lattice community \cite{13–20}. So, most of our knowledge of the physics of QCD at $\theta \neq 0$ has been gleaned from effective theories. One of the most striking examples of novel physics is the emergence of two CP violating degenerate vacua separated by a potential energy barrier at $\theta = \pi$ known as Dashen’s phenomenon \cite{21}. While QCD is seemingly invariant under the discrete CP group for $\theta$ equal to integer values of $\pi$, this invariance is spontaneously broken in a first–order phase transition at $\theta = \pi$. Chiral effective Lagrangians in the large-$N_c$ limit were used to investigate this and other properties of the $\theta$-vacua in Refs. \cite{22} and \cite{23}. Subsequent elaborations and refinements using this approach were made in Refs. \cite{24–29}. Additionally, random matrix models \cite{30,31} as well as numerical simulations of $CP^{N-1}$ models \cite{32,33} have also been employed to investigate the physics of nonzero values of $\theta$.

In this work, we investigate the properties of QCD at $\theta \neq 0$ in the Leutwyler–Smilga finite volume regime \cite{36}, also known as the mesoscopic regime. Here, chiral perturbation theory is valid but the volume is taken such that the Goldstone modes are constant and their kinetic term can be ignored. This approach differs from those of Refs. \cite{22,29}, in which the large-$N_c$ is taken and the Lagrangian is studied to lowest order in the chiral fields. The Leutwyler–Smilga regime, on the other hand, enables exact, analytical predictions to be made. Indeed, this limit is realized in many lattice simulations \cite{37}. Many of the low-energy aspects of QCD have been studied using effective chiral Lagrangians in a finite volume \cite{38}. In Ref. \cite{38}, Leutwyler and Smilga demonstrated that such theories contain information beyond pion dynamics and the spontaneous breaking of chiral symmetry, including the low-lying spectrum of the QCD Dirac operator and the topology of the gauge fields. The purpose of this work is twofold. First, we reduce the QCD partition function for $N_f \geq 3$ in the Leutwyler-
Smilga scaling regime including the contributions from all topological sectors to $N_f - 2$ angular integrations over single Bessel functions. The latter half of this work is devoted to examining the vacuum properties of QCD in the Leutwyler-Smilga scaling regime at nonzero values of $\theta$.

The partition functions for one and two flavors of quarks including contributions from all topological sectors were computed in Refs. [39] and [40]. As emphasized in Ref. [41], the contributions to the partition function from sectors with nonzero topological charge are crucial in the finite volume regime. For example, if one considers the partition function at any fixed topological charge (with the exception of $\nu = 0$), then chiral condensate diverges as one of the quark masses approaches zero. This completely unphysical behavior is remedied after summing over all topological charges, a procedure which becomes significantly more complicated for three or more quark flavors. We show in the following that the summation over all topological sectors can be performed for arbitrary $N_f$ and $\theta$ with the reduction of the partition function to $N_f - 2$ angular integrations over single Bessel functions.

This paper is organized as follows. In Sec. II, we briefly review the reduction of the QCD partition function to a finite dimensional group integral in the Leutwyler-Smilga scaling regime. In Sec. III, we review the summation over all topological charges for the partition function for $N_f = 1$ and 2. We then calculate the summation for arbitrary $N_f$ and quark masses. While the full partition function for $N_f = 2$ has been known for some time [36], there has not been a detailed study of the vacuum properties of this theory for $\theta \neq 0$. In Sec. IV, we examine the $\theta$ dependence of the chiral condensate, chiral susceptibility, topological density and topological susceptibility for two flavors. In Sec. V, we extend this discussion to three flavors. Finally, we give concluding remarks in Sec. VI.

II. PARTITION FUNCTIONS IN THE LEUTWYLER–SMILGA REGIME

Consider a $SU(N_c)$ gauge theory with $N_f$ flavors of fermions in the fundamental representation on a four-dimensional torus of volume $V = L^4$. The Lagrangian is

$$\mathcal{L} = \frac{1}{4g^2} F_{\mu\nu}^a F_{\mu\nu}^a - \sum_{f=1}^{N_f} \bar{\psi}_f (i\slashed{D} - m_f) \psi_f - i \theta \tilde{F}_{\mu\nu} F_{\mu\nu}^a ,$$

(1)

where $\tilde{F}_{\mu\nu} = \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} F_{\rho\sigma}^a$. The last term in eq. (1) is a total derivative and so does not affect the field equations or any of the perturbative aspects of the theory. The integral of this term over the four-volume is quantized and is given by

$$\nu = \frac{1}{32\pi^2} \int d^4 x \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x) \in \mathbb{Z} .$$

(2)

This quantity, known as the topological charge, contributes a phase factor to the path integral and is associated with transitions between topologically nontrivial gauge field configurations. The full partition function is given by a weighted sum over the partition function for each topological sector:
\[ Z^{(N_f)}(\theta, \{m_k\}) = \sum_{\nu=-\infty}^{\infty} e^{i\nu \theta} Z^{(N_f)}_{\nu}(\{m_k\}). \]  

The individual contributions are

\[ Z^{(N_f)}_{\nu}(\{m_k\}) = \int [dA]_{\nu} \prod_{f=1}^{N_f} \text{det} [iD[A] - m_f] \exp \left( - \int_V d^4x L_{YM}[A] \right), \]

where the integration is taken only over gauge field configurations with topological charge \( \nu \).

In principle, all of the observables of QCD can be calculated by evaluating eq. (3) and its various functional derivatives. Typically, however, this can only be done in some approximation since the integration is taken over an infinite dimensional functional space and there are ultraviolet and infrared divergences. Formulating the theory on a discrete, Euclidean lattice has the advantage of eliminating the ultraviolet divergences on account of a nonzero lattice spacing, \( a \), and the infrared divergences on account of a necessarily finite volume. A second approach is to analyze the partition function for the effective theory which describes the low–energy behavior. For QCD, this is chiral perturbation theory. Restricting the Euclidean four-volume, \( V = L^4 \), to the range

\[ \frac{1}{\Lambda} \ll L \ll \frac{1}{m_\pi}, \]

where \( \Lambda \) is the typical hadronic scale and \( m_\pi \) is the mass of the Goldstone excitations, results in tremendous simplifications and exact analytical predictions are possible \([38,36]\). This is possible since the lower limit ensures that the partition function is dominated by Goldstone modes and the upper limit ensures that these modes are constant, i.e. that the kinetic term in the partition function factorizes from the mass dependent term.

There have been a number of advances in recent years towards evaluating the QCD finite volume partition function. With the four-volume taken according to eq. (5), the partition function was shown in Refs. \([38,36]\) to reduce to the finite dimensional group integration

\[ Z^{(N_f)}(\theta, \{m_i\}, V) = \int_{SU(N_f)} dU \text{ exp} \left[ V \Sigma \text{Re} \left( e^{i\theta/N_f} \text{Tr} M U^\dagger \right) \right], \]

where \( M = \text{diag}(m_1, \ldots, m_{N_f}) \) is the mass matrix for the quark fields and \( \Sigma \) is the chiral condensate in the chiral and infinite volume limit. We shall henceforth refer to \( \Sigma \) as the macroscopic chiral condensate. The integration is taken over the group manifold of the Goldstone modes, \( SU(N_f) \). Note that the dependence on the volume, the macroscopic chiral condensate and the quark masses is only through the dimensionless scaling variable

\[ \mu_i = \Sigma V m_i. \]

The Fourier coefficients conjugate to \( Z^{(N_f)}(\theta, \{\mu_i\}) \) are obtained by taking the Fourier transformation of eq. (3),
They have been computed for arbitrary \( N_f \) and \( N_c \geq 3 \) \cite{42,39}, and can be expressed as

\[
Z^{(N_f)}(\{\mu_i\}) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \ Z^{(N_f)}(\theta, \{\mu_i\}) e^{-i\nu \theta} .
\]  

(8)

Combinatorial formulas for generating the character expansions of the \( U(N) \) group were recently given in Ref. \cite{13} and used to very efficiently derive eq. (9). The close connection to random matrix theory was firmly established in Refs. \cite{14,06}.

The vacuum properties of the theory are defined by eq. (6) and its derivatives. Recall that the first derivative of the logarithm of the partition function with respect to a parameter determines the mean value of the conjugate variable to the parameter, while the second derivative serves as a measure for the fluctuations around the average value. We focus on the derivatives with respect to the quark masses, \( m_i \), and the vacuum angle, \( \theta \). The chiral condensate for the \( i \)-th quark species is

\[
\Sigma^{(N_f)}(\theta, \{m_k\}, V) = \frac{1}{V N_f} \frac{\partial}{\partial m_i} \log Z^{(N_f)}(\theta, \{m_i\}, V) ,
\]

(12)

with the average value

\[
\Sigma^{(N_f)}(\theta, \{m_k\}, V) = \sum_{i=1}^{N_f} \Sigma^{(N_f)}_{(i)}(\theta, \{m_k\}, V) .
\]

(13)

This quantity should approach macroscopic chiral condensate, \( \Sigma \), at \( \theta = 0 \) and for large values of the scaling variable, \( \mu \). The chiral (scalar) susceptibility is defined as
\[
\chi^{(N_f)}_{ij}(\theta, \{m_k\}, V) = \frac{1}{V} \frac{\partial^2}{\partial m_i \partial m_j} \log Z^{(N_f)}(\theta, \{m_k\}, V) .
\]

(14)

Vacuum properties associated with the vacuum angle, \( \theta \), can be analogously defined. The topological density is

\[
\sigma(\theta, \{m_k\}, V) = -\frac{1}{V} \frac{\partial}{\partial \theta} \log Z^{(N_f)}(\theta, \{m_k\}, V) ,
\]

(15)

which at \( \theta = 0 \) has the interpretation of the mean topological charge. From eqs. (3) and (9), one can see that the topological density vanishes if \( \theta \) is an integer multiple of \( \pi \). The topological susceptibility is defined by

\[
\chi_{\text{top}}(\theta, \{m_i\}, V) = -\frac{1}{V} \frac{\partial^2}{\partial \theta^2} \log Z^{(N_f)}(\theta, \{m_i\}, V) ,
\]

(16)

which at \( \theta = 0 \) is the mean square deviation of the topological charge and is in general nonzero.

III. SUMMATION OVER TOPOLOGICAL CHARGES

When studying the vacuum properties, e.g. the chiral condensate, in the Leutwyler–Smilga regime, the necessity of including the contributions to the partition function from every topological sector was established in Ref. [41]. For one and two quark flavors, the summation can be performed using standard Bessel function identities. For \( N_f \geq 3 \), however, the summation is more complicated and to the best of our knowledge has not been performed previously in the literature. It is instructive to review the derivation of the results for one and two flavors before proceeding to the derivation for \( N_f \geq 3 \).

A. \( N_f = 1 \)

For \( N_f = 1 \), the summation over all topological sectors is straightforward to calculate. Using the definition of the generating function for modified Bessel functions [47],

\[
\exp \left[ \frac{x}{2} (t + t^{-1}) \right] = \sum_{\nu=-\infty}^{\infty} t^\nu I_\nu(x) ,
\]

(17)

the summation can be performed:

\[
Z^{(N_f=1)}(\theta, \mu) = \sum_{\nu=-\infty}^{\infty} e^{i\nu \theta} I_\nu(\mu)
= \exp \left[ \frac{\mu}{2} (e^{i\theta} + e^{-i\theta}) \right]
= \exp [\mu \cos \theta] .
\]

(18)

This result was first found in Ref. [30].
B. $N_f = 2$

For two flavors, the calculation is more involved but the method generalizes very naturally to $N_f \geq 3$. From eq. (3), the partition function is

$$Z^{(N_f=2)}(\theta, \mu_1, \mu_2) = \frac{1}{\mu_2 - \mu_1^2} \sum_{\nu=-\infty}^{\infty} e^{i\nu\theta} \left[ \mu_2 I_\nu(\mu_1) I_{\nu+1}(\mu_2) - \mu_1 I_\nu(\mu_2) I_{\nu+1}(\mu_1) \right].$$  (19)

Since the partition function is symmetric in the two scaling variables, we consider only the first term between the brackets in eq. (19). Following Ref. [47], we use the contour integral representation for $I_\nu(x)$ which follows from eq. (17),

$$I_\nu(x) = \oint \frac{ds}{2\pi i} s^{-\nu-1} \exp \left[ \frac{x}{2} (s + s^{-1}) \right],$$  (20)

where the contour is the standard Bessel function contour surrounding the negative real axis and the origin in a counterclockwise fashion. Using this representation, the summation can be calculated:

$$\sum_{\nu=-\infty}^{\infty} e^{i\nu\theta} I_\nu(\mu_1) I_{\nu+1}(\mu_2) = \sum_{\nu=-\infty}^{\infty} e^{i\nu\theta} I_\nu(\mu_1) \oint \frac{ds}{2\pi i} s^{-\nu-2} \exp \left[ \frac{\mu_2}{2} (s + s^{-1}) \right]$$  (21a)

$$= \oint \frac{ds}{2\pi i} s^{-2} \exp \left[ \frac{\mu_2}{2} (s + s^{-1}) \right] \sum_\nu (e^{i\theta} s^{-1})^\nu I_\nu(\mu_1)$$  (21b)

$$= \oint \frac{ds}{2\pi i} s^{-2} \exp \left[ \frac{\mu_2}{2} (s + s^{-1}) \right] \exp \left[ \frac{\mu_1}{2} (s e^{-\theta} + s^{-1} e^{\theta}) \right].$$  (21c)

By making the change of variables,

$$\omega = \frac{(\mu_2 + \mu_1 e^{-i\theta})}{\mu_{12}(\theta)} s$$  (22a)

$$\omega^{-1} = \frac{(\mu_2 + \mu_1 e^{i\theta})}{\mu_{12}(\theta)} s^{-1},$$  (22b)

where

$$\mu_{12}(\theta) \equiv \sqrt{\mu_1^2 + \mu_2^2 + 2 \mu_1 \mu_2 \cos \theta}.$$  (22c)

eq (21a) can then be simplified to yield

$$\sum_{\nu=-\infty}^{\infty} e^{i\nu\theta} I_\nu(\mu_1) I_{\nu+1}(\mu_2) = \frac{\mu_2 + \mu_1 e^{-i\theta}}{\mu_{12}(\theta)} \oint \frac{d\omega}{2\pi i} \omega^{-2} \exp \left[ \frac{\mu_{12}(\theta)}{2} (\omega + \omega^{-1}) \right]$$  (23)

$$= \frac{\mu_2 + \mu_1 e^{-i\theta}}{\mu_{12}(\theta)} I_1(\mu_{12}(\theta)) .$$

Combining the two contributions, the partition function for $N_f = 2$ is

$$Z^{(N_f=2)}(\theta, \mu_1, \mu_2) = \frac{I_1(\mu_{12}(\theta))}{\mu_{12}(\theta)} .$$  (24)

Equation (22c) defines a reduced mass determined by a triangle law. The triangle has sides $\mu_1$, $\mu_2$ and $\mu_{21}$ and the angle subtended by $\mu_1$ and $\mu_2$ is $\pi - \theta$. 

C. \( N_f \geq 3 \)

For \( N_f \geq 3 \), we consider cases of degenerate and nondegenerate quark masses separately. In the case of nondegenerate quark masses, the summation over topological charge is a generalization of the summation for \( N_f = 2 \). In the process of the derivation, we find interesting relationships between sums of products of arbitrarily many Bessel functions and angular integrations over single Bessel functions.

1. Nondegenerate quark masses

From eq. (9), the quantity that needs to be calculated is a summation of products of \( N_f \) modified Bessel functions weighted by a phase, since

\[
\det \mathcal{A}_\nu(\{\mu_i\}) = \varepsilon_{i_1 \ldots i_{N_f}} \prod_{j=1}^{N_f} \mu_{i_j}^{j-1} I_{\nu+j-1}(\mu_{i_j}) .
\]

Each term in the summation is of the form

\[
B = \sum_{\nu = -\infty}^{\infty} e^{\nu \theta} I_{\nu+m_1}(x_1) I_{\nu+m_2}(x_2) \cdots I_{\nu+m_{N_f}}(x_{N_f}) \quad (26)
\]

\[
= e^{-im_1 \theta} \sum_{\nu = -\infty}^{\infty} e^{\nu \theta} I_{\nu}(x_1) I_{\nu+n_2}(x_2) \cdots I_{\nu+n_{N_f}}(x_{N_f}) \equiv e^{-im_1 \theta} C,
\]

where \( n_j = m_j - m_1 \). For the calculation of the partition function, \( B \) is actually more general than necessary and the particular choices of \( x_j = \mu_{i_j} \) and \( m_j = j - 1 \) specialize to the appropriate terms in the partition function.

By expressing all but the first of the modified Bessel functions by their contour integral representations, \( C \) can be written as

\[
C = \sum_{\nu = -\infty}^{\infty} e^{\nu \theta} I_\nu(x_1) \prod_{j=2}^{N_f} \theta \left( \frac{ds_j}{2\pi i s_j} \right)^{-\nu-n_j-1} \exp \left[ \frac{x_j}{2} (s_j + s_j^{-1}) \right] .
\]

The definition of the generating function for \( I_n(x) \), eq. (17), can be used to perform the summation over \( \nu \):

\[
C = \prod_{j=2}^{N_f} \theta \left( \frac{ds_j}{2\pi i s_j} \right)^{-n_j-1} \exp \left[ \frac{x_j}{2} (s_j + s_j^{-1}) \right] \exp \left[ x_1 \left( \frac{e^{i\theta}}{s_2 \cdots s_{N_f}} + \frac{s_2 \cdots s_{N_f}}{e^{i\theta}} \right) \right] .
\]

We now make a change of variables which is suggested by eqs. (22a) and (22b):

\[
\omega = \left( x_2 + x_1 \frac{s_3 \cdots s_{N_f}}{e^{i\theta}} \right) \frac{s_2}{\psi} ,
\]

\[
\omega^{-1} = \left( x_2 + x_1 \frac{e^{i\theta}}{s_3 \cdots s_{N_f}} \right) \frac{s_2^{-1}}{\psi} ,
\]
where
\[ \psi^2 = x_1^2 + x_2^2 + x_1 x_2 \left( \frac{e^{i\theta}}{s_3 \ldots s_{N_f}} + \frac{s_3 \ldots s_{N_f}}{e^{i\theta}} \right). \] (31)

The contour integration over \( s_2 \) is rewritten as
\[
\oint \frac{ds_2}{2\pi i} s_2^{-n_2-1} \exp \left[ \frac{s_2}{2} \left( x_2 + x_1 \frac{s_3 \ldots s_{N_f}}{e^{i\theta}} \right) + \frac{1}{2s_2} \left( x_2 + x_1 \frac{e^{i\theta}}{s_3 \ldots s_{N_f}} \right) \right] = \left( \frac{x_2 + x_1 s_3 \ldots s_{N_f} e^{-i\theta}}{\psi} \right)^{n_2} \oint \frac{d\omega}{2\pi i} \omega^{-n_2-1} \exp \left( \frac{\psi}{2} (\omega + \omega^{-1}) \right).
\] (32)

Making the second change of variables, \( s_k = e^{i\theta_k} \), for \( k = 3, \ldots, N_f \), and deforming the contours to the unit circle, the final expression for \( C \) is obtained:
\[
C = \oint \prod_{j=3}^{N_f} \left( \frac{ds_j}{2\pi i} s_j^{-n_j-1} \exp \left( \frac{s_j}{2} (s_j + s_j^{-1}) \right) \right) \left( \frac{x_2 + x_1 s_3 \ldots s_{N_f} e^{-i\theta}}{\psi} \right)^{n_2} I_{n_2}(\psi).
\] (33)

Collecting the various contributions, the partition function for \( N_f \) quark flavors is
\[
Z^{(N_f)}(\theta, \mu_i) = \frac{1}{\Delta(\mu_i)} \varepsilon_{i_1 \ldots i_{N_f}} \left( \prod_{k=1}^{N_f} \mu_{i_k}^{k-1} \right) \mu_{i_2} S(\mu_{i_1}, \mu_{i_2}; \mu_{i_3}, \ldots, \mu_{i_{N_f}}),
\] (34)

where
\[
S(\mu_{i_1}, \mu_{i_2}; \mu_{i_3}, \ldots, \mu_{i_{N_f}}) = \oint_0^{2\pi} \prod_{k=3}^{N_f} \left( \frac{d\phi_k}{2\pi} \exp \left[ -i(k-1)\phi_k + \mu_{i_k} \cos(\phi_k) \right] \right) \frac{I_{i_1 i_2 i_3}(\theta; \phi_3, \phi_{N_f}, \ldots)}{\mu_{i_1 i_2}(\theta; \phi_3, \phi_{N_f}, \ldots)},
\] (35)

and
\[
\mu_{i_1 i_2}(\theta, \phi_3, \phi_{N_f}, \ldots) = \sqrt{\mu_{i_1}^2 + \mu_{i_2}^2 + 2\mu_{i_1 i_2} \cos (\phi_3 + \ldots + \phi_{N_f} - \theta)}.
\] (36)

Note that \( S(\mu_{i_1}, \mu_{i_2}; \mu_{i_3}, \ldots, \mu_{i_{N_f}}) \) is symmetric under the interchange of \( \mu_{i_1} \) and \( \mu_{i_2} \).

In the case of complete nondegeneracy, \( \mu_i \neq \mu_j \) for all \( i \neq j \), the partition function and its derivatives are analytic functions to all orders. Any potential nonanalyticities in eq. (33) and its
derivatives occur when $\mu_{i_1 j_2}(\theta, \phi_3, \ldots, \phi_{N_f})$ vanishes which is only possible if at least two quark masses become degenerate. This becomes apparent when eq. (34) is rewritten in the form

$$
\lim_{\mu_{i_1 j_2} \to \mu} \mu_{i_1 j_2}(\theta, \phi_3, \ldots, \phi_{N_f}) = \mu \sqrt{2 + 2 \cos \left( \frac{\phi_3 + \ldots + \phi_{N_f} - \theta}{2} \right)}
$$

(37)

which has a cusp at $\phi_3 + \ldots + \phi_{N_f} - \theta = \pi$. This behavior is a necessary condition for the derivatives of eq. (34) to have discontinuities. On account of the integration, this is not a sufficient condition.

2. Degenerate Quark Masses

The limit of equal quark masses, $\mu_i \to \mu$, can be calculated either by summing over all topological sectors for nondegenerate quark masses and then taking the limit $\mu_i \to \mu$, or starting from the equal mass partition function in a given topological sector, eq. (11) and then summing over all topological charges. Using the first approach, one can derive equal mass limit from eqs. (34)-(36) and the resulting expression for the partition function involves derivatives up to order $N_f - 1$ of modified Bessel functions with respect to the masses. This approach is quite cumbersome and, moreover, the derivatives are by construction taken at the cusps given by eq. (37). The second approach is more tractable and is the one used here. After expanding the determinant in eq. (11),

$$
Z^{(N_f)}_{\nu}(\mu) = \varepsilon_{i_1 \ldots i_{N_f}} \prod_{j=1}^{N_f} I_{\nu+j-i_j}(\mu),
$$

(38)

and using the contour integral representation for each Bessel function, the expression for the equal mass partition function in a sector of given topological charge becomes

$$
Z^{(N_f)}_{\nu}(\mu) = \oint \prod_{j=1}^{N_f} \left( \frac{d\phi_j}{2\pi} \exp \left[ \mu \cos(\phi_j) - i \nu \phi_j - i j \phi_j \right] \right) \varepsilon_{i_1 \ldots i_{N_f}} e^{i\phi_{i_1}} \ldots e^{i\phi_{i_{N_f}}}
$$

(39)

The last equality is obtained by change of variables, $s_j = e^{i\phi_j}$, deforming the integration contours to the unit circle, and making use of the identity

$$
\varepsilon_{k_1 \ldots k_{N_f}} e^{i\phi_{k_1}} \ldots e^{i\phi_{k_{N_f}}} = \varepsilon_{k_1 \ldots k_{N_f}} e^{ik_1 \phi_{k_1}} \ldots e^{ik_{N_f} \phi_{k_{N_f}}}
$$

(40)

This is true for finite $\mu_i$. As shown for $N_f = 2$ in Ref. [48], there can be a nonanalyticity if the two scaling variables are taken to infinity such that $\lim_{\mu_{i_1 j_2} \to \infty} \frac{1}{\mu_{i_1 j_2}^2} \to 0$. We expect that this limit can be generalized to arbitrary $N_f$ in a straightforward manner.
The authors of Ref. [36] showed using a result of Weyl that
\[ Z^{(N_f)}_\nu(\mu) = \frac{1}{N_f!} \int_0^{2\pi} \prod_{j=1}^{N_f} \left( \frac{d\phi_j}{2\pi} \exp[\mu \cos(\phi_j) + i\nu \phi_j] \right) \prod_{k<l} |e^{i\phi_k} - e^{i\phi_l}|^2 . \] (41)

Equations (39) and (41) can be transformed into one another by observing that
\[ \varepsilon_{i_1 \ldots i_{N_f}} e^{i\phi_{i_1}} \ldots e^{iN_f \phi_{i_{N_f}}} = \Delta\{e^{i\phi_j}\} = \prod_{k<l} (e^{i\phi_k} - e^{i\phi_l}) \] (42)

is a Vandermonde determinant, and so
\[ \prod_{k<l} |e^{i\phi_k} - e^{i\phi_l}|^2 = \Delta\{e^{i\phi_j}\} \Delta\{-e^{i\phi_j}\} . \] (43)

By expanding \( \Delta\{e^{-i\phi_j}\} \), one can transform both expressions into one another by an appropriate relabeling of the integration variables.

The summation over the topological charges can be performed using
\[ \int_0^{2\pi} \frac{d\phi_1}{2\pi} f(\phi_1, \ldots, \phi_{N_f}, \theta) \sum_{\nu=-\infty}^{\infty} e^{i\nu(\theta - \phi_1 - \ldots - \phi_{N_f})} = f(\phi_2 + \ldots + \phi_{N_f} - \theta, \phi_2, \ldots, \phi_{N_f}, \theta) , \] (44)

provided \( f \) is \( 2\pi \)-periodic in \( \phi_1 \). For the subsequent integration over \( \phi_2 \), an integral representation of the Bessel functions is used. The details of the calculation are given in the appendix. The result is
\[ Z^{(N_f)}(\theta, \mu) = \varepsilon_{a_1 \ldots a_{N_f}} (a_2 - a_1) \prod_{m=3}^{N_f} \left( \int_0^{2\pi} \frac{d\phi_m}{2\pi} e^{\mu \cos(\phi_m)} \right) \frac{I_{a_1 - a_2}(\mu(\phi_3, \ldots, \phi_{N_f}, \theta))}{\mu(\phi_3, \ldots, \phi_{N_f}, \theta)} \times \cos\left\{ (3 - a_1 - a_2)(\theta + \phi_3 + \ldots + \phi_{N_f})/2 - (3 - a_3)\phi_3 - \ldots - (N_f - a_{N_f})\phi_{N_f} \right\} , \] (45)

where
\[ \mu(\phi_3, \ldots, \phi_{N_f}, \theta) = \mu\sqrt{2 + 2 \cos (\phi_3 + \ldots + \phi_{N_f} - \theta)} . \] (46)

The summation over the completely antisymmetric tensor can be simplified to give a \( (N_f - 2) \)-fold integration over a sum of \( N_f - 1 \) Bessel functions multiplied by some phases,
\[ Z^{(N_f)}(\theta, \mu) = -2 e^{-i\phi/2} \int_0^{2\pi} \prod_{m=3}^{N_f} \left( \frac{d\phi_m}{2\pi} e^{\mu \cos(\phi_m) - i(m-3/2)\phi_m} \right) \times \sum_{r=1}^{N_f-1} \sum_{m=3}^{N_f} r(-1)^r \frac{I_r(\mu(\phi_3, \ldots, \phi_{N_f}, \theta))}{\mu(\phi_3, \ldots, \phi_{N_f}, \theta)} \alpha_r^{(N_f)}(\phi_3, \ldots, \phi_{N_f}, \theta) . \] (47)

The phases \( \alpha_r^{(N_f)}(\phi_3, \ldots, \phi_{N_f}, \theta) \) are given by
\[ \alpha_r^{(N_f)}(\phi_3, \ldots, \phi_{N_f}, \theta) = \sum_{j=1}^{N_f-r} e^{-i(j+r/2)(\phi_3 + \ldots + \phi_{N_f} - \theta)} \beta_{j+1}^{(N_f)}(\phi_3, \ldots, \phi_{N_f}) , \] (48)
with

$$
\beta_{k,l}^{(N_f)}(\phi_3, \ldots, \phi_{N_f}) = \begin{vmatrix}
1 & \ldots & e^{i(k-2)\phi_3} & e^{ik\phi_3} & \ldots & e^{i(l-2)\phi_3} & e^{il\phi_3} & \ldots & e^{i(N_f-1)\phi_3} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
1 & \ldots & e^{i(k-2)\phi_{N_f}} & e^{ik\phi_{N_f}} & \ldots & e^{i(l-2)\phi_{N_f}} & e^{il\phi_{N_f}} & \ldots & e^{i(N_f-1)\phi_{N_f}} 
\end{vmatrix}. \quad (49)
$$

Despite appearances, this last expression is real. As mentioned above, the possible emergence of a cusp in the integrand occurs in the ratios of the Bessel functions and $$\mu(\phi_3, \ldots, \phi_{N_f}, \theta)$$. At this stage, it is not \textit{a priori} obvious that there are nonanalyticities after the integrations are performed. Thus, one must consider them on a case by case basis. This is done for $$N_f = 2$$ and 3 in the following sections.

\section*{IV. Vacuum Properties for $$N_f = 2$$}

Since the partition function for $$N_f = 2$$, eq. (24), can be expressed in closed form even after summing over all topological charges, calculating the vacuum observables is straightforward. Most of the work in the literature has focused upon the behavior of the chiral condensate and the topological susceptibility as functions of the scaling variable for either $$\theta = 0$$ or in a sector of fixed topological charge. In this section, we demonstrate that QCD in the Leutwyler–Smilga scaling regime exhibits a great deal of nontrivial behavior at nonzero values of $$\theta$$ for $$N_f = 2$$.

\subsection*{A. Partition Function}

The partition function for two quark flavors is

$$
Z^{(N_f=2)}(\theta, \mu_1, \mu_2) = \frac{I_1(\sqrt{\mu_1^2 + \mu_2^2 + 2\mu_1\mu_2 \cos \theta})}{\sqrt{\mu_1^2 + \mu_2^2 + 2\mu_1\mu_2 \cos \theta}}. \quad (50)
$$

At $$\theta = (2n+1)\pi$$, where $$n$$ is an integer, it reduces to

$$
Z^{(N_f=2)}(\theta = (2n+1)\pi, \mu_1, \mu_2) = \frac{I_1(|\mu_1 - \mu_2|)}{|\mu_1 - \mu_2|}, \quad (51)
$$
i.e. the theory at $$\theta = \pi$$ is equivalent to the theory at $$\theta = 0$$ but taking one quark masses to be negative. This is in accordance with the standard lore. Taking the two quark masses to be equal, however, leads to the surprising result that the partition function is \textit{independent} of the scaling variable,

$$
Z^{(N_f=2)}(\theta = (2n+1)\pi, \mu) = \frac{1}{2}. \quad (52)
$$

This can be seen also by starting from the equal mass partition function:
Since \( Z^{(N_f=2)}(\theta, \mu_1, \mu_2) \) is a smooth function of \( \mu_1, \mu_2 \) and \( \theta \), it does not matter in which order the limits of degenerate masses and \( \theta = (2n+1)\pi \) are taken. This result may be understood in terms of the microscopic spectral density. As shown in Ref. \[41\], after summing over all topological charges, the full microscopic spectral density is related to a particular quotient of the partition function for \( N_f \) flavors at \( \theta \) and the partition function for \( N_f + 2 \) flavors at \( \theta + \pi \). Thus, the partition function for two flavors at \( \theta = \pi \) is related to the quenched \((N_f = 0)\) theory at \( \theta = 0 \). This fact also demonstrates at a qualitative level that the partition function becomes independent of the quark masses if and only if \( N_f = 2 \) and \( \theta = \pi \) [49]. It is apparent already at the level of the partition function that, at least in the Leutwyler–Smilga scaling regime, QCD is very different qualitatively at \( \theta = n\pi \) than at all other values of \( \theta \).

This can also be understood directly from chiral perturbation theory. For \( N_f = 2 \), the leading order term in chiral perturbation theory, \( \Sigma \text{Re} \left\{ \text{Tr} \left\{ \mathcal{M} e^{i\theta/N_f} U^1 \right\} \right\} \), vanishes at \( \theta = \pi \) when \( \mathcal{M} = m\mathbf{1} \) since the trace of an \( SU(2) \) matrix is always real. This term, however, is the only relevant term in the Leutwyler–Smilga scaling regime as can be seen from eq. (5). From this observation, it is clear that the partition function at \( \theta = \pi \) is simply a constant in this case. The resolution to this problem was given in Ref. \[24\] where higher order terms quadratic in masses were included in the effective chiral Lagrangian. A more extensive analysis in terms of chiral perturbation theory was given in Refs. \[28,29\]. By including higher order terms in the chiral expansion, the energy density then depends once again explicitly on the quark masses. These terms, however, are suppressed in the Leutwyler-Smilga regime and so we do not include them.

The most fundamental quantity that can be derived from the partition function is the energy density which is defined by

\[
E(\theta, \mu_1, \mu_2) = -\frac{1}{V} \log Z^{(N_f=2)}(\theta, \mu_1, \mu_2).
\]  

An expansion for large \( \mu_{12}(\theta) \) gives

\[
E(\theta, \mu_1, \mu_2) = -\frac{\mu_{12}(\theta)}{V} + \mathcal{O}(\log \mu_{12}(\theta)).
\]  

Note that the volume dependence drops out in the leading order term. In the macroscopic limit, \( \mu_{12}(\theta) \gg 1 \),

\[
\lim_{V \to \infty} E(\theta, m_1, m_2, V) = \begin{cases} 
-\Sigma m_1 - \Sigma m_2 \cos \theta + \mathcal{O}(m_2/m_1), & m_1 \gg m_2 \\
-2m \Sigma |\cos(\theta/2)|, & m_1 = m_2 = m
\end{cases}
\]  

There is a constant shift, \( E_0 = -\Sigma m_1 \), in the energy density which we subtract in the following. The energy density in both limits is plotted in Fig. 1. It is minimized at \( \theta = 0 \) and maximized at \( \theta = \pi \). For degenerate quark masses, there is a cusp at \( \theta = \pi \).
FIG. 1. The energy density for $N_f = 2$ in the macroscopic limit. The lower curve corresponds to degenerate quark masses, while the upper curve corresponds to an infinite mass splitting. The region between the two curves contains all finite mass splittings. The global minimum of the energy density for all cases occurs at $\theta = 0$.

B. Chiral Condensate

The chiral condensate is calculated from eq. (12) and for the first quark flavor is

$$\Sigma^{(N_f=2)}_{(1)}(\theta, \mu_1, \mu_2) = \frac{\Sigma (\mu_1 + \mu_2 \cos \theta)}{\mu_{12}(\theta)} I_2(\mu_{12}(\theta)) I_1(\mu_{12}(\theta)).$$

(57)

The condensate for the second quark flavor is given by the same expression with $\mu_1$ and $\mu_2$ interchanged. The total chiral condensate given by the sum is

$$\Sigma^{(N_f=2)}(\theta, \mu_1, \mu_2) = \frac{\Sigma (\mu_1 + \mu_2)(1 + \cos \theta)}{\mu_{12}(\theta)} I_2(\mu_{12}(\theta)) I_1(\mu_{12}(\theta)).$$

(58)

For $\theta = 0$, the individual contributions are equal. For $\theta = \pi$, however, they are equal in magnitude but opposite in sign:

$$\Sigma^{(N_f=2)}_{(1)}(\pi, \mu_1, \mu_2) = \text{sign}(\mu_1 - \mu_2) \frac{\Sigma I_2(\mu_{12}(\pi))}{I_1(\mu_{12}(\pi))} = -\Sigma^{(N_f=2)}_{(2)}(\pi, \mu_1, \mu_2),$$

(59)

with their sum, the total chiral condensate, vanishing for any value of the quark masses.

Taking of the limit of degenerate quark masses, the chiral condensate is

$$\Sigma^{(N_f=2)}_{(1,2)}(\theta, \mu) = \frac{\Sigma \sqrt{2 + 2 \cos \theta} I_2(\mu \sqrt{2 + 2 \cos \theta})}{4 I_1(\mu \sqrt{2 + 2 \cos \theta})}.$$

(60)

$$= \frac{\Sigma^{(N_f=2)}_{(1,2)}(\theta, \mu)}{2}.$$
Three observations may be made based upon eq. (60) about the physics of QCD in the Leutwyler–Smilga scaling regime at nonzero values of $\theta$:

- For fixed $\mu$, the chiral condensate decreases monotonically in the interval $\theta \in [0, \pi)$ and increases monotonically for $\theta \in (\pi, 2\pi)$.
- As $\mu = m \Sigma V \to \infty$, the chiral condensate develops a cusp at $\theta = \pi$.
- For any value of $\mu$, the chiral condensate vanishes identically at $\theta = \pi$.

This behavior is shown in Figs. 2 and 3. The last observation follows of course from the constancy of the partition function for $N_f = 2$ at $\theta = \pi$ and is not expected to be true outside the Leutwyler–Smilga regime.

![Figure 2](image)

**FIG. 2.** The chiral condensate in the macroscopic limit as a function of $\theta$ normalized to the infinite volume value, $\Sigma$. The lower curve corresponds to asymptotically large quark mass splitting and the upper curve is limit of degenerate quark masses. The area between the two curves contains all finite mass splittings between the quark masses. There is a cusp at $\theta = \pi$ for equal quark masses.

For small values of the scaling variable, the chiral condensate has the expansion

$$\frac{\Sigma(N_f=2)(\theta, \mu)}{\Sigma} = \cos^2(\theta/2) \mu - \frac{\cos^4(\theta/2)}{12} \mu^3 + \frac{\cos^6(\theta/2)}{48} \mu^5 + \mathcal{O}(\mu^7).$$  \hspace{1cm} (61)

As expected, the chiral condensate is linear to lowest order in the quark mass and vanishes term-by-term at $\theta = (2n+1)\pi$. The expression for the chiral condensate simplifies in the limit of degenerate quark masses and in the limit of large quark mass splitting:
The volume dependence of the chiral condensate in these two limits is easily calculated. In the limit of small volume, the chiral condensate vanishes in both limits of degenerate quark masses and large mass splittings. In the macroscopic limit, \( V \gg 1/\Sigma m \), the chiral condensate is

\[
\lim_{V \to \infty} \Sigma^{(N_f=2)}(\theta, m_1, m_2, V) = \begin{cases} 
\Sigma \cos^2(\theta/2) + O(m_2/m_1) , & m_1 \gg m_2 \\
\Sigma \frac{\sqrt{2} + 2 \cos \theta}{2} \frac{T_2(m \Sigma V \sqrt{2 + 2 \cos \theta})}{T_1(m \Sigma V \sqrt{2 + 2 \cos \theta})} , & m_1 = m_2 = m
\end{cases}
\]

and is independent of the quark masses in both cases. Any nonzero quark mass splitting, \( m_1 \neq m_2 \), interpolates between these two cases as shown in Fig. 3. The value of the chiral condensate is remarkably insensitive to the magnitude of the quark mass splitting.

In Fig. 3, the chiral condensate as a function of the scaling variable is plotted for \( \theta = 0, \pi/2 \), and \( \pi \). As \( \theta \) increases from zero to \( \pi \), the condensate decreases and vanishes identically at \( \theta = \pi \). The monotonic decrease in the chiral condensate can be understood from the underlying QCD Lagrangian [49]. If one performs a chiral rotation by an angle \( \alpha \), then \( \theta \to \theta - \alpha \) and the chiral condensate, \( \langle \bar{\psi} \gamma_5 \psi \rangle \) rotates into \( \langle \bar{\psi} \gamma_5 \psi \rangle \). For \( N_f = 2 \), the (scalar) chiral condensate is completely...
rotated into the pseudoscalar chiral condensate at $\theta = \pi$. This can be demonstrated analytically by introducing a complex mass matrix as a source for both the scalar and pseudoscalar chiral condensates.

C. Chiral Susceptibility

The chiral susceptibility has been previously studied in Ref. [50] but the analysis was restricted to fixed values of $\nu$. As shown in Ref. [41], however, the contributions from all topological sectors can be important in the mesoscopic regime. Defining

\[ S(\mu_{12}(\theta)) = \left[ \frac{I_3(\mu_{12}(\theta))}{I_1(\mu_{12}(\theta))} - \frac{I_2(\mu_{12}(\theta))^2}{I_1(\mu_{12}(\theta))^2} \right] \]  
\[ T(\mu_{12}(\theta)) = \frac{1}{\mu_{12}(\theta)} \frac{I_2(\mu_{12}(\theta))}{I_1(\mu_{12}(\theta))} \]  

the diagonal terms in the chiral susceptibility are

\[ \chi_{11} = \sum \nu \left[ \frac{(\mu_1 + \mu_2 \cos \theta)^2}{\mu_{12}(\theta)^2} S(\mu_{12}(\theta)) + T(\mu_{12}(\theta)) \right] \]  
\[ \chi_{22} = \sum \nu \left[ \frac{(\mu_2 + \mu_1 \cos \theta)^2}{\mu_{12}(\theta)^2} S(\mu_{12}(\theta)) + T(\mu_{12}(\theta)) \right] . \]  

The off-diagonal terms are

\[ \chi_{12} = \chi_{21} = \sum \nu \left[ \frac{(\mu_1 + \mu_2 \cos \theta)(\mu_2 + \mu_1 \cos \theta)}{\mu_{12}(\theta)^2} S(\mu_{12}(\theta)) + \cos \theta T(\mu_{12}(\theta)) \right] . \]  

In the limit of degenerate quark masses, $m_1 = m_2 = m$, chiral susceptibilities become

\[ \chi_{11} = \chi_{22} = \sum \nu \left[ \frac{\nu \cos^2(\theta/2)}{4m} S(\mu_{12}(\theta)) + \mu \cos \theta T(\mu_{12}(\theta)) \right] \]  
\[ \chi_{12} = \chi_{21} = \sum \nu \left[ \frac{\nu \cos^2(\theta/2)}{4m} S(\mu_{12}(\theta)) + \mu \cos \theta T(\mu_{12}(\theta)) \right] . \]

At $\theta = \pi$, the diagonal and off-diagonal elements are maximally different,

\[ \chi_{11}(\theta = \pi) = \chi_{22}(\theta = \pi) = \frac{\sum \nu}{4m} = \frac{\sum \nu}{4} \]  
\[ \chi_{12}(\theta = \pi) = \chi_{21}(\theta = \pi) = - \frac{\sum \nu}{4m} = - \frac{\sum \nu}{4} . \]

An expansion in small $\mu$ yields

\[ \chi_{11} = \chi_{22} = \sum \nu \left[ \frac{\mu}{4} - \frac{1}{24} \cos^2(\theta/2)(2 + \cos \theta) \mu^3 + \mathcal{O}(\mu^5) \right] \]  
\[ \chi_{12} = \chi_{21} = \sum \nu \left[ \frac{\mu \cos \theta}{4} - \frac{1}{24} \cos^2(\theta/2)(1 + 2 \cos \theta) \mu^3 + \mathcal{O}(\mu^5) \right] . \]

On the other hand, in the limit $\mu \gg 1$ for $\theta \neq \pi$, 17
\[ \chi_{11} = \chi_{22} = \frac{\sum m}{m} \left[ \frac{\sin^2(\theta/2)}{2[\cos(\theta/2)]} + \frac{3\cos \theta}{8\mu \cos(\theta/2)^2} + O(1/\mu^2) \right] \]  
\[ \chi_{12} = \chi_{21} = -\frac{\sum m}{m} \left[ \frac{\sin^2(\theta/2)}{2[\cos(\theta/2)]} + \frac{3}{8\mu \cos(\theta/2)^2} + O(1/\mu^2) \right], \]  
for leading order in $1/\mu$, $\chi_{11} = \chi_{22} = -\chi_{12} = -\chi_{21}$. The chiral susceptibility was shown to be proportional to $3/8m^2V$ at $\theta = 0$ in Ref. [50]. The importance of summing over all topological charges is clear in this expression, since the leading order terms in eqs. (70a) and (70b) vanish at $\theta = 0$.

D. Topological Density: First–Order Phase Transition at $\theta = \pi$

The topological density, defined by eq. (15), is
\[ \sigma(\theta, \mu_1, \mu_2) = \frac{1}{V} \frac{\mu_1 \mu_2 \sin \theta}{2} \frac{I_2(\mu_1^2(\theta))}{I_1(\mu_1^2(\theta))}. \]  
At $\theta = 0$, $\sigma(\theta, \mu_1, \mu_2)$ has the strict interpretation as the mean topological charge. Since in a large enough ensemble of gauge fields the average number of instantons should be equal to average number of anti-instantons, the topological density should be zero at $\theta = 0$, and, indeed, the right hand side of eq. (71) vanishes for $\theta$ equal to any integer multiple of $\pi$.

In the limit of degenerate quark masses, the topological density becomes
\[ \sigma(\theta, \mu) = \frac{1}{V} \frac{\mu \sin \theta}{\sqrt{2 + 2 \cos \theta}} \frac{I_2(\mu \sqrt{2 + 2 \cos \theta})}{I_1(\mu \sqrt{2 + 2 \cos \theta})}. \]  
The most interesting property of this relation is that in the limit of very large scaling variable, $\mu \gg 1$, $\sigma(\theta, \mu)$ develops a discontinuity at $\theta = \pi$. This is the first–order phase transition proposed by Dashen [21].

\[ \sigma(\theta, m_1, m_2, V) = \begin{cases} 
\sum m_2 \sin \theta \frac{I_2(\Sigma V m_1)}{I_1(\Sigma V m_1)} + O(m_2/m_1), & m_1 \gg m_2 \\
\sum m \sin(\theta/2) \frac{I_2(2\Sigma V m \cos(\theta/2))}{I_1(2\Sigma V m \cos(\theta/2))}, & m_1 = m_2 = m 
\end{cases} \]  
Then, in the infinite volume limit,
\[ \lim_{V \to \infty} \sigma(\theta, m_1, m_2, V) = \begin{cases} 
\sum m_2 \sin \theta + O(m_2/m_1), & m_1 \gg m_2 \\
\sum m \sin(\theta/2) \text{sign}(\cos(\theta/2)), & m_1 = m_2 = m. 
\end{cases} \]  
The limit $m_1 \gg m_2$ coincides with the one-flavor case. For two flavors of degenerate quarks, there is a first–order phase transition at $\theta = \pi$, while for two flavors of non-degenerate quarks the phase transition disappears as long as the quark masses are kept finite. As mentioned above, it was shown
in Ref. [48] that there exists a particular scaling limit in which there may be a phase transition for nondegenerate quark masses.

FIG. 4. The topological density of the $\theta$ vacua. The solid line corresponds to the limit where one quark mass is very heavy, $m_1 \gg m_2$, the long dashed line to mass splitting of $m_1/m_2 = 2$, and the dashed line to the case of degenerate masses, $m_1 = m_2 = m$. A first-order phase transition occurs at $\theta = \pi$ in the case of degenerate quark masses. The transition is washed out by mass splitting between the quarks. The topological density is measured in units of $m_2 \Sigma$, where $m_2$ denotes the mass of the lighter quark.

E. Topological Susceptibility

The topological susceptibility reads

$$\chi^{(N_f=2)}(\theta, m_1, m_2, V) = \frac{1}{V} \frac{I_2(\mu_{12}(\theta))}{I_1(\mu_{12}(\theta))} \frac{\mu_{12}(\theta)}{\mu_1 \mu_2} \left( \frac{\mu_{12}(\theta) \cos \theta}{\mu_1 \mu_2} \left( \frac{4}{\mu_{12}(\theta)} + \frac{I_2(\mu_{12}(\theta))}{I_1(\mu_{12}(\theta))} - \frac{I_1(\mu_{12}(\theta))}{I_2(\mu_{12}(\theta))} \right) \sin^2(\theta) \right).$$

For equal quark masses, one has

$$\chi^{(N_f=2)}(\theta, m, V) = \frac{\Sigma m}{2} \frac{2 - \cos \theta}{\cos(\theta/2)|I_1(\mu(\theta))} + \frac{\Sigma^2 m^2 V}{4} \frac{\sin^2(\theta)}{\cos^2(\theta/2)} \left( \frac{I_2(\mu(\theta))^2}{I_1(\mu(\theta))^2} - 1 \right).$$

This reduces at $\theta = \pi$ to

$$\chi^{(N_f=2)}(\theta = \pi, m, V) = - \frac{\Sigma^2 m^2}{4} V,$$

which diverges in the infinite volume limit on account of the first-order phase transition. For $\theta \neq \pi$, however, the limit is finite,
\[
\lim_{V \rightarrow \infty} \chi^{(N_f=2)}(\theta, m, V) = \frac{\Sigma m}{2} |\cos(\theta/2)|, \quad \theta \neq \pi.
\]  
(78)

This is completely consistent with the expectation from the flavor singlet Ward–Takahashi identity at \(\theta = 0\) which predicts a linear rise in topological susceptibility with mass \([51]\),

\[
\lim_{V \rightarrow \infty} \chi^{(N_f)}(\theta = 0, m, V) = \frac{\Sigma m}{N_f} + \mathcal{O}(m^2).
\]  
(79)

Equation (78) may be considered to be a generalization of eq. (79) to nonzero values of \(\theta\).

In the limit of large mass splitting, the topological susceptibility reduces to

\[
\chi^{(N_f=2)}(\theta, m_1, m_2, V) = \Sigma m_2 \cos \theta \frac{I_2(\Sigma V m_1)}{I_1(\Sigma V m_1)} + \mathcal{O}(m_2/m_1), \quad m_1 \gg m_2,
\]  
(80)

which in the macroscopic limit is

\[
\lim_{V \rightarrow \infty} \chi^{(N_f=2)}(\theta, m_1, m_2, V) = \Sigma m_2 \cos \theta + \mathcal{O}(m_2/m_1), \quad m_1 \gg m_2.
\]  
(81)

**FIG. 5.** The topological susceptibility as a function \(\theta\) in the macroscopic limit. The solid, long dashed, and dashed line represent \(m_1 \gg m_2\), \(m_1/m_2 = 2\), and \(m_1 = m_2\), respectively.

**V. VACUUM PROPERTIES FOR \(N_F = 3\)**

The summation over all topological charges in the partition function for \(N_f \geq 3\) was performed in Sec. \([1]\). In this section, we complement the analysis of Sec. \([1]\) by examining the \(\theta\) dependence of the QCD vacuum for three flavors of quarks. The partition function for \(N_f = 3\) involves a single
integration which we were not able to calculate analytically. Since the partition function has a group–theoretic origin, we expect that the integrals that result after summing over all topological charges provide some functional representation of the Goldstone manifold. However, since the integrand is a smooth function of $\theta$ and $\mu$ except possibly at a single point in the interval of integration and the integral is taken over a compact interval, the numerical evaluation of the partition function is straightforward. Additionally, the derivatives of the partition function with respect to $\theta$ and $\mu$ can be commuted past the integration. Explicit expressions are only given for the chiral condensate and the topological density since the expressions for the chiral and topological susceptibilities become quite complicated and are not particularly enlightening even in the limit of degenerate quark masses.

We focus on a triplet of quark masses, $(m_{\text{light}}, m_{\text{light}}, m_{\text{heavy}})$, between the limits of total degeneracy, $m_{\text{light}} = m_{\text{heavy}}$, and very large mass splitting, $m_{\text{light}} \ll m_{\text{heavy}}$.

### A. Partition Function

For three degenerate masses, the partition function can be written in the compact form:

$$Z^{(N_f=3)}(\theta, \mu) = \frac{2}{\pi} \int_0^{2\pi} d\phi e^{\mu \cos \phi} \left[ \cos \left( \frac{3\phi - \theta}{2} \right) \left( I_1(\mu(\theta, \phi)) - \cos \left( \frac{3\phi - \theta}{2} \right) I_2(\mu(\theta, \phi)) \right) \right]$$

$$= \frac{2}{\pi} \int_0^{2\pi} d\phi e^{\mu \cos \phi} \frac{I_1(\mu(\theta, \phi))}{\cos \left( \frac{3\phi - \theta}{2} \right)} \frac{I_2(\mu(\theta, \phi))}{\cos \left( \frac{3\phi - \theta}{2} \right)} ,$$

where $\mu(\theta, \phi) = 2\mu \left| \cos \left( \frac{\phi - \theta}{2} \right) \right|$. Unlike the $N_f = 2$ partition function, we find that $Z^{(N_f=3)}(\theta, \mu)$ does not become independent of $\mu$ at $\theta = \pi$ which is consistent with the discussion in Sec. [IV A]. As discussed in Refs. [28,29], the leading order term in the chiral expansion does not vanish at $\theta = \pi$ for $N_f \geq 3$.

The dependence of the energy density as a function of $\theta$, however, is similar to the two flavor case. The energy density in the macroscopic limit is shown in Fig. 6 shifted by its zero point, $E_0 = -\Sigma m_{\text{heavy}}$. The global minimum and maximum of the energy density in the macroscopic limit are at $\theta = 0$ and $\pi$, respectively. As long as two quark masses are degenerate, there seems to be a cusp at $\theta = \pi$. In general, the positions for the global minimum and maximum are $\theta = 0$ and $\pi$, respectively, for any value of $\mu$. The zero point energy is dominated by the heavy quark mass. After subtracting this physically irrelevant zero point contribution, the energy density is relatively insensitive to taking the heavy quark mass to infinity.

### B. Chiral Condensate

For three degenerate quark masses, the chiral condensate is
\[
\Sigma^{(N_f=3)}(\theta, \mu) = \frac{2}{\pi} \frac{\Sigma}{2^{(N_f=3)}(\theta, \mu)} \int_0^{2\pi} d\phi e^{\mu \cos \phi} \left[ a_1 I_1(\mu(\theta, \phi)) + a_2 I_2(\mu(\theta, \phi)) \right],
\]

(83a)

where

\[
a_1 = \cos \left( \frac{3\phi - \theta}{2} \right) \left[ \cos \phi \cos \left( \frac{3\phi - \theta}{2} \right) - \left| \cos \left( \frac{\phi - \theta}{2} \right) \right| \right]
\]

(83b)

\[
a_2 = \cos \left( \frac{3\phi - \theta}{2} \right) \left[ \frac{3}{\mu} - \cos \phi + 2 \cos \left( \frac{3\phi - \theta}{2} \right) \left| \cos \left( \frac{\phi - \theta}{2} \right) \right| \right].
\]

(83c)

In many respects, the behavior of the equal mass chiral condensate for two and three quark flavors is again similar. The chiral condensate as a function of the scaling variable is plotted in Fig. 7. The chiral condensate decreases monotonically as \(\theta\) increases from zero to \(\pi\) like the \(N_f = 2\) case. However, it is nonzero at \(\theta = \pi\) unlike the \(N_f = 2\) chiral condensate. For small values of \(\mu\), the chiral condensate is linear in \(\mu\) and independent of \(\theta\).

FIG. 6. The energy density in the macroscopic limit as a function of \(\theta\). The upper (lower) curve corresponds to infinite (zero) mass splitting between the two degenerate quark masses and the third quark mass. All finite mass splittings are contained in the region between the two curves.

Figure 8 shows the chiral condensate as a function of \(\theta\) in the macroscopic limit, \(\mu \to \infty\). In this limit, \(\Sigma^{(N_f=3)}(\theta, \mu)\) has a cusp at \(\theta = \pi\), but otherwise is a smooth function. In the macroscopic limit with two degenerate quark masses, the value of the chiral condensate is very insensitive to the mass of the third nondegenerate quark. For any nonzero value of \(\theta\), the chiral condensate is always less than the \(\theta = 0\) chiral condensate. We find numerically that
\[
\Sigma(\theta = \pi, m_{\text{light}}, m_{\text{heavy}}) = \begin{cases} 
1/2, & m_{\text{light}} = m_{\text{heavy}} \\
1/3, & m_{\text{light}} \ll m_{\text{heavy}}
\end{cases}
\] (84)

to a very high precision.

FIG. 7. The mass dependence of the chiral condensate for various values of \(\theta\) for three degenerate quark flavors. The upper, middle and lower curves correspond to \(\theta = 0, \pi/2,\) and \(\pi\), respectively. As \(\theta\) is increased from zero to \(\pi\), the chiral condensate decreases in magnitude for a given \(\mu\).

C. Topological Density: First-Order Phase Transition at \(\theta = \pi\)

For degenerate quark masses, the topological density is given by

\[
\sigma(\theta, \mu, V) = \frac{2}{\pi} \frac{1}{Z(N_f=3)} \frac{1}{V} \int_0^{2\pi} d\phi \frac{e^{\mu \cos \phi}}{\mu(\theta, \phi)} \left[ b_1 I_1 (\mu(\theta, \phi)) + b_2 I_2 (\mu(\theta, \phi)) \right] 
\] (85a)

where the coefficients are given by

\[
b_1 \equiv \cos \left( \frac{3\phi - \theta}{2} \right) \left[ -\mu \sin \left( \frac{\phi - \theta}{2} \right) + \sin \left( \frac{3\phi - \theta}{2} \right) \right] 
\] (85b)

\[
b_2 \equiv \cos \left( \frac{3\phi - \theta}{2} \right) \left[ \mu \cos \left( \frac{3\phi - \theta}{2} \right) \sin \left( \frac{\phi - \theta}{2} \right) + \frac{3}{2} \tan \left( \frac{\phi - \theta}{2} \right) - \frac{1}{2} \tan \left( \frac{3\phi - \theta}{2} \right) \right] . 
\] (85c)

The topological density as a function of \(\theta\) is shown in Fig. 8 in the macroscopic limit. For three degenerate quark masses, there is a discontinuity at \(\theta = \pi\) which is simply Dashen’s phenomena.
This discontinuity is washed out for any nonzero mass splitting, however, for any mass splitting between $m_{\text{heavy}}$ and $m_{\text{light}}$, the transition is always extremely rapid.

\[ \lim_{V \to \infty} \chi^{(N_f=3)}(\theta = 0, m_{\text{light}}, m_{\text{heavy}}, V) = \begin{cases} \frac{\Sigma m_{\text{light}}}{3}, & m_{\text{light}} = m_{\text{heavy}} \\ \frac{\Sigma m_{\text{light}}}{2}, & m_{\text{light}} \ll m_{\text{heavy}} \end{cases} \] (86)

which is consistent with the Ward–Takahashi identity. [24]
FIG. 9. The $N_f = 3$ topological density as a function of $\theta$ in the macroscopic limit for which at least two of the quark masses are degenerate. The solid, dashed and long–dashed curves correspond to the mass splittings $m_{\text{heavy}} \gg m_{\text{light}}$, $m_{\text{heavy}} = 2m_{\text{light}}$, and $m_{\text{heavy}} = m_{\text{light}}$, respectively. For completely degenerate masses, there is a first–order phase transition at $\theta = \pi$. Even for large mass splittings, however, there is still a very rapid crossover.
FIG. 10. The $N_f = 3$ topological susceptibility as a function of $\theta$ in the macroscopic limit for which at least two of the quark masses are degenerate. The solid, dashed and long–dashed curves correspond to the mass splittings $m_{\text{heavy}} \gg m_{\text{light}}$, $m_{\text{heavy}} = 2m_{\text{light}}$, and $m_{\text{heavy}} = m_{\text{light}}$, respectively. For completely degenerate masses, the topological susceptibility diverges at $\theta = \pi$ on account the first-order phase transition.

VI. CONCLUSION

In this paper, we investigated the properties of the QCD partition function in the Leutwyler–Smilga finite volume scaling regime. The full partition function including the contributions from all topological sectors for $N_f = 2$ has been previously calculated. We extended these results by performing the summation over all topological charges for arbitrary $N_f$. For $N_f \geq 3$, the partition function can be expressed as a $(N_f - 2)$–fold angular integration over a finite sum of modified Bessel functions. We considered both the cases of degenerate and nondegenerate quark masses. The partition function remains $2\pi$-periodic in $\theta$ after summing over all topological charges.

We systematically investigated the $\theta$ dependence of the QCD vacuum in the Leutwyler–Smilga regime. In this limit, the partition function only depends on $\theta$ and the scaling variables, $\mu_i = m_i \Sigma V$. In the limit of degenerate quark masses, the $N_f = 2$ partition function is independent of the scaling variable at $\theta = \pi$. As a consequence, the chiral condensate vanishes identically at $\theta = \pi$ for all values of $\mu$. For fixed $\mu$, the chiral condensate decreases monotonically as $\theta$ is increased from 0 to $\pi$.

In the macroscopic limit, i.e. for $\mu \to \infty$, the behavior of the two-flavor partition function is particularly striking. For degenerate quark masses, the first derivative of the energy density with respect to $\theta$ has a discontinuity at $\theta = \pi$ corresponding to the spontaneous breaking of the discrete CP symmetry. This phenomena was predicted by Dashen and was subsequently demonstrated by Di Vecchia and Veneziano and Witten using large-$N_c$ chiral perturbation theory. The chiral condensate also develops a cusp at $\theta = \pi$ for degenerate quark masses in the macroscopic limit.

For $N_f = 3$, we find that all the examined quantities are very insensitive to the mass splitting between two degenerate flavors and the third heavy flavor in the macroscopic limit. When compared to those of $N_f = 2$, the vacuum properties for three flavors are quite similar. While the partition function for $N_f = 2$ can be expressed in closed form, the partition function for $N_f = 3$ requires the straightforward numerical evaluation of a single integral. Unlike the $N_f = 2$ case, the $N_f = 3$ partition function is not independent of the scaling variables at $\theta = \pi$ and subsequently the chiral condensate is nonzero at $\theta = \pi$ even in the macroscopic limit. The chiral condensate does, however, exhibit the same monotonicity in $\theta$ as the $N_f = 2$ chiral condensate and in the macroscopic limit there is a cusp at $\theta = \pi$. Dashen’s phenomena, a first-order phase transition at $\theta = \pi$, is also realized in this limit.

Many of our results are corroborated by general $\theta = 0$ field theoretic identities, for example, the Ward–Takahashi identity. Our analysis naturally extends these results to nonzero values of $\theta$. 

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We have also demonstrated that QCD in the mesoscopic regime exhibits Dashen’s phenomena. We examined the physics of QCD at \( \theta \neq 0 \) in a nonperturbative framework. While the existence of Dashen’s phenomena has been known for thirty years and studied using chiral perturbation theory and numerical simulations, we have demonstrated the spontaneous breaking of the CP symmetry at \( \theta = \pi \) in a way that is both nonperturbative and analytic. We have also provided a further step towards the full evaluation of the path integral for chiral perturbation theory. We hope that this work helps elucidate a parameter space of QCD which has been largely unexplored.

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APPENDIX A: EXPLICIT CALCULATION OF THE DEGENERATE MASS PARTITION FUNCTION

Starting with the representation

\[
Z^{(N_f)}(\nu)(\mu) = \frac{2\pi}{2\pi} \prod_{j=1}^{N_f} \left( \frac{d\phi_j}{2\pi} \exp \left[ \mu \cos(\phi_j) - i\nu \phi_j - i\frac{j-3}{2} \phi_j \right] \right) \delta_{i_1...i_{N_f}} e^{i\phi_{i_1}}...e^{i\phi_{i_{N_f}}},
\]

(A1)

the summation \( Z^{(N_f)}(\theta, \mu) = \sum_{\nu} e^{i\nu \theta} Z^{(N_f)}(\nu)(\mu) \) can be performed by the use of

\[
\int_0^{2\pi} \frac{d\phi_1}{2\pi} f(\phi_1, ..., \phi_{N_f}, \theta) \sum_{\nu = -\infty}^{\infty} e^{i\nu(\theta - \phi_1 - ... - \phi_{N_f})} = f(\phi_2 + ... + \phi_{N_f} - \theta, \phi_2, ..., \phi_{N_f}, \theta),
\]

(A2)

After a change of integration variables

\[
e^{i\phi_2}(1 + e^{i(\phi_3 + ... + \phi_{N_f} - \theta)}) = \psi e^{i\varphi}
\]

(A3)

\[
e^{-i\phi_2}(1 + e^{-i(\phi_3 + ... + \phi_{N_f} - \theta)}) = \psi e^{-i\varphi}
\]

(A4)

with

\[
\psi = \sqrt{2 + 2 \cos (\phi_3 + ... + \phi_{N_f} - \theta)}
\]

(A5)

one arrives at

\[
Z^{(N_f)}(\theta, \mu) = e^{-i\theta/2} \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{i\mu \cos \varphi - i\varphi} \prod_{j=3}^{N_f} \left( \frac{d\phi_j}{2\pi} e^{i\mu \cos(\phi_j) - i(j-3)/2} \phi_j \right) \Gamma(\varphi, \phi_3, ..., \phi_{N_f}, \theta)
\]

(A6)
From that the final expression for the partition function with degenerate masses is

\[ Z = \exp \left( \frac{1}{2} \phi_{N_j} - i \phi_{N_j} \right) \cdots \exp \left( \frac{1}{2} \phi_{N_j} + i \phi_{N_j} \right) \]

Expanding the determinant around the first two rows leads to

\[ \Gamma(\varphi, \phi_3, \ldots, \phi_{N_j}, \theta) = \sum_{r=1}^{N_j-1} (-1)^r (e^{ir\varphi} - e^{-ir\varphi}) \alpha_r^{(N_j)}(\phi_3, \ldots, \phi_{N_j}, \theta), \tag{A8} \]

where the phases \( \alpha_r^{(N_j)} \) are given by

\[ \alpha_r^{(N_j)}(\phi_3, \ldots, \phi_{N_j}, \theta) = \sum_{j=1}^{N_j-r} e^{-i(j+r/2)(\phi_3 + \phi_{N_j} - \theta)} \beta_{r,j}^{(N_j)}(\phi_3, \ldots, \phi_{N_j}) \tag{A9} \]

with

\[ \beta_{r,k}^{(N_j)}(\phi_3, \ldots, \phi_{N_j}) = \begin{vmatrix} 1 & \ldots & e^{i(k-2)\phi_3} & e^{ik\phi_3} & \ldots & e^{i(l-2)\phi_3} & e^{i(2l-3)\phi_3} & \ldots & e^{i(N_j-1)\phi_3} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \ldots & e^{i(k-2)\phi_{N_j}} & e^{ik\phi_{N_j}} & \ldots & e^{i(l-2)\phi_{N_j}} & e^{i(2l-3)\phi_{N_j}} & \ldots & e^{i(N_j-1)\phi_{N_j}} \end{vmatrix}. \tag{A10} \]

The integration over the angle \( \varphi \) can be easily performed, since

\[ \int_0^{2\pi} d\varphi \mu \psi \cos(\varphi) (e^{ir\varphi} - e^{-ir\varphi}) = I_{r+1}(\mu \psi) - I_{r-1}(\mu \psi) = -2r \frac{I_r(\mu \psi)}{\mu \psi}. \tag{A11} \]

From that the final expression for the partition function with degenerate masses is

\[ Z^{(N_j)}(\theta, \mu) = -2e^{-\theta/2} \prod_{m=3}^{N_j} \left( \frac{d \phi_m}{2\pi} \mu \cos(\phi_m - i(m-3/2)\phi) \right)^{N_j-1} \sum_{r=1}^{N_j-1} (-1)^r \frac{I_r(\mu \psi)}{\mu \psi} \alpha_r^{(N_j)}(\phi_3, \ldots, \phi_{N_j}, \theta). \tag{A12} \]

Alternatively, from eq. (11), the equal mass partition function is

\[ Z^{(N_j)}(\theta, \mu) = \varepsilon_{a_1 \ldots a_{N_j}} \sum_{\nu=-\infty}^{\infty} e^{i\nu\theta} \prod_{m=1}^{N_j} I_{\nu+m-a_m}(\mu) \tag{A13a} \]

\[ = \varepsilon_{a_1 \ldots a_{N_j}} \sum_{\nu=-\infty}^{\infty} e^{i\nu\theta} \prod_{m=1}^{N_j} \int_0^{2\pi} \frac{d \phi_m}{2\pi} \exp [\mu \cos(\phi_m) + i(\nu + m - a_m)\phi_m]. \tag{A13b} \]
Using eq. (44), the summation over $\nu$ gives a delta function which facilitates the integration $\phi_a$:

\[ Z^{(N_f)}(\theta, \mu) = \frac{\varepsilon_{a_1...a_{N_f}}}{(2\pi)^{N_f-1}} \int_0^{2\pi} d\phi_2 \ldots d\phi_N \exp \left[ \mu \cos(\theta + \phi_2 + \ldots + \phi_{N_f}) \right] \]

\[ \times \exp \left[ \mu \cos(\phi_2) + \mu \cos(\phi_3) + \ldots \mu \cos(\phi_{N_f}) \right] \]

\[ \times \cos \left\{ (a_1 - 1)(\theta + \phi_2 + \ldots + \phi_{N_f}) + (2 - a_2)\phi_2 + \ldots + (N_f - a_{N_f})\phi_{N_f} \right\} . \]

The integration over $\phi_2$ can be done analytically [52] by expanding $\cos(\theta + \phi_2 + \ldots + \phi_{N_f}) = \cos(\phi_2)\cos(\theta + \phi_3 + \ldots + \phi_{N_f}) - \sin(\phi_2)\sin(\theta + \phi_3 + \ldots + \phi_{N_f})$.

The result is

\[ Z^{(N_f)}(\theta, \mu) = \varepsilon_{a_1...a_{N_f}} \prod_{m=3}^{N_f} \left\{ \int_0^{2\pi} d\phi_m e^{\mu \cos(\phi_m)} \right\} \]

\[ \times I_{a_1-a_2+1} \left( 2\mu \cos \left( \frac{\theta + \phi_3 + \ldots + \phi_{N_f}}{2} \right) \right) \]

\[ \times \cos \left\{ (3 - a_1 - a_2)(\theta + \phi_3 + \ldots + \phi_{N_f})/2 - (3 - a_3)\phi_3 - \ldots - (N_f - a_{N_f})\phi_{N_f} \right\} . \]

Using the addition rules for modified Bessel functions, one arrives at eq. (45).

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