Complex saddle points in QCD at finite temperature and density

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Abstract
The sign problem in QCD at finite temperature and density leads naturally to the consideration of complex saddle points of the action or effective action. The global symmetry $C\mathcal{K}$ of the finite-density action, where $C$ is charge conjugation and $\mathcal{K}$ is complex conjugation, constrains the eigenvalues of the Polyakov loop operator $P$ at a saddle point in such a way that the action is real at a saddle point, and net color charge is zero. The values of $Tr_F P$ and $Tr_F P^\dagger$ at the saddle point, are real but not identical, indicating the different free energy cost associated with inserting a heavy quark versus an antiquark into the system. At such complex saddle points, the mass matrix associated with Polyakov loops may have complex eigenvalues, reflecting oscillatory behavior in color-charge densities. We illustrate these properties with a simple model which includes the one-loop contribution of gluons and massless quarks moving in a constant Polyakov loop background. Confinement-deconfinement effects are modeled phenomenologically via an added potential term depending on the Polyakov loop eigenvalues. For sufficiently large $T$ and $\mu$, the results obtained reduce to those of perturbation theory at the complex saddle point. These results may be experimentally relevant for the CBM experiment at FAIR.
The sign problem is a fundamental issue in the study of QCD at finite density, manifesting as complex weights in the path integral that make lattice simulations extremely problematic [1–3]. However, the sign problem also appears in analytical calculations of mean-field type. Here we show that the sign problem can be solved in such calculations provided a fundamental symmetry of finite density models, CK symmetry, is respected. This leads to the analytic continuation of Polyakov loop eigenvalues into the complex plane from the unit circle.

Let us consider an $SU(N)$ gauge theory coupled to fermions in the fundamental representation. It is well known that the log of the fermion determinant, $\log \det (\mu, A)$, which is a function of the chemical potential $\mu$ and the gauge field $A$, can be formally expanded as a sum over Wilson loops with real coefficients. For a gauge theory at finite temperature, the sum includes Wilson loops that wind non-trivially around the Euclidean timelike direction; Polyakov loops, also known as Wilson lines, are examples of such loops. At $\mu = 0$, every Wilson loop $Tr_{F}W$ appearing in the expression for the fermion determinant is combined with its conjugate $Tr_{F}W^{\dagger}$ to give a real contribution to path integral weighting. This can be understood as a consequence of charge conjugation invariance $C$, which acts on the gauge field as

$$C : A_{\mu} \rightarrow -A_{\mu}^{t} \quad (1)$$

and thus exchanges $Tr_{F}W$ and $Tr_{F}W^{\dagger}$. When $\mu \neq 0$, Wilson loops with non-trivial winding number $n$ in the $x_{4}$ direction receive a weight $e^{n\beta\mu}$ while the conjugate loop is weighted by $e^{-n\beta\mu}$. Thus it is seen that these loops break charge conjugation invariance when $\mu \neq 0$. However, $Tr_{F}W$ transforms into itself under the combined action of $CK$, where $K$ is the fundamental antilinear operation of complex conjugation. Thus the theory is invariant under $CK$ even in the case $\mu \neq 0$. For fermions, $CK$ symmetry implies the well-known relation $\det (-\mu, A_{\mu}) = \det (\mu, A_{\mu})^{*}$ for Hermitian $A_{\mu}$, but can be used with bosons as well as fermions.

Given the existence of the symmetry $CK$ at finite density, we wish to ensure that, in the absence of spontaneous symmetry breaking, calculational methods of all types respect the symmetry. For perturbative or mean-field type calculations, this leads naturally to the consideration of complex but $CK$-symmetric saddle points for some effective potential at finite temperature and density $V_{\text{eff}}$, such that the free energy density is given by the value
of $V_{eff}$ at the dominant saddle point. Such saddle points have been seen before in finite density calculations [4–7]. A field configuration is $\mathcal{C}\mathcal{K}$-symmetric if $-A_\mu^\dagger$ is equivalent to $A_\mu$ under a gauge transformation. For such a field configuration, it is easy to see that every Wilson loop is real and thus $\det (\mu, A_\mu)$ is real and positive.

Let us consider the Polyakov loop $P$ associated with some particular field configuration that is $\mathcal{C}\mathcal{K}$-symmetric. We can transform to Polyakov gauge where $A_4$ is diagonal and time-independent, and work with the eigenvalues $\theta_j$ defined by

$$P_{jk}(\vec{x}) = \delta_{jk}e^{i\theta_j(\vec{x})}$$

where the $\theta_j$’s are complex but satisfy $\sum_j \theta_j = 0$. Because we are primarily interested in constant saddle points, we suppress the spatial dependence hereafter. Invariance under $\mathcal{C}\mathcal{K}$ means that the set $\{-\theta_j^*\}$ is equivalent to the $\{\theta_j\}$ although the eigenvalues themselves may permute. In the case of $SU(3)$, we may write this set uniquely as

$$\{\theta - i\psi, -\theta - i\psi, 2i\psi\}.$$ (3)

This parametrizes the set of $\mathcal{C}\mathcal{K}$-symmetric $SU(3)$ Polyakov loops. Notice that both

$$Tr_F P = e^{\psi}2\cos \theta + e^{-2\psi}$$ (4)

and

$$Tr_F P^\dagger = e^{-\psi}2\cos \theta + e^{2\psi}$$ (5)

are real, but they are equal only if $\psi = 0$. In the usual interpretation of the Polyakov loop expectation value, this implies that the free energy change associated with the insertion of a fermion is different from the free energy change associated with its antiparticle. It is easy to check that the trace of all powers of $P$ or $P^\dagger$ are all real, and thus all group characters are real as well. This parametrization represents a generalization of the Polyakov loop parametrization used in the application of mean-field methods to confinement, e.g., in PNJL models [8] or in gauge theories with double-trace deformations [9, 10]. This parametrization can be generalized to include finite density models for arbitrary $N$.

The existence of complex $\mathcal{C}\mathcal{K}$-symmetric saddle points provides a fundamental approach to non-Abelian gauge theories that is similar to the heuristic introduction of color chemical potentials, and naturally ensures the system has zero color charge, i.e., all three charges contribute equally [11]. In the case of $SU(3)$, extremization of the thermodynamic potential
with respect to $\theta$ leads to the requirement $\langle n_r \rangle - \langle n_g \rangle = 0$ where $\langle n_r \rangle$ is red color density, including the contribution of gluons. Similarly, extremization of the thermodynamic potential with respect to $\psi$ leads $\langle n_r \rangle + \langle n_g \rangle - 2\langle n_b \rangle = 0$. Taken together, these two relations imply that $\langle n_r \rangle = \langle n_g \rangle = \langle n_b \rangle$.

We demand that any saddle point solution be stable to constant, real changes in the Polyakov loop eigenvalues, corresponding for $SU(3)$ to constant real changes in $A_3^3$ and $A_8^4$. Consider the $(N-1) \times (N-1)$ matrix $M_{ab}$, defined in Polyakov gauge as

$$M_{ab} \equiv g^2 \frac{\partial^2 V_{\text{eff}}}{\partial A_{a}^4 \partial A_{b}^4}.$$  

(6)

The stability criterion is then that the eigenvalues of $M$ must have positive real parts. At $\mathcal{CK}$-symmetric saddle points, the eigenvalues will be either real or part of a complex conjugate pair. In the case of $SU(3)$, the matrix $M$ may also be written in terms of derivatives with respect to $\theta$ and $\psi$ as

$$M = \frac{g^2}{T^2} \left( \begin{array}{cc} \frac{1}{4} \frac{\partial^2 V_{\text{eff}}}{\partial \theta^2} & i \frac{\partial^2 V_{\text{eff}}}{\partial \theta \partial \psi} \\ i \frac{\partial^2 V_{\text{eff}}}{\partial \theta \partial \psi} & \frac{1}{4\sqrt{3}} \frac{\partial^2 V_{\text{eff}}}{\partial \psi^2} \end{array} \right).$$  

(7)

This stability criterion generalizes the stability criterion used previously for color chemical potentials, which was $\partial^2 V_{\text{eff}}/\partial \psi^2 < 0$. Crucially, the mass matrix $M$ is invariant under $M^* = \sigma_3 M \sigma_3$, which is a generalized $\mathcal{PT}$ (parity-time) symmetry transformation [12, 13]. It is easy to see that this relation implies that $M$ has either two real eigenvalues or a complex eigenvalue pair.

We first illustrate the working of $\mathcal{CK}$ symmetry using the well-known one-loop expressions for the effective potential of particles moving in a constant background Polyakov loop. The one-loop contribution to the effective potential of $N_f$ flavors of fundamental fermions moving in a background gauge field $A$ is given by

$$\beta V_{\text{eff}}^f = -N_f \log [\det (\mu, A)]$$  

where $\det$ again represents the functional determinant of the Dirac operator and $\beta V$ is the volume of spacetime. A compact expression for the effective potential of massless fermions when the eigenvalues of $P$ are complex was derived using zeta function methods in [14]. It will be useful in what follows to repeat their derivation and check the reality of $V_{\text{eff}}^f$ for $\mathcal{CK}$-symmetric backgrounds. Out starting point is the finite-temperature contribution to the effective potential of a single Dirac fermion in a $U(1)$ background Polyakov loop characterized by an angle $\theta$:
\[ v_f(\theta) = -2T \int \frac{d^3k}{(2\pi)^3} \left\{ \log\left[1 + e^{-\beta \omega_k + i\theta}\right] + \log\left[1 + e^{-\beta \omega_k - i\theta}\right] \right\}. \] (8)

Setting the fermion mass to zero, and expanding the logarithms, we obtain

\[ v_f(\theta) = -\frac{4T^4}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^4} \cos(n\theta). \] (9)

After expanding the cosine and interchanging the order of summation, we get

\[ v_f(\theta) = -\frac{4T^4}{\pi^2} \sum_{m=0}^{\infty} \frac{(-1)^m \theta^{2m} \eta(4 - 2m)}{(2m)!}. \] (10)

where \( \eta \) is the Dirichlet eta function. Only the first three terms of the expansion are non-zero, and we arrive at

\[ v_f(\theta) = -\frac{4T^4}{\pi^2} \left( \frac{\theta^4}{48} - \frac{\pi^2 \theta^2}{24} + \frac{7\pi^4}{720} \right). \] (11)

This expression is valid provided \( \text{Re}[\theta] \in (-\pi, \pi) \). In general, if \( \theta \) is complex, so is \( v_f \). However, the free energy of quarks in a \( CK \)-symmetric background Polyakov loop is always real. For \( SU(3) \), we have

\[ V_f(\theta, \psi, T, \mu) = N_f \left( v_f\left(\theta - i\psi - \frac{i\mu}{T}\right) + v_f\left(-\theta - i\psi - \frac{i\mu}{T}\right) + v_f\left(2i\psi - \frac{i\mu}{T}\right) \right) \] (12)

which is explicitly real:

\[ V_f(\theta, \psi, T, \mu)/N_f = -\frac{\mu^4}{2\pi^2} + T^2 \left( -\mu^2 + \frac{2\theta^2 \mu^2}{\pi^2} - \frac{6\mu^2 \psi^2}{\pi^2} \right) + \frac{4T^3 \left( \theta^2 \mu \psi + \mu \psi^3 \right)}{\pi^2} \]
\[ + \frac{T^4 \left( -7\pi^4 + 20\pi^2 \theta^2 - 10\theta^4 - 60\pi^2 \psi^2 + 60\theta^2 \psi^2 - 90\psi^4 \right)}{30\pi^2}. \] (13)

Because we are interested in the analytic continuation of Polyakov loop eigenvalues into the complex plane, we need expressions for the gauge bosons as well as for fermions. Our starting point is

\[ v_b(\theta) = 2T \int \frac{d^3k}{(2\pi)^3} \left\{ \log\left[1 - e^{-\beta \omega_k + i\theta}\right] + \log\left[1 - e^{-\beta \omega_k - i\theta}\right] \right\}. \] (15)

which represent the one-loop of two gauge bosons of opposite \( U(1) \) charge. A naive repetition of the zeta-function argument that was successful for fermions fails for boson even in the case where \( \theta \) is real. However, it is possible to define the bosonic analog of \( v_f(\theta) \) by [15]

\[ v_b(\theta) = -v_f(\theta - \pi) \] (16)
and this leads to the correct expression when $Re \{ \theta \} \in (0, 2\pi)$:

$$v_b (\theta) = - \frac{(-15\theta^4 + 60\pi\theta^3 - 60\pi^2\theta^2 + 8\pi^4) T^4}{180\pi^2}.$$

(17)

As in the fermionic case, $v_b (\theta)$ is generally complex if $\theta$ is complex. However, the one-loop gluonic contribution for a $\mathcal{C}\mathcal{K}$-symmetric Polyakov loop background, given by

$$V_g (P) = v_b (0) + v_b (2\theta) + v_b (\theta + i3\psi) + v_b (\theta - i3\psi)$$

(18)

is real. Explicitly, we have for $SU(3)$

$$V_g (P) = \frac{T^4 (135 (\theta^2 - 3\psi^2)^2 + 180\pi^2 (\theta^2 - 3\psi^2) + 60\pi\theta (27\psi^2 - 5\theta^2) - 16\pi^4)}{90\pi^2}$$

(19)

which is real. Note that the valid range of $\theta$ is $(0, \pi)$ due to the appearance of $2\theta$ as an eigenvalue in the adjoint representation. The one-loop effective potential is simply the sum of $V_g (\theta)$ and $V_f (\theta)$. As is the case when $\mu = 0$, the dominant saddle point remains at $\theta = 0$ when $\mu \neq 0$.

We now consider a simple phenomenological model that combines the one-loop result with the effects of confinement for the case of $SU(3)$ gauge bosons and massless fermions at finite temperature and density. The model is described by an effective potential which is the sum of three terms:

$$V_{eff} (P) = V_g (P) + V_f (P) + V_d (P)$$

(20)

where $V_g (P) + V_f (P)$ is the one-loop effective potential for gluons and quarks given above and $V_d (P)$ is an additional term that favors the confined phase [9, 16–18]. There are two different points of view that can be taken on this model. In one view, $V_d (P)$ represents a deformation of the original model. In typical applications, the temperature $T$ is taken to be large such that perturbation theory is reliable in the chromoelectric sector because the running coupling $g^2 (T)$ is small. The deformation term is taken to respect center symmetry and is used to move between the confined and deconfined phases in a controlled way. The gauge contribution $V_g (P)$ favors the deconfined phase, and in the pure gauge theory ($N_f = 0$) the deconfinement transition arises out of the competition between $V_g (P)$ and $V_d (P)$ . The confined phase arising from models of this type are known to be analytically connected to the usual low-temperature confined phase of $SU(3)$ gauge theory [9]. This point of view emphasizes analytic control at the price of deforming the original gauge theory by the
addition of \( V_d(P) \). From the second point of view, the entire model is phenomenological in nature, with the potential \( V_d(P) \) models the unknown confining dynamics of the pure gauge theory. The parameters of \( V_d(P) \) are set to reproduce the deconfinement temperature of the pure gauge theory, known from lattice simulations to occur at \( T_d \approx 270 \text{ MeV} \).

We will take the second point of view, using a simple expression for \( V_d(P) \) that reproduces much of the thermodynamic behavior seen in lattice simulations of the pure gauge theory. The specific form used is Model A of [16], where the two terms \( V_g(P) + V_d(P) \) can be written together as

\[
V_A(\theta) = -\sum_{j,k=1}^{N} \frac{1}{\pi^2} \left( 1 - \frac{1}{N} \delta_{jk} \right) \left[ -\frac{2\pi^4}{3\beta^4} B_4 \left( \frac{\Delta \theta_{jk}}{2\pi} \right) - \frac{m^2 \pi^2}{2\beta^2} B_2 \left( \frac{\Delta \theta_{jk}}{2\pi} \right) \right]
\]  

(21)

where \( \Delta \theta_{jk} = |\theta_j - \theta_k| \) are the adjoint Polyakov loop eigenvalues and \( B_j \) is the \( j \)'th Bernoulli polynomial. This expression gives a simple quartic polynomial in the Polyakov loop eigenvalues and thus can be thought of as a form of Landau-Ginsburg potential for the Polyakov loop eigenvalues. For the \( SU(3) \) parametrization used here, \( V_d(P) \) takes the simple form

\[
V_d(P) = \frac{m^2 T^2 ((2\pi - 3\theta)^2 - 27\psi^2)}{6\pi^2}.
\]  

(22)

The parameter \( m \) controls the location of the deconfinement transition in the pure gauge theory, and is set to 596 MeV. At low temperatures, this term dominates the pure gauge theory effective potential. The variable \( \psi \) is zero, and \( V_d(P) \) is minimized when \( \theta = 2\pi/3 \). For this value of \( \theta \), the eigenvalues of \( P \) are uniformly spaced around the unit circle, respecting center symmetry, and \( TrP = TrP^\dagger = 0 \). As the temperature increases, \( V_g(P) \) becomes relevant, and gives rise to the deconfined phase where center symmetry is spontaneously broken. The addition of light fundamental quarks via \( V_f(P) \) explicitly breaks center symmetry. For all non-zero temperatures, center symmetry is broken and \( \langle TrF \rangle \neq 0 \). However, a remnant of the deconfinement transition remains in the form of a rapid crossover from smaller value of \( TrP \) to larger ones as \( T \) and \( \mu \) are varied. Note that this simple model neglects both chiral symmetry breaking and the formation of a color superconductor, both of which are important at low temperatures.

For a given \( T \) and \( \mu \), the free energy and other thermodynamic quantities are obtained from the saddle point of \( V_{eff}(P) \). Figure [1] shows \( TrP \) and \( TrP^\dagger \) as functions of \( T \) at constant \( \mu \) for values up to \( \mu = 450 \text{ MeV} \). There is a rapid crossover in \( TrP \) and \( TrP^\dagger \) for smaller values of \( \mu \) that becomes less dramatic as \( \mu \) increases. There is a small difference
Figure 1: $\frac{1}{3}TrP$ (solid line) and $\frac{1}{3}TrP^\dagger$ (dotted line) as functions of $T$ at constant $\mu$ for values up to $\mu = 450\, MeV$.

between $TrP$ and $TrP^\dagger$ in the crossover region when $\mu \neq 0$, with $TrP^\dagger > TrP$, indicating that it is easier to insert a heavy antiquark into the system than a heavy quark. Figure 2 shows $TrP$ and $TrP^\dagger$ as functions of $\mu$ at constant $T$ for values up to $T = 250\, MeV$. Similar behavior is obtained as that shown in figure 1 but the crossover is less abrupt and almost gone at $T = 250\, MeV$. These results are consistent with more complicated models that include the effects of chiral symmetry and color superconductivity.

As discussed above, the mass matrix associated with the fields $A_3^3$ and $A_8^\psi$ has the property that the eigenvalues are either both real or form a complex conjugate pair. The most physically interesting region for this model occurs when $T$ is larger than the $\mu = 0$ crossover temperature. In this region, we can safely assume that chiral symmetry is approximately restored, and the use of zero-mass quarks is a reasonable approximation. Working in this region also excludes color superconducting phases. Useful analytic results can be obtained in the region $T, \mu \gg m$, where the saddle point is given approximately by

$$\theta \approx \frac{3m^2\pi}{8\pi^2T^2 + 6\mu^2},$$

$$\psi \approx \frac{9m^4\pi^2T\mu}{4(4\pi^2T^2 + 3\mu^2)^3}. \quad (23)$$

$$ (24)$$
The corresponding mass matrix eigenvalues are given by to order $m^2$ by

$$g^2 \left( \frac{4T^2}{3} + \frac{\mu^2}{\pi^2} \right) + \frac{g^2 m^2 \left( 9\mu^2 - 12\pi^2 T^2 \pm 2\pi T \sqrt{9\pi^2 T^2 - 12\mu^2} \right)}{4\pi^2 (3\mu^2 + 4\pi^2 T^2)}, \quad (25)$$

a formula that combines the one-loop formula for the screening masses $g^2 \left( \frac{4T^2}{3} + \frac{\mu^2}{\pi^2} \right)$ with corrections due to the confining term $V_d$ in $V_{\text{eff}}$ that are proportional to $m^2$. If $T > 2\mu/\sqrt{3}\pi$, there are two real, non-degenerate eigenvalues. However, if $T < 2\mu/\sqrt{3}\pi$, the two eigenvalues form a conjugate pair. The occurrence of such pairs is unusual in a Euclidean field theory, and is associated with the sign problem at finite density \[13\]. In a $d$-dimensional theory, a boson of mass $m_B$ contributes a term

$$\frac{1}{2} \int \frac{d^d k}{(2\pi)^d} \log \left[ k^2 + m_B^2 \right], \quad (26)$$

to the effective potential. A negative value for $m_B^2$ leads to an imaginary part for the effective potential, indicating instability, as would a complex value. However, in the case where there are complex conjugate pairs of mass eigenvalues where $m_B^2 = a \pm ib$, the contribution of the two terms is now

$$\frac{1}{2} \int \frac{d^d k}{(2\pi)^d} \log \left[ (k^2 + a + ib)(k^2 + a - ib) \right] = \frac{1}{2} \int \frac{d^d k}{(2\pi)^d} \log \left[ (k^2 + a)^2 + b^2 \right] \quad (27)$$
which is always positive. If $a > 0$ (the case here), there is no instability whatsoever, but correlation functions will exhibit modulated decay. If $a < 0$ (not the case here), the system becomes unstable to spatial modulation of the ground state at $k^2 = -a$. This is a form of the Lifshitz mechanism for a spatially modulated state, when the Landau-Ginzburg theory for the lightest field has the form $(\partial^2 \phi)^2 + 2a(\partial \phi)^2 + (a^2 + b^2)\phi^2$.

The occurrence of complex eigenvalues indicates periodic modulation in the spatial decay of color-color density correlation functions reminiscent of similar oscillations in density-density correlation functions in liquids. Figure 3 shows the region where the exact mass matrix is complex, along with high-$T$ and low-$T$ approximations to the boundary of the region. This result may depend strongly on the choice of $V_d$, an issue we plan to address in later work. Patel has suggested that a signal for such oscillatory behavior might appear in baryon number correlators in heavy ion collisions at RHIC and the LHC [19, 20]. Based on the results reported here, it would be more natural to observe this behavior in the CBM experiment at FAIR, but much work is needed to determine a useful experimental signature.
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