Analyticity and the phase diagram of QCD

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Abstract

Some consequences of the analyticity of the free energy (pressure) of QCD at finite chemical potential are deduced. These include a method for numerical exploration of the full phase diagram by a novel use of simulations at imaginary chemical potential to extract Yang-Lee zeroes of the grand-canonical partition function. We make use of, and comment on, CPT symmetries, positivity of non-linear susceptibilities and the finiteness of screening lengths. We also comment on the structure of zeroes expected for the usual picture of the phases of QCD, following a discussion of the physics of imaginary chemical potential.

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Motivated by the complex phase structure of QCD at finite chemical potential, \( \mu \), predicted by effective theories and perturbative analyses \[1\], there has been a spate of work extending lattice computations to finite \( \mu \) \[2, 3, 4, 5, 6\]. Most of these methods extrapolate data obtained at \( \mu = 0 \) out to finite \( \mu \) using, implicitly or explicitly, a Taylor expansion in \( \mu \) of the free energy. As a result, these expansions cannot be continued beyond the nearest phase transition to \( \mu = 0 \). Much of the interesting phase structure of QCD then lies beyond their scope. This paper explores consequences of the analyticity of the free energy (guaranteed by time reversal invariance) as a function of complex \( \mu \) to suggest a numerical technique for exploring the QCD phase diagram. It turns out that analyticity also has many other consequences, some of which are touched upon.

The plan of this paper is the following. First it is shown how analyticity is guaranteed by time reversal symmetry. This material is known to practitioners, but serves to introduce notation and several concepts I use later. Next I write down the canonical product representation for the partition function and make contact with the Yang-Lee theory of phase transitions. A numerical technique is developed to explore the phase diagram using simulations at imaginary chemical potential, which goes beyond using Taylor series for analytic continuation. The need for a different approach is discussed next, with remarks on the phase diagram.

The partition function of QCD, i.e., \( SU(N_c) \) gauge theory, with \( N_f \) flavours of fermions, each subjected to a common chemical potential, \( \mu \), is

\[
Z(T, \mu) = \int DU e^{-S_g(T)} \prod_{f=1}^{N_f} \text{Det} M(m_f, \mu, T),
\]

where \( M \) is the Dirac operator, \( S_g \) the gauge part of the action and the temperature \( T \) enters the action through boundary conditions on the fields. The free energy, \( F \) and the pressure are defined by

\[
P(T, \mu) = -\frac{1}{V} F(T, \mu) = \left( \frac{T}{V} \right) \log Z(T, \mu).
\]

At any purely real or imaginary value of the chemical potential, the free energy (or the pressure) is purely real \[7\]. Is it possible then for the free energy to be an analytic function of a general complex \( \mu \)? Recall that this requires the real and imaginary parts of \( F \), \( F_r \) and \( F_i \) respectively, to satisfy the Cauchy-Riemann equations, implying that they are conjugate harmonic functions. This rules out \( F_i = 0 \) unless \( F \) is constant.
The answer is that it is entirely possible to have a harmonic function (i.e., a function satisfying Laplace’s equation) which is zero along the real and imaginary axes and is non-trivial elsewhere. Since all even powers of the complex number \( \mu \) satisfy these requirements, it seems that analyticity of \( F(\mu) \) (at fixed \( T \)) requires that it be even in \( \mu \).

Now recall that the transformation \( \mu \to -\mu \) can be compensated by time-reversal, i.e., by interchanging particles and anti-particles. However, this definition is arbitrary; in the absence of CP violating terms in the action, thermodynamics remains unchanged by such a relabelling. The physics is therefore unchanged by changing the sign of \( \mu \). In other words, CP symmetry (same as time reversal, by the CPT theorem) implies that \( F(\mu) \) is an even function of \( \mu \), i.e., only even powers of \( \mu \) appear in the Taylor expansion. Since the whole chain of logic above can be inverted, this means that CP symmetry is necessary and sufficient for the analyticity of \( F \), and its reality along the coordinate axes of \( \mu \) in the complex plane.

The simplest use of analyticity is to expand the pressure in a Taylor series \(^5, 6\) and to determine the coefficients by direct lattice simulations at \( \mu = 0 \) \(^6, 8\) or by fitting to results obtained at imaginary \( \mu \) \(^4\). However, this approach is limited, since it only gives information on the phase connected to \( \mu = 0 \). The first phase transition encountered stops the extrapolation, and more machinery is required to get around this barrier. This is what we develop in this paper.

At real \( \mu \), the path integral measure in eq. \(^\Pi\) is complex \(^9\) and importance sampling in a Monte Carlo procedure fails although the integral is real. From the argument above, it seems that by grouping together configurations related by CP, it should be possible to construct a real weight by summing over each such “CP orbit”. Since CP symmetry forms a \( Z_2 \) group, each orbit consists of exactly two configurations, and the sum of the weights in these two configurations (for real \( \mu \)) must be real. The simplest example is the Gibbs model \(^10\).

This model contains Fermions on a 1-dimensional lattice (\( N_t \) sites in the temporal direction) and \( U(1) \) gauge fields on the links. Since there are no plaquettes, the gauge action is trivial and the path integral can be performed easily. The model is a zero (spatial) dimensional field theory, and, therefore is the quantum mechanics of a single fermion subjected to a constant \( U(1) \) field. It is possible to choose a gauge where all links have equal value \( U = \exp(i\theta) \). With fermion mass \( m \), chemical potential \( \mu \) and defining \( q^{N_t} = z = \exp(\mu/T) \),
the Fermion matrix is—

\[
M = \begin{pmatrix}
  m & qU & \cdots & -U^\dagger/q \\
-\frac{U^\dagger}{q} & m & qU & \cdots \\
  & \vdots & \vdots & \vdots \\
qU & \cdots & -\frac{U^\dagger}{q} & m
\end{pmatrix}.
\] (3)

The determinant is—

\[
\text{Det } M = w^N + 1/w^N - 2 \cosh \frac{1}{2} N m'
\] (4)

where \( w = qU \) and \( ma/2 = \sinh m' a/2 \). The lattice spacing is \( a = 1/T N_t \). The partition function is

\[
Z(N, z) = \int_{-\pi}^{\pi} d\theta \det M,
\] (5)

which is real, although the weight is complex. In this simple model a CP transformation induces the mapping \( U \rightarrow U^\dagger \). Then, summing over each CP orbit one gets

\[
\sum_{CP} \det M = 4 \cosh(\mu/T) \cos(N_t\theta) - 4 \cosh(m'/2T),
\] (6)

which is real. In the partition function one should compensate the double counting by dividing by a factor of two. This is immaterial for expectation values.

In a more realistic model, the gauge configurations connected by a CP transformation are harder to construct. It turns out to be easier to implement the symmetry transformation \( C \) (which is the same as PT) which is local and maps each link matrix \( U \rightarrow U^\dagger \). The T part of the transformation can be used as before to prove that the free energy is even in \( \mu \). Moreover, this symmetry transformation preserves the values of \( S_g \) and \( \text{Det } M \) (see eq. 11) separately. As a result, for the Taylor expansion of \( \text{Det } M \) summed over each PT orbit—

\[
\text{Det } M(m, T, \mu) = \text{Det } M(m, T, 0) \left[ 1 + a_1 \mu + \frac{a_2}{2} \mu^2 + \frac{a_3}{3!} \mu^3 + \cdots \right],
\] (7)

one has \( \Re a_i = \Im a_i = 0 \) for all odd \( i \). In other words, summed over PT orbits, the measure is even in \( \mu \).

Since this summation over a symmetry orbit leads to a weight that is the sum of two determinants, it is clear that the measure cannot be rewritten using local pseudo-fermion fields. Disappointingly, these symmetries turn out to be unexploitable in this form for molecular dynamics algorithms paralleling those which are used at zero chemical potential.
However, by ensuring analyticity, they lead to other numerical approaches to the problem, as I show next.

From the Hamiltonian expression for the partition function,

$$Z(T, \mu) = \text{Tr} \exp \left[ -\frac{\hat{H}}{T} - \frac{\mu \hat{N}}{T} \right],$$

(8)

(where $\hat{H}$ is the Hamiltonian and $\hat{N}$ the number operator) it is clear that $Z$ has a periodicity of $2\pi T$ in the imaginary part of the chemical potential—

$$Z(T, \mu) = Z(T, \mu + 2\pi ikT) \text{ for any integer } k.$$  (9)

Functions with such periodicity are best analysed in terms of the fugacity, $z = \exp(\mu/T)$. Entire functions in $\mu$ are regular in the complex $z$ plane without the origin, i.e., the punctured $z$ plane [12]. Then the partition function can be written in the canonical product form [13]

$$Z(T, z) = e^{-\overline{F}(T,z)/T} \prod \left( 1 - \frac{z}{z_n(T)} \right),$$

(10)

where $z_n(T)$ are the zeroes of $Z$, and $\overline{F}$ is the regular part of the free energy. CP symmetry constrains the set of zeroes, $\{z_n\}$ to be symmetric under inversions in the unit circle. Branch points in the full free energy, $F = -T \log Z$, then do not appear in the regular part $\overline{F}$. The periodicity of $Z$ in $\mu$ also implies that

$$\overline{F}(T, \mu) = \overline{F}(T, \mu + 2\pi ikT) \text{ for any integer } k.$$  (11)

The appropriate setting for further analysis is the Yang-Lee theory of phase transitions [14].

According to this theory, phase transitions occur at points in the parameter space where dense sets of zeroes develop into pinch points. In the present understanding of the phase diagram of QCD, one expects pinch points on the real $\mu$ axis at small $T$ where interesting new phases of QCD appear [1]. We shall come back to this after a digression on ideal gases which throws more light on the question of periodicity in the imaginary part of $\mu$.

An ideal gas has the free energy—

$$F(T, \mu) = N_c N_f V \left[ \frac{7\pi^2}{180} T^4 + \frac{1}{6} \mu^2 T^2 + \frac{1}{12\pi^2} \mu^4 \right],$$

(12)

which does not have the required periodicity; no polynomial in $\mu$ can. By examining the Hamiltonian formulation of an ideal gas, we can show where the periodicity is hidden. The free energy can be written as

$$F(\mu, T) = \frac{N_c N_f V T^4}{3\pi^2} \int_0^\infty dx x^3 \left[ \frac{1}{ze^x + 1} + \frac{1}{e^x/z + 1} \right].$$

(13)
Since \( z \) is unchanged under \( \mu \to \mu + 2\pi iT \), this has explicitly the required periodicity. By the substitution \( y = \exp x \), the integral can be written in terms of fourth order Euler Polylogarithm functions [15]—

\[
F(\mu, T) = -\frac{2N_cN_fVT^4}{\pi^2} \left[ \text{Li}_4 \left( -\frac{1}{z} \right) + \text{Li}_4 (-z) \right],
\]

(14)

which also explicitly retains the periodicity. In fact, each of the terms has this periodicity explicitly. This property is lost in a Taylor expansion of the polylogs in \( \mu/T \)—

\[
\text{Li}_4 (-e^x) = -\frac{7\pi^4}{720} - \frac{3\zeta_3}{4}x - \frac{\pi^2}{24}x^2 - \frac{\log 2}{6}x^3 - \frac{x^4}{48} - \frac{x^5}{480} + \frac{x^7}{40320} - \frac{x^9}{1451520} + \cdots
\]

(15)

where the remaining terms are odd in the expansion parameter. The reason is that in taking the logarithm of the argument one makes a choice of the Riemann sheet, which is precisely equivalent to working within a single strip of width \( 2\pi iT \). When the sum in eq. (14) is expanded in a Taylor series in \( \mu \), it is clear that every term cancels, apart from those which appear in eq. (12). Periodicity can be restored by averaging this expression over all Riemann sheets of the logarithm, the result of which is expressed concisely in eq. (14) [16]. In general, interactions modify the integral expression in eq. (13), without spoiling the periodicity. This upsets the conspiracy which cancels all higher terms in \( F \), leading to non-vanishing values for general Taylor coefficients, i.e., the non-linear number susceptibilities [6].

We return now to considerations of phase transitions in QCD through the Yang-Lee mechanism. The set of zeroes, \( z_n(T) \), of the partition function contains the full information needed to identify all the phase transitions in the theory through the Yang-Lee mechanism [14]. But for all this to make sense, one needs to check that a thermodynamic limit exists, and that, in this limit, the pressure is a continuous and monotonically increasing function of \( z \). This is Theorem I of [14], and is proven there in the non-relativistic limit when interparticle potentials obey two conditions—first that there should be a limit to the number of particles that can be accommodated in a finite box, and second that the interactions between them be of finite range. Non-intuitive phenomena can occur when these conditions are violated [17]. All work on QCD assumes the validity this theorem. However, it is useful to first examine the basis for this assumption.

In the low temperature phase, where the carriers of baryon number are the baryons themselves, the problem is essentially non-relativistic, since the baryon mass is much greater than the temperature. There is ample experimental evidence that the inter-nucleon potential satisfies both conditions necessary for the theorem to hold—the baryon-baryon interaction has
a hard core repulsion and a short ranged Yukawa interaction at long distances. In the high-
temperature phase the problem is relativistic, since one expects that the carriers of baryon
number are the quarks, whose masses are much less than the temperature. Quarks and
antiquarks are freely created and destroyed, and, as is well-known, the correct reformulation
of the problem is to work in ensembles where the excess (or deficit) of quarks over antiquarks
is fixed (the canonical ensemble) or is conjugate to the chemical potential (the grand canoni-
cal ensemble). The second requirement, of finite range of interactions, is straightforward.
The gauge interaction, which could be long-ranged, is known to be screened in the electric
sector \[18\]. In the magnetic sector there is no evidence for screening, but there is evidence
of confinement and hence a mass-gap \[19\]. All other screening lengths are smaller in the
continuum limit \[8\]. While these phenomena are best established for \(N_c = 2\) and 3, they are
expected to hold also for other \(N_c\).

If we accept these arguments, or otherwise directly assume the first theorem of \[14\]— that
the pressure is a continuous increasing function for \(z \geq 1\), then an immediate consequence
is that the Taylor expansion coefficients of \(P(T, z)\) in \(z\) at fixed \(T\) are non-negative. Now,
the generalised susceptibilities \[6\], are Taylor coefficients of \(P(T, \mu)\) in an expansion in \(\mu\).
Since the expansion in \(\mu\) can be obtained from that in \(z = \exp(\mu/T)\) by expanding out
the exponential, which is itself a convex function, it follows that the sum of all generalised
susceptibilities of a given order are strictly positive.

This theorem of Yang and Lee is expected to hold for a continuum theory in the ther-
modynamic limit of infinite volume. It is also expected to hold for a continuum theory in
a finite volume much bigger than the range of interactions, even when the limit is taken
with a sequence of cutoffs, holding the physical volume fixed. On the other hand, at any
intermediate step in this procedure, the convexity argument may fail if some of the screening
masses are far from their continuum limits and not sufficiently small. Negative values of
some of the susceptibilities may then be observed at finite volume. However, convexity is
regained either by increasing the spatial volume or on taking the continuum limit \[20\].

Further practical use of this theory necessitates estimation of the set of zeroes, \(\{z_n(T)\}\).
Further information hinges on the connection between the grand-canonical and the canonical
partition functions. The partition function in eq. (11) generates expectation values in a grand
canonical ensemble with respect to quark number. A partition function for fixed quark
number, \(Q\), i.e., in a canonical ensemble has also been used before \[7, 21, 22, 23\]. One
defines this canonical partition function by the Fourier transform

$$Q(T, Q) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi Z(T, i\phi) \cos Q\phi,$$

where $Z(T, i\phi)$ denotes the grand canonical partition function in an imaginary chemical potential $\mu = i\phi$. One can invert this formula to write

$$Z(T, z) = \prod_{Q=1}^{V N_s N_f N_c} Q(T, Q) \left[ z^Q + \frac{1}{z^Q} \right],$$

where $N_s$ is the number of components of the Dirac spinor ($N_s = 4$ in four dimensions). Note that on any lattice with $V$ sites on each spatial slice, $Z$ is a polynomial in $z$ of degree $V N_s N_f N_c$. The $Z_{N_c}$ symmetry of the gauge action can be used to show that $Q_n = 0$ unless $n$ is a multiple of $N_c$. The remaining coefficients are real and non-negative. Hence the $V N_s N_f$ distinct zeroes of $Z$ cannot lie on the positive real axis of $z$. The Yang-Lee picture now follows, with phase transitions occurring when $V \to \infty$ and the zeroes pinch the positive real $z$ axis. Note that the finite Laurent series on the right of eq. (17) is typical of a relativistic theory with its CP symmetry. In non-relativistic theories this is just a finite polynomial.

This gives a method for determining the transition line in the $(\mu, T)$ plane. Construct the partition function at imaginary chemical potential and, by Fourier transforming it, build up the coefficients of the polynomial in $z$. Transform this information into that of the zeroes of the polynomial and check whether they begin to pinch the positive real $z$ axis. Since this information finds all the pinch points, this is one way to go beyond the present day lattice computations and look for signals of phase transitions to the conjectured colour superconducting phases. Some results will be presented elsewhere.

This is an appropriate place to discuss a couple of interesting points about this algorithm. An absolute normalisation for $Z$ is not needed in any practical implementation of this method. An overall multiplicative factor in $Z$ appears as such in the $Q$’s, and hence is irrelevant to the zeroes of eq. (17). Simulations will never give an absolute normalisation for $Z$. However, combinations of simulations at several different values of $\phi$ can be combined to give the relative values of $Z$, as is done in setting up a multi-histogram reweighting. There have been preliminary investigations of methods for constructing $Q$’s.

A second practical question is that of statistical errors. Any simulation will necessarily contain statistical errors, and the question naturally arises whether they allow a determina-
tion of the pinch point of the Lee-Yang zeroes with any degree of accuracy. Since the pinch points lie on the real axis, after appropriate scaling, the zeroes in the vicinity of this point are the solution of $z^N + 1 = 0$, with $N$ being a large integer of the order of $V$. The zeroes of this polynomial lie at the points $z_n = \exp[2\pi i (n + 1/2)/N]$. The effect of simulation errors is to change this equation to a general polynomial of order $k$—

$$\sum_{i=0}^{N} \alpha_i z^i = 0,$$

where the coefficients are real and we can write $|\alpha_N - 1| = \epsilon_N$, $|\alpha_0 - 1| = \epsilon_0$ and $|\alpha_i| = \epsilon_i$ (for $0 < i < N$). We model the errors $\epsilon_i$ as being independent random numbers drawn from Gaussians of width $\sigma$. For sufficiently large statistics $\sigma$ is small, and the deviations of the roots of eq. (18) from $z_n$, $\delta_n$, can be treated as linear in the $\epsilon_i$. It is then a straightforward exercise to show that $\langle \delta_n \rangle = 0$ and the RMS error, $\sqrt{\langle \delta_n^2 \rangle - \langle \delta_n \rangle^2} = \sigma z_n/N$. Thus the problem is statistically well conditioned. The estimates of zeroes are unbiased and the errors fall inversely with the square root of the statistics and inversely with the system volume.

We turn to the question of phase transitions at purely imaginary $\mu$, since this yields further insight into the locations of the zeroes of the partition function. We note at the outset that crucial convexity theorems (such as the second law) fail at imaginary $\mu$, and hence thermodynamics in its usual sense does not apply. The idea of $[3]$ is to use the peak in a response function, $\chi$, (i.e., second derivative of the free energy with respect to an intensive parameter) to identify putative critical points at imaginary $\mu$ and finite volume, analytically continue them to real $\mu$, and then take the infinite volume limit. Note several subtleties in the argument. First, for a function $\chi(\mu^2)$, the extrema for imaginary chemical potential, $\mu_\ast^2 < 0$, are obtained by solving for the zeroes of the first derivative. This does not necessarily give the extrema at real chemical potential, since the solution of $\chi'(\mu_\ast^2) = 0$ does not guarantee that $\chi'(-\mu_\ast^2)$ also vanishes. A second, related subtlety can be seen in a double Taylor expansion for any response function at finite volume—

$$\chi(T/T_c, \mu/T) = \sum_{nm} c_{nm} (1 - T/T_c)^n \left( \frac{\mu}{T} \right)^{2m},$$

where the Taylor coefficients $c_{nm}$ are independent of $T$ and $\mu$. At the critical end-point, $T_E(\mu_E)$ this series must sum to the divergent quantity $|1 - T/T_E(\mu_E)|^{-\gamma}$ (with $\gamma > 0$) in the infinite volume limit. There may also be a critical point, $(T'_E, \mu'_E)$ at an imaginary chemical
potential, \((\mu'_E)^2 < 0\). Clearly the sum in eq. (19) differs at the two points, i.e., even if \(\chi(T_E/T_c, \mu_E/T_E)\) and \(\chi(T'_E/T_c, \mu'_E/T'_E)\) are both divergent, neither \(\chi(T_E/T_c, i\mu_E/T_E)\) nor \(\chi(T'_E/T_c, i\mu'_E/T'_E)\) need to diverge [24].

![Graph](diagram.png)

**FIG. 1:** Number densities, \(\langle n \rangle\) in the model of [25] for the values of \(Q(T, 0)\) marked in the figure.

In the context of our earlier arguments, it is more natural to look for accumulation points of zeroes of the partition function for imaginary chemical potential. This leads to the third subtlety, and a genuine difference between real and imaginary chemical potential due to the lack of convexity mentioned earlier. The theorem of Yang and Lee which we have earlier quoted allowed us to express the partition function as a finite (at all finite volumes) Laurent series in \(z\) with non-negative coefficients (eq. 17). This constraint on the coefficients ensures convexity and prevents zeroes at real positive \(z\), i.e., for real \(\mu\). Only in the limit of infinite volume can the zeroes pinch the real line and cause a phase transition. However, this same structure allows, (and, in some models, may force) the occurrence of zeroes on the unit circle in \(z\) (i.e., for imaginary \(\mu\)) even at finite volume.

Examples abound. We point out the extension of the Gibbs model to \(SU(N_c)\) gauge group where the partition function has been computed [25], and found to be

\[
Z = 2 \cosh[N_c \mu/T] + \sinh[(N_c + 1)m'/T]/\sinh[m'/T].
\] (20)
This is of the form in eq. (17), with $Q(T, N_c) = 2$, $Q(T, 0)$ being the second term in the expression on the right, and all other coefficients vanishing. In the limit $m \to 0$, $Z = 2 \cosh[N_c \mu/T]$, and the zeroes of $Z$ are at

$$z_n = e^{i(2n+1)\pi/2N_c}, \quad (0 \leq n < N_c).$$

Note that there are no positive real $z_n$. The zeroes lie exclusively on the imaginary axis in the $\mu$-plane. The nearest zeroes to the positive real $z$ axis are at $z = \exp(\pm i\pi/2N_c)$. In this 0+1 dimensional problem there is no phase transition for any finite $N_c$. However, a pinch point develops at $z = 1$ as $N_c \to \infty$, very beautifully illustrating van Hove’s theorem.

FIG. 2: Phase diagrams along the real and imaginary axes in $\mu$ for $N_c = 3$ and $N_f = 2$ for finite quark mass. The two insets show the lines of Yang-Lee zeroes pinching the phase transition points on the real $z$ axis. The phase diagram on the left constrains only the pinch points for the lines marked a and b, not their shapes and orientations. CP symmetry causes the whole phase diagram to be replicated for $\Re \mu < 0$, and the corresponding Lee-Yang zeroes to be replicated inside the unit circle (dotted line) by inversion.

The zeroes on the imaginary $\mu$ axis give rise to logarithmic branch point singularities of the free energy evaluated at imaginary chemical potential. The quark number density, all quark number susceptibilities, the energy density and all its derivatives diverge at all these points for all values of $N_c$. These divergences are thermodynamically meaningless since they occur without the necessity of taking a thermodynamic or continuum limit. At finite quark mass, the zeroes remain on the unit circle but move about as long as $Q(T, 0) \leq 1$. When the mass becomes larger, these zeroes leave the imaginary axis, but they are still visible as maxima of these observables (see Figure 2), and can be interpreted as crossover points. The
effect of mass seems to be one of the main differences between the perturbative and strong coupling computations of [7].

These crossovers are generic at imaginary chemical potential—Potts models (or $O(N)$ models) with an ordering field in one direction and an imaginary transverse field show such behaviour, as do massive fermions subjected to imaginary chemical potential. Removing the first ordering field converts them into branch point singularities. Both pose dangers to numerical simulations, since these non-thermodynamical singularities are easily misinterpreted as strong first order transitions, or developing critical points. If one indeed misidentifies such points, then finite size scaling studies are also misleading, since one tries to apply inappropriate homogeneity relations arising from thermodynamic considerations. The idea of locating the zeroes of the partition function using data collected at imaginary chemical potential is to bypass these problems altogether.

The connection of the results of [7] and the phase diagram of QCD at real $\mu$ seems to be rather subtle. Here we make a hypothesis which is consistent with the observed absence of a critical point with $Z_3$ symmetry [26] and with present understanding of the physics of the $Z_Nc$ phases [27]. Figure 2 is a cartoon of the conjectured phases of QCD ($N_c = 3$ and $N_f = 2$) with finite quark mass [1]. There are three lines of first order phase transitions (labelled A, B and C) in the figure. These meet at a triple point, where the normal phase, the plasma phase and a colour-superconducting phase coexist. The line A, separating the normal and plasma phases ends in a critical point [28]. The line B is expected to continue to infinity. For imaginary chemical potential, only the locus of zeroes of the partition function, the lines F and G, are shown.

There are also two insets showing the positions of Yang-Lee zeroes which might lead to such phase diagrams. In this figure only the pinch points are constrained—the remainder of the lines 'a' and 'b' are allowed to twist, merge or intersect without changing the phase diagram [29]. The important point is that in a range of temperatures, there are two pinch points on the real axis [30]. As the temperature rises, the pinch point on the right, labelled 'b', moves to higher and higher $\mu_r$, whereas the one on the left, labelled 'a', lifts away from the real axis at the critical end point, $T_E$. Its effect can still be felt at the crossover temperature, $T_c$, seen in finite temperature simulations at $\mu = 0$. Above $T_c$ the line 'b' continues to move outwards, but there remain isolated $N_c$ zeroes on or near the unit circle (drawn with a dotted line), depending on the quark mass, which give rise to the crossovers.
We end by summarizing the contents of this paper. The complex analytic structure of the free energy (pressure) of QCD was investigated. It was shown that CP symmetry makes the free energy an analytic function of the chemical potential $\mu$ at all temperatures $T$. This symmetry is unexploitable to give an algorithm for a Monte Carlo procedure that works through a molecular dynamics algorithm. Exploiting analyticity, it is possible to write a canonical product representation of the partition function, and made contact with the Yang-Lee theory. It was argued that analyticity, monotonicity and continuity of the pressure implies that non-linear susceptibilities of arbitrary order must exist and be non-negative at all $T$. It was further argued that this is connected with electric screening and magnetic confinement in high temperature QCD. I showed how to use canonical partition functions, derived from Monte Carlo simulations at purely imaginary chemical potential, to obtain information on the phase structure of QCD. Finally, a plausible phase diagram of QCD was used to anticipate the behaviour of the zeroes that such numerical techniques might give rise to.

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CP symmetry then implies that $Z$ is symmetric under inversions in the unit circle, $z \to 1/z$. In the remaining part of this paper all statements should be interpreted as pertaining to one part of the $z$ plane unless otherwise stated. We will usually examine the region outside the unit circle, i.e., for $\Re \mu > 0$. By inversion, i.e., CP transformations, the physics inside the unit circle can be reconstructed.

See, for example, chapter 5, section 2.8 of L. Ahlfors, *Complex Analysis*, Mc Graw Hill Book Company, New York, 1966.

C. N. Yang and T. D. Lee, *Phys. Rev.*, 87 (1952) 404.

Li$_n(z)$ has no poles or essential singularities in the complex $z$ plane, has branch points at $z = 1$ and $\infty$, is single valued on the complex plane cut between these points, where it is continuous from below. For more information see A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions*, Vol. 1, Krieger, New York, 1981; L. Lewin, *Polylogarithms and Associated Functions*, North Holland, New York, 1981.

In a path-integral approach one obtains directly the expression in eq. (12) and periodicity can only be obtained then by summing over all the strips of width $2\pi i T$. The enhanced periodicity noticed in [7] implies that one sums over strips of width $2\pi i T/N_c$.

See J. Barré et al., cond-mat/0102036 for a recent take on these problems.

A. Rebhan, *Nucl. Phys.*, B 430 (1994) 319; K. Kajantie et al., *Phys. Rev. Lett.*, 79 (1997) 3130; S. Datta and S. Gupta, *Phys. Rev.*, D 67 (2003) 054503.

D. G. Gross et al., *Rev. Mod. Phys.*, 53 (1981) 43; G. S. Bali et al., *Phys. Rev. Lett.*, 71 (1993) 3059; S. Datta and S. Gupta, *Nucl. Phys.*, B 534 (1998) 392; M. Laine, [hep-ph/0301011](http://arxiv.org/abs/hep-ph/0301011).

Other examples are known where convexity arguments fail at each step of a limiting procedure, while being true in the limit. See, for example, K. Binder, *Phys. Rev.*, B 25 (1982) 1699; A. Billoire et al., *Nucl. Phys.*, B 358 (1991) 231; A. Irbäck et al., *Nucl. Phys.*, B 409 (1993) 663; A. Billoire, *Nucl. Phys. Proc. Suppl.*, 42 (1995) 21.

D. E. Miller and K. Redlich, *Phys. Rev.*, D 35 (1987) 2524.

I. M. Barbour et al., *Phys. Lett.*, B 215 (1988) 567.

A. Hasenfratz and D. Toussaint, *Nucl. Phys.*, B 371 (1992) 539.

These are straightforward consequences of comparison of general alternating series and absolutely convergent series.

N. Bilic and K. Demeterfi, *Phys. Lett.*, B 212 (1988) 83.
[26] For details on the failure of previous searches for a critical point in models with $Z_3$ symmetry, see, for example, R. V. Gavai and F. Karsch, Phys. Lett., B 233 (1989) 417; S. Gupta et al., Nucl. Phys., B 329 (1990) 263; A. Billoire, R. Lacaze and A. Morel, Nucl. Phys., B 340 (1990) 542.

[27] A. Gocksch and R. Pisarski, Nucl. Phys., B 402 (1993) 657; C. Korthals-Altes, K. Lee and R. Pisarski, Phys. Rev. Lett., 73 (1994) 1754; I. Kogan, Phys. Rev., D 49 (1994) 6799; T. Hansson, H. B. Nielsen and I. Zahed, Nucl. Phys., B 451 (1995) 162; V. Belyaev et al., Phys. Lett., B 277 (1992) 331; W. Chen et al., Phys. Rev., D 46 (1992) R1223; K. Sailer, [hep-ph/9403367], A. Smilga, Ann. Phys., 234 (1994) 1; J. Kiskis, Phys. Rev., D 51 (1995) 3781.

[28] At zero quark mass the critical point may be pushed to $\mu = 0$, or may change into a tricritical point from which a critical line emerges. While there are theoretical biases towards the latter alternative, deciding between them is one of the goals of future lattice simulations.

[29] For known constraints on the locus of zeroes, see M. Biskup et al., [math-ph/0004003], ibid., math-ph/0304007.

[30] For certain classes of models the zeroes lie only on a circle. This gives a single phase transition at any temperature. QCD is expected to fall outside this class of theories. However, at the triple point, the two pinch points are expected to merge. It is interesting to speculate that across the triple point the potential between effective baryonic degrees of freedom changes in character.