

TRIAGE OF THE SIGN PROBLEM*

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We discuss the sign problem in QCD at nonzero chemical potential and its relation with chiral symmetry breaking and the spectrum of the Dirac operator using the framework of chiral random matrix theory. We show that the Banks–Casher formula is not valid for theories with a sign problem and has to be replaced by an alternative mechanism that is worked out in detail for QCD in one dimension at nonzero chemical potential.

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1. Introduction

Despite tremendous efforts [1–5], the phase diagram of QCD in the chemical potential temperature plane is only known for $\mu = 0$ and at asymptotically large densities. In between these extreme limits, the only firm result at low temperatures is the transition to nuclear matter when the sum of the chemical potential and the binding energy of nuclear matter is equal to the nucleon mass. Most results at intermediate values of the chemical potential are based on models such as the Nambu–Jona–Lassinio model [6, 7], strong coupling expansions [8, 9], ADS–CFT dualities [10–12] and random matrix theory [13, 14].

The reason for the lack of first principle calculations is the phase of the fermion determinant at nonzero chemical potential which invalidates probabilistic methods. When the sign problem is mild, though, simulations can be performed by absorbing the phase in the observable which is known as re-weighting. The real merit of the work by Fodor and Katz [15] is the

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realization that the sign problem is much less severe close to T_c so that sophisticated re-weighting methods have a chance to work. In fact, results close to T_c and small chemical potential obtained with a variety of methods such as imaginary chemical potential [16,17], Taylor expansion [18,19], re-weighting [15], the canonical ensemble [20] and the density of state method [21,22], are in close agreement.

In this lecture we will discuss the average phase factor of the fermion determinant. It provides a direct measure for the severity of the sign problem. We will focus on the average phase factor in the microscopic domain of QCD where *nonperturbative* analytical results can be obtained by exploiting the equivalence of QCD and chiral random matrix theory [23,24]. *Perturbatively*, the average phase factor can be calculated by means of chiral perturbation theory up to temperatures close to T_c and chemical potentials up to the pion mass [25]. We will find that the sign problem is necessarily severe when $\mu > m_\pi/2$. The reason is that exponentially large contributions to the partition function have to be canceled in order to obtain a chiral condensate that has sensible physical properties such as a discontinuity when the quark mass crosses the imaginary axis.

One disturbing observation is that the relation between the spectral density of the Dirac operator and the discontinuity of the chiral condensate seems to be violated for QCD at nonzero chemical potential. From an analysis in the microscopic domain of QCD it was found [26] that the discontinuity arises due to an alternative mechanism. Lending support to its universality, the same mechanism is at work [27] for QCD in one dimension. This case, because of its simplicity, will be discussed in detail below.

In this lecture we will show that chiral random matrix theory has added significantly to our understanding of chiral symmetry breaking and the sign problem for QCD at nonzero chemical potential. This adds to a long list of successes of random matrix theory in this field such as the understanding of quenched approximation [28], the critical endpoint in QCD [13,14], the macroscopic spectral density [28–34], the microscopic spectral density [35–41] and Yang–Lee zeros [28,42,43]. For more successes we refer to reviews of this subject [44,45].

After some introductory remarks on QCD at nonzero chemical potential in Sec. 2, we will discuss the sign problem in Sec. 3. The microscopic domain of QCD will be introduced in Sec. 4. Results for the average phase factor will be presented in Sec. 5 and their relation with the Dirac spectrum is examined in Sec. 6. Sec. 7 contains a detailed discussion of the alternative to the Banks–Casher formula for the example of one-dimensional QCD at nonzero chemical potential. Concluding remarks are made in Sec. 8.

2. QCD at nonzero chemical potential

The QCD partition at temperature $1/\beta$ and chemical potential μ is given by

$$Z_{\text{QCD}} = \sum_k e^{-\beta(E_k - \mu)}, \quad (1)$$

where the sum is over all states. This partition function can be rewritten as a Euclidean quantum field theory

$$Z_{\text{QCD}} = \left\langle \prod_f \det(D + m_f + \mu\gamma_0) \right\rangle_{\text{YM}}, \quad (2)$$

where the average is over the Yang–Mills action. The Dirac operator is denoted by D and the product is over N_f flavors with mass m_f . The Dirac operator is nonhermitean whereas $\mu\gamma_0$ is Hermitean so that the total Dirac operator has no hermiticity properties. In lattice QCD, the chemical potential enters on each time-like link such that forward hopping is enhanced by $\exp(\mu)$ whereas backward hopping is suppressed by $\exp(-\mu)$ [46]. The asymmetry between forward and backward propagation also implies that the Dirac operator is nonhermitean for $\mu \neq 0$:

$$\det(D + m + \mu\gamma_0) = |\det(D + m + \mu\gamma_0)|e^{i\theta} = \prod_k (\lambda_k + m). \quad (3)$$

If the average phase factor vanishes in the thermodynamic limit, Monte Carlo simulations are not possible. This problem is known as the sign problem. Nevertheless, we emphasize that it is our aim to understand QCD at $\mu \neq 0$ starting from *first* principles.

Let us now discuss the phase diagram in the chemical potential temperature plane. A schematic phase diagram is shown in Fig. 1. Even though the $\mu = 0$ axis is rather well-understood, there is still an ongoing controversy about the value of the crossover temperature. Whether it is value of 190 MeV [47] or 170 MeV [48] or somewhere in between, will definitely be resolved by future lattice simulations. At asymptotically large values of the chemical potential, perturbative calculations, show that QCD is superconducting [49]. We will not further discuss this region.

At low temperature and $\mu < (m_N - E_{\text{binding}})/3$ with E_{binding} the binding energy per nucleon of nuclear matter, only the vacuum state contributes to the QCD partition function, and its free energy is μ -independent. At $\mu = (m_N - E_{\text{binding}})/3$ a transition to nuclear matter takes place. These are the only solid results at intermediate densities. All other results at intermediate density are model dependent. We agree with McLerran and Pisarski [50] that confining forces play an essential role, and that one better

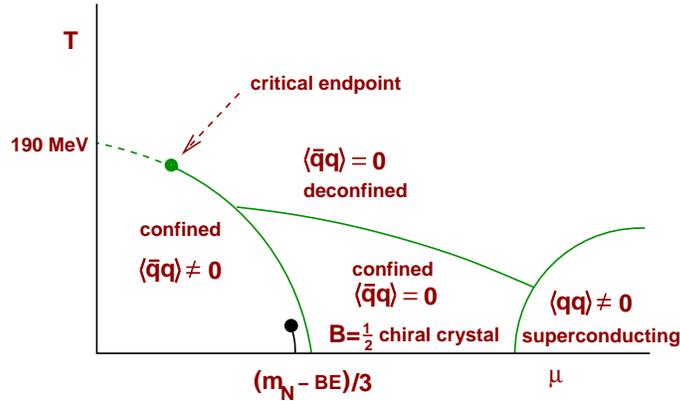


Fig. 1. A schematic phase diagram of QCD in the temperature chemical potential plane.

relies on models where confinement is manifest. One such model is the Skyrme model which is believed to be an accurate description of QCD at large N_c . With increasing density this model undergoes a transition [51] to a qualitatively different phase. It was shown in [52, 53] that the dense phase that minimizes the energy is a chiral crystal of $B = 1/2$ objects [54] which has restored chiral symmetry. This state is strongly bound with a binding energy of at least 100 MeV per nucleon over nuclear matter. We expect that it takes similar temperatures to melt this phase. Most recently such scenario was advocated in [50] for the large N_c phase diagram of QCD. If indeed the phase transition to the chiral symmetric phase is of first order, the critical line should end in a critical endpoint to allow for a crossover transition at small chemical potential.

3. Triage of the sign problem

A quantitative measure for the severity of the sign problem is given by the ratio of the QCD partition function and the phase quenched QCD partition function

$$\frac{\langle \det^2(D + m + \mu\gamma_0) \rangle}{\langle |\det(D + m + \mu\gamma_0)|^2 \rangle} \sim e^{-V(F_{N_f=2} - F_{\text{pq}})}. \quad (4)$$

Because both the numerator and denominator are physical partition functions they can be expressed in terms of an extensive free energy. At nonzero temperature, the difference $F_{N_f=2} - F_{\text{pq}}$ is always nonzero so that, in the thermodynamic limit, the sign problem becomes prohibitively severe. There is no reason, though, to doubt that, despite these cancellations, the large

volume limit is still smooth. What happens is that, with increasing volume, it becomes more and more difficult to generate the QCD partition function from the phase quenched ensemble. By factoring the determinant of the Dirac operator into its absolute and phase factor, $\exp(i\theta)$, the ratio (4) can be interpreted as the phase quenched expectation value of $\exp(2i\theta)$,

$$\frac{\langle \det^2(D + m + \mu\gamma_0) \rangle}{\langle |\det(D + m + \mu\gamma_0)|^2 \rangle} = \langle e^{2i\theta} \rangle_{\text{pq}}. \quad (5)$$

The phase quenched QCD partition function can be rewritten as the expectation value

$$\langle |\det(D + m + \mu\gamma_0)|^2 \rangle = \langle \det(D + m + \mu\gamma_0) \det(D + m - \mu\gamma_0) \rangle. \quad (6)$$

This means that the two flavors have opposite charge with respect to the chemical potential. In other words, μ can be interpreted as an isospin chemical potential. Therefore, in the low-temperature limit, the free energy of phase quenched QCD remains constant for $\mu < m_\pi/2$. At $\mu = m_\pi/2$ a phase transition to a Bose-condensed phase of pions takes place so that the free energy becomes μ -dependent for $\mu > m_\pi/2$ [55–57]. In the low temperature limit, the free energy of QCD is μ -independent for $\mu < (m_N - E_{\text{binding}})/3$. This implies that the free energy of QCD and phase quenched QCD are different for $m_\pi/2 < \mu < (m_N - E_{\text{binding}})/3$ resulting in a severe sign problem.

Below we will analyze the average phase factor in the microscopic domain of QCD and for one-dimensional QCD.

4. Microscopic domain of QCD and random matrix theory

The QCD Dirac spectrum can be probed by including additional bosonic and fermionic determinants in the partition function with quark masses equal to complex parameters that can be varied independent of the QCD quark masses. For definiteness let us assume that we have N_f original quarks and s additional quarks with masses given by

$$m_1, \dots, m_{N_f} \quad \text{and} \quad z_1, \dots, z_s, \quad (7)$$

respectively. For fixed QCD quark masses, it is always possible to choose these additional quark masses such that the associated Goldstone bosons are much lighter than the Goldstone bosons of the original quarks (the case of massless quarks has to be treated separately; we assume that all quark masses are nonzero). Using the same arguments as given by Gasser and Leutwyler for the ε -domain of QCD [58], to leading order in the chiral expansion of the z_k -quarks, the partition function factorizes as [59]

$$Z(m_1, \dots, m_{N_f}, z_1, \dots, z_s) = Z_{\text{QCD}}(m_1, \dots, m_{N_f}) Z(z_1, \dots, z_s) \quad (8)$$

if the Compton wave lengths of the additional bosons containing the quark masses z_k are much larger than the size of the box. Using the Gell–Mann–Oakes–Renner relation, the *microscopic* domain of QCD is given by [59]

$$|z_k| \ll \frac{F^2}{\Sigma\sqrt{V}}, \quad (9)$$

where Σ is the chiral condensate, F the pion decay constant and V the volume of the box. In solid state physics, this scale for z is known as the Thouless energy and was discussed in the context of QCD in [60–62]. Of course, we can consider QCD with quark masses m_k in the microscopic domain (9) which is also known as the ε -domain of QCD. This domain will also be called the microscopic domain of QCD.

In the domain (9), the z_k dependent part of the partition function is given by a unitary matrix integral. At $\mu \neq 0$ invariance arguments lead to the following partition function of a form [34, 55]

$$Z(z_1, \dots, z_s) = \int dU \text{Sdet}^\nu U e^{V\Sigma[\text{Str}(MU^\dagger + M^\dagger U)] - \frac{1}{4}F^2 V \text{Str}[B, U][B, U^\dagger]}, \quad (10)$$

with quark mass matrix given by $M = \text{diag}(z_1, \dots, z_s)$ and charge matrix equal to $B = \text{diag}(q_1, \dots, q_s)$. The superdeterminant and the supertrace are denoted by Sdet and Str , respectively. If we have f fermionic quarks and $s-f$ bosonic quarks, the integral is over a supergroup with bosonic sector equal to the product of $U(f)$ and the positive definite matrices $Gl(s-f)/U(s-f)$. For convergence reasons, the quark mass matrix involving the bosonic quarks has to be properly adjusted [35] and additional conjugate quarks may have to be introduced [63].

Another representation of the partition function (10) is the large- N limit of a random matrix model with the symmetries of $Z(z_1, \dots, z_s)$. This random matrix model is obtained by replacing the matrix elements of the Dirac operator by Gaussian random numbers [64, 65],

$$D = \begin{pmatrix} m & iW + \mu \\ iW^\dagger + \mu & m \end{pmatrix}, \quad P(W) \sim e^{-N\text{Tr}W^\dagger W}, \quad (11)$$

where W is in general an $N \times (N + \nu)$ matrix with ν the topological charge. As was shown in [66], the properties of this theory in the microscopic domain are not sensitive to the details of the probability distribution. The reason is that for $N \rightarrow \infty$ with mN fixed, the random matrix model has a mass gap, so that it becomes a theory of Goldstone bosons dictated by the pattern of spontaneous symmetry breaking with partition function given by (10).

Philosophically, this is important because of the realization that chaotic motion dominates the dynamics of quarks at low energy. Practically, this is useful because it enables us to use powerful random matrix techniques to calculate physical observables.

5. The phase of the fermion determinant

Let us now calculate the average phase factor in the microscopic domain of QCD. For simplicity we consider the quenched case so that

$$\langle e^{2i\theta} \rangle = \left\langle \frac{\det(D + m + \mu\gamma_0)}{\det(D^\dagger + m + \mu\gamma_0)} \right\rangle. \tag{12}$$

Since the average phase factor is the ratio of two partition functions, its value is necessarily real and nonnegative. We evaluate the ratio (12) in the microscopic domain of QCD where only the contribution of the zero momentum Goldstone modes has to be taken into account. The partition function (12) has four different Goldstone modes. If we denote the fermionic quark by f and the bosonic quark by b , they are given by

$$\bar{f}f, \quad \bar{b}b, \quad \bar{b}f, \quad \bar{f}b. \tag{13}$$

The first two are neutral, but because the charge of conjugate quarks is opposite to that of regular quarks, the last two have charge ± 2 . The masses of the corresponding Goldstone bosons are thus given by

$$m_{\bar{f}f} = m_\pi, \quad m_{\bar{b}b} = m_\pi, \quad m_{\bar{b}f} = m_\pi + 2\mu, \quad m_{\bar{f}b} = m_\pi - 2\mu. \tag{14}$$

When $\mu < m_\pi/2$ only the vacuum state contributes to the partition function so that the free energy is a μ -independent constant and the average phase factor is given by the product of the square root of the curvatures of the Goldstone modes,

$$\langle e^{2i\theta} \rangle = \frac{(m_\pi - 2\mu)(m_\pi + 2\mu)}{m_\pi^2}. \tag{15}$$

For $\mu > m_\pi/2$ the massless pion Bose condenses, and the free energy becomes μ -dependent so that the average phase factor becomes zero in the thermodynamic limit. We thus find

$$\langle e^{2i\theta} \rangle = \theta(m_\pi - 2|\mu|) \left(1 - \frac{4\mu^2}{m_\pi^2} \right). \tag{16}$$

In [23] the average phase factor was calculated by means of the complex orthogonal polynomial method of [36, 68]. The result is given by

$$\begin{aligned} \langle e^{2i\theta} \rangle_{N_f=0} &= 1 - 4\hat{\mu}^2 I_0(\hat{m}) K_0(\hat{m}) - \frac{1}{4\hat{\mu}^2} e^{-2\hat{\mu}^2 - \frac{\hat{m}^2}{8\hat{\mu}^2}} \\ &\times \int_{\hat{m}}^{\infty} dx x e^{-\frac{x^2}{4\hat{\mu}^2}} K_0\left(\frac{x\hat{m}}{4\hat{\mu}^2}\right) (I_0(x)\hat{m}I_1(\hat{m}) - xI_1(x)I_0(\hat{m})). \end{aligned} \tag{17}$$

The average phase factor can also be calculated using an imaginary chemical potential [67]. However, this gives only the first two terms and misses the non-analytic term in the above expression. The non-analytic term is essential when μ approaches $m_\pi/2$ and cancels the analytic term for $\mu > m_\pi/2$.

In Fig. 2 we show the analytical result for the average phase factor weighted with the determinant for two flavors (left figure). The solid curve is the mean field result. In the right figure we compare the quenched average “phase factor” for imaginary chemical potential with lattice simulations on an 8^4 lattice (see [67]). The solid curve is given by the analytical continuation ($\mu^2 \rightarrow -\mu^2$) of the first two terms in (17).

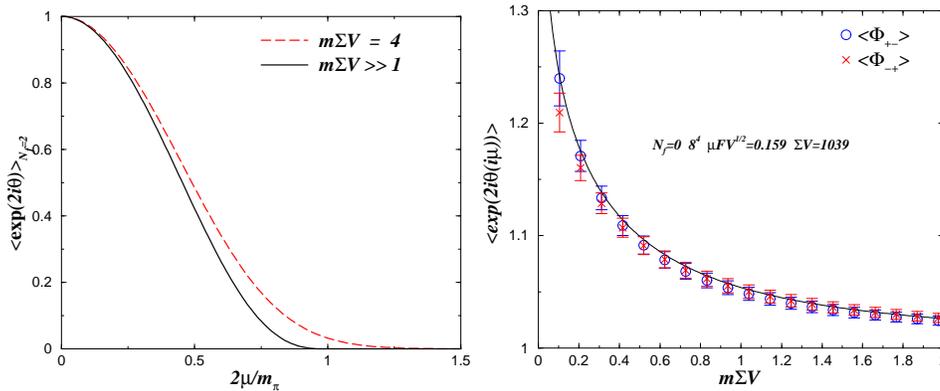


Fig. 2. The microscopic result of the average phase factor (left) and the average phase factor for imaginary chemical potential (right). The points with error bars in the right figure are lattice results obtained in [67].

6. Average phase factor and Dirac spectrum

The sign problem becomes inevitable when the quark mass is inside the domain of eigenvalues. This should be obvious because for eigenvalues close to the mass, small variations of the gauge field result in large phase fluctuations. In Fig. 3 we illustrate the distribution of the Dirac eigenvalues. The width of the spectrum can be obtained from chiral perturbation theory [34] or chiral random matrix theory [28]. In the quenched case or the phase quenched case the chiral condensate at m can be interpreted as the planar electric field at m of charges located at the position of the eigenvalues. Elementary electrostatics dictates that the chiral condensate behaves as the green curve in the right panel of Fig. 3. In particular, there is no discontinuity at $m = 0$. Because the low temperature limit of the free energy of full QCD does not depend on the chemical potential, the chiral condensate

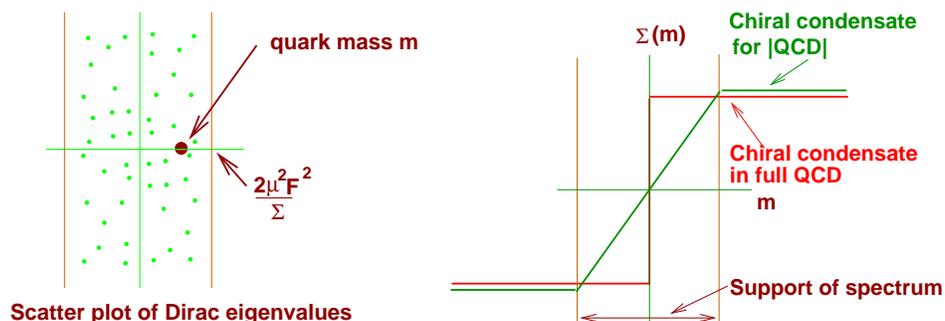


Fig. 3. Scatter plot of Dirac eigenvalues and $\mu \neq 0$ (left), and in the right panel, we show the mass dependence the chiral condensate for full QCD (red curve) and quenched or phase quenched QCD (green curve).

of full QCD should have a discontinuity at $m = 0$ for $\mu < m_N/3$. What has to happen is that the phase of the fermion determinant has to cancel the decrease in free energy that takes place in the quenched or phase quenched theory for $\mu > m_\pi/2$. Therefore, we necessarily have a severe sign problem in this domain.

The puzzle that the chiral condensate remains the same as the result of strong cancellations is known as the “Silver Blaze Problem” [69]. This name has been inspired by the title of a Sherlock Holmes novel by Conrad Doyle. The analogy is that the dog did not bark although the racing horse “Silver Blaze” disappeared.

In the literature it has been stated that average spectral density of full QCD will show an accumulation of spectral density on the imaginary axis consistent with the Banks–Casher formula. We now understand that this is not the case. The average spectral density for full QCD was evaluated in the microscopic domain of full QCD using the method of complex orthogonal polynomials [36]. It was found that it has oscillations in a macroscopic region of the complex plane with an amplitude that increases exponentially with the volume and a period that is inversely proportional to the volume [38]. The cancellations of the exponential large contributions result in a condensate that has a discontinuity in the thermodynamic limit [26].

The same phenomenon occurs for QCD in one dimension. Although the eigenvalues of the Dirac operator are located on an ellipse instead of being scattered in the complex plane, the mechanism for generating a discontinuity in the chiral condensate is the same as for QCD. To simplify the argument we will restrict ourselves to giving a detailed discussion for the case of QCD in one dimension only.

7. One-dimensional QCD

All gauge fields in one-dimensional QCD can be gauged away with the exception of the gauge field at the boundary of the manifold. Therefore, one-dimensional lattice QCD is given by the random matrix theory

$$Z_{1d} = \int dU \det^{N_f} D \quad (18)$$

with Dirac operator for n lattice points given by

$$D = \begin{pmatrix} mI & e^\mu & \dots & e^{-\mu}U^\dagger \\ -e^{-\mu} & mI & \dots & 0 \\ \vdots & & & \vdots \\ 0 & \dots & mI & e^\mu \\ -e^\mu U/2 & \dots & -e^{-\mu} & mI \end{pmatrix}. \quad (19)$$

The chemical potential can also be gauged to the boundary. The full theory does not have charged excitations resulting in a chiral condensate that is μ -independent. The phase quenched theory, on the other hand, undergoes a phase transition at $\mu = m_\pi/2$ resulting in a different free energy. This can be easily shown in the limit of large n by using the explicit result for the determinant of the Dirac operator (19)

$$\det D = 2^{-nN_c} \det[e^{n\mu_c} + e^{-n\mu_c} + e^{n\mu_c} + e^{n\mu_c}U + e^{-n\mu_c}U^\dagger]. \quad (20)$$

Here, we introduced the critical chemical potential μ_c given by the relation $\sinh \mu_c = m$. For gauge group $U(N)$ the integrals are particularly simple, and we obtain in the limit of large n

$$\begin{aligned} F_{N_f=2} &= -nN_f|\mu_c|, \\ F_{N_f=2, \text{pq}} &= -nN_f|\mu_c| - nN_f(|\mu| - |\mu_c|)\theta(|\mu| - |\mu_c|), \end{aligned} \quad (21)$$

resulting in a chiral condensate with a mass dependence as shown in Fig. 4. Although nothing happens to the $N_f = 2$ free energy, this comes only as a result of exponentially large cancellations in the partition function. This is the ‘‘Silver Blaze Problem’’ [69] mentioned before. We will now illustrate how this problem manifests itself in spectrum of the Dirac operator and the chiral condensate.

For simplicity we will only consider the case $N_f = 1$ with $U(1)$ as gauge group. Because the phase angles of the eigenvalues are uniformly distributed along an ellipse with semi-minor axis equal to $\sinh \mu$ and semi-major axis equal to $\cosh \mu$ (see Fig. 4; notice that the figure is for large N_c , for $U(1)$ the

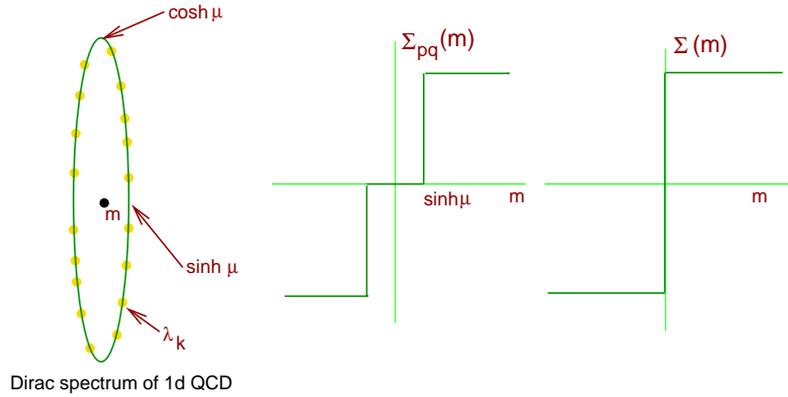


Fig. 4. The eigenvalue distribution of the one-dimensional QCD Dirac operator at nonzero chemical potential and large N_c (left). The graphs show the mass dependence of chiral condensate of the partially quenched theory (middle) and the full theory (right).

phase angles of the eigenvalues are equally spaced), the eigenvalue density of the $N_f = 1$ theory is given by

$$\rho_{N_f=1}(z)d^2z = \frac{1}{2\pi} \frac{e^{n\mu_c} + e^{-n\mu_c} - e^{n(i\alpha+\mu)} - e^{-n(i\alpha+\mu)}}{e^{n\mu_c} + e^{-n\mu_c}} \delta(r-\mu)dr d\alpha \quad (22)$$

with the original variables z parameterized as

$$z = \frac{1}{2} (e^{r+i\alpha} - e^{-r-i\alpha}), \quad r > 0, \alpha \in [0, 2\pi]. \quad (23)$$

The chiral condensate for $N_f = 1$ given by

$$\Sigma(m) = \frac{\left\langle \sum_k \frac{1}{\lambda_k+m} \prod_k (\lambda_k + m) \right\rangle}{\left\langle \prod_k (\lambda_k + m) \right\rangle} \quad (24)$$

can then be expressed as

$$\begin{aligned} \Sigma_{N_f=1} &= \int d^2z \frac{\rho_{N_f=1}(z)}{z+m} \\ &= \int \frac{d\alpha}{2\pi} \frac{e^{n\mu_c} + e^{-n\mu_c} - e^{n(i\alpha+\mu)} - e^{-n(i\alpha+\mu)}}{(e^{n\mu_c} + e^{-n\mu_c})(m + (e^{\mu+i\alpha} - e^{-\mu-i\alpha})/2)} \\ &= \frac{\tanh(n\mu_c)}{\cosh \mu_c}. \end{aligned} \quad (25)$$

When $|\mu| < |\mu_c|$, all four terms in the numerator contribute to the integrand. When $|\mu| > |\mu_c|$, *i.e.* the domain where the quark mass is inside the ellipse of eigenvalues, the quenched chiral condensate, given by the first two terms of the numerator, is zero resulting in a chiral condensate that behaves as the phase quenched theory (see middle panel of Fig. 4). Therefore, the condensate for $|\mu| > |\mu_c|$ is due to the oscillating terms in the numerator. A finite result is obtained because the oscillations cancel the exponential growth with n of the amplitude. In the thermodynamic limit the $\tanh(n\mu_c)$ results in a discontinuity at $m = 0$ (see Fig. 4).

8. Conclusions

Random matrix theory has been invaluable for understanding QCD at nonzero chemical potential. In this lecture we have discussed applications involving the phase of the fermion determinant at nonzero chemical potential. We have shown that QCD has a severe sign problem if the quark mass is inside the domain of eigenvalues. In this domain strong cancellations lead to a free energy that does not depend on the chemical potential and a chiral condensate that has a discontinuity when the quark mass crosses the imaginary axis. The latter happens without an accumulation of eigenvalues on the imaginary axis, but due to oscillations in the spectral density with an amplitude that increases exponentially with the volume. This mechanism occurs both in the random matrix limit of QCD and in one dimensional QCD which strongly suggests that it is the generic replacement of the Banks–Casher formula for theories with a sign problem.

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