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Subsets of configurations and canonical partition functions

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Abstract

We explain the physical nature of the subset solution to the sign problem in chiral random matrix theory: The subset sum over configurations is shown to project out the canonical determinant with zero quark charge from a given configuration. As the grand canonical chiral random matrix partition function is independent of the chemical potential, the zero quark charge sector provides the full result.

I. INTRODUCTION

Chiral random matrix theory [1] has given us several deep insights into the QCD sign problem which prohibits direct application of lattice QCD methods at nonzero quark chemical potential [2]. The random matrix framework has allowed us to understand the failure of the quenched approximation [3], to formulate the OSV relation [4] which replaces the Banks-Casher relation [5] and to derive the first analytical result for the average phase factor of the fermion determinant [6].

These lessons from chiral random matrix theory apply directly to QCD at nonzero chemical potential since the two are equivalent in the microscopic limit (this limit is also known as the ϵ-regime of chiral perturbation theory). For this reason it is most interesting that the sign problem in a chiral random matrix theory can be solved by means of the subset method [7, 8]. In particular this subset method works even in the region of $\mu > m_\pi/2$ where the sign problem is severe.

The aim of the present paper is to provide the physical explanation of why the subset method introduced in [7, 8] solves the sign problem in chiral random matrix theory: As we will show in detail below the subset construction projects out the canonical determinant with zero quark charge from the fermion determinant. Since the chiral random matrix partition function is independent of the chemical potential the zero charge part makes up the full result.

In this paper we start from a random matrix theory for QCD that is μ-independent even for finite size of the random matrix. This choice has a direct physical motivation: First, in the microscopic domain (where the size, n, of the random matrix goes to infinity while the quark mass times n and the square of the chemical potential times n are held fixed) the random matrix partition function is identical to the partition function of chiral perturbation theory in the ϵ-regime [9, 10]. Second, being a theory of pions, which are bound states of quarks and anti-quarks, chiral perturbation theory naturally does not couple to the quark chemical potential. As chiral perturbation theory is the effective theory for QCD at low temperatures and $\mu < m_N/3$ the μ-independence of the partition function is natural in this regime.

In general, random matrix partition functions for QCD only need to be μ-independent in the microscopic domain. In the present context it is convenient to work with a random matrix theory where this μ-independence is manifest even at finite n.

II. SUBSET AND CANONICAL DETERMINANTS IN CHIRAL RANDOM MATRIX THEORY

Our starting point is a variation of the chiral random matrix theory at non-zero chemical potential μ introduced in [11] (see [12] for a review). It is defined by

$$Z(m,\mu) = \int d\Phi_1 d\Phi_2 \det \begin{pmatrix} m & e^{\mu}\Phi_1 - e^{-\mu}\Phi_2^\dagger \\ -e^{-\mu}\Phi_1^\dagger + e^{\mu}\Phi_2 & m \end{pmatrix} e^{-n\mathrm{Tr}(\Phi_1\Phi_1^\dagger + \Phi_2\Phi_2^\dagger)}, \tag{1}$$

where Φ_1 and Φ_2 are complex $n \times n$ matrices. We have chosen to work with this form of the partition function because it is independent of μ even for finite n (this was also the case for the partition function used in [11], see the appendix), and because the chemical potential appears in the form $\exp(\pm\mu)$ which allows us to project out the canonical partition function in the same way as in lattice QCD. The μ-independence of the partition function follows immediately by using that the Gaussian integral is only nonzero for terms that have an equal number of factors Φ_i and $\Phi_i^\dagger$ for $i = 1, 2$. The relation to the form used in [7, 8] is given in the appendix.

In the subset method of [7, 8], one first performs a sum over a subset of roots of unity contained in the integral over the matrices Φ_1 and Φ_2. The critical observation in [7, 8] is that the determinants

$$d(\mu,\theta_k) \equiv \det \begin{pmatrix} m & e^{\mu+i\theta_k}\Phi_1 - e^{-\mu-i\theta_k}\Phi_2^\dagger \\ -e^{-\mu-i\theta_k}\Phi_1^\dagger + e^{\mu+i\theta_k}\Phi_2 & m \end{pmatrix}, \tag{2}$$

where $\theta_k = 2k\pi/N_s$ with $N_s \geq 2n+1$ [19] sum up to a positive real number

$$\frac{1}{N_s}\sum_{k=0}^{N_s-1} d(\mu,\theta_k) \in \mathbf{R}_+. \tag{3}$$

This number can then in turn be used to generate a Monte Carlo ensemble of configurations and subsequently the unquenched expectation values. Note the invariance of the Gaussian measure under these phase rotations (the arguments below apply to any measure with the same invariance properties). Next we show that the measure Eq. (3) is a canonical determinant with zero baryon number which is manifestly positive.

For a given configuration (Φ_1, Φ_2) we decompose the fermion determinant

$$D(\mu) \equiv \det \begin{pmatrix} m & e^{\mu}\Phi_1 - e^{-\mu}\Phi_2^\dagger \\ -e^{-\mu}\Phi_1^\dagger + e^{\mu}\Phi_2 & m \end{pmatrix} \tag{4}$$

into canonical determinants

$$D(\mu) = \sum_{q=-2n}^{2n} e^{\mu q} D_q, \tag{5}$$

where

$$D_q \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \; e^{-iq\theta} D(i\theta). \tag{6}$$

(See [13–15] for applications of canonical determinants to lattice QCD.) Likewise we decompose the partition function, Z, into canonical partition functions

$$Z(\mu) = \sum_{q=-2n}^{2n} e^{\mu q} Z_q, \tag{7}$$

where

$$Z_q = \langle D_q \rangle, \tag{8}$$

and $\langle \ldots \rangle$ is the expectation value with respect to the Gaussian weight for $\Phi_{1,2}$. As Z is independent of μ we necessarily have $Z_q = 0$ for $q \neq 0$. For odd q the canonical determinants vanish as well, $D_{q=2l+1} = 0$. This follows trivially from $D(i(\mu+\pi)) = D(i\mu)$ and $\exp(-iq(\mu+\pi)) = \exp(-iq\mu)(-1)^q$. For even index, however, the canonical determinants are nonzero for a typical configuration (Φ_1, Φ_2), and only after averaging will one find $Z_{q=2l} = 0$ for $l \neq 0$.

To make the connection to the subset construction of [7, 8] we first rewrite the canonical partition functions

$$\begin{aligned} D_q &= \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \; e^{-iq(-i\mu+\theta)} D(i(-i\mu+\theta)) \\ &= \frac{1}{2\pi} e^{-q\mu} \int_{-\pi}^{\pi} d\theta \; e^{-iq\theta} D(\mu + i\theta), \end{aligned} \tag{9}$$

where in the first line we shifted the contour into the complex plane. The determinant inside the integrand is now

$$D(\mu + i\theta) \; = \; \det \begin{pmatrix} m & e^{\mu+i\theta}\Phi_1 - e^{-\mu-i\theta}\Phi_2^\dagger \\ -e^{-\mu-i\theta}\Phi_1^\dagger + e^{\mu+i\theta}\Phi_2 & m \end{pmatrix}. \tag{10}$$

To establish the relation between this subset construction and the canonical determinants introduced above first note that we can replace the subset-sum over θ_k in Eq. (3) by an integral

$$\frac{1}{N_s}\sum_{k=0}^{N_s-1} d(\mu,\theta_k) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta\; d(\mu,\theta). \tag{11}$$

This follows from the observation that the integrand is a polynomial in $e^{\pm i\theta}$ of maximum order $2n$ and that all integrals follow from the orthogonality relations

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta\; e^{i(j-l)\theta} = \delta_{jl}. \tag{12}$$

The same orthogonality relation holds for the sum

$$\frac{1}{N_s}\sum_{q=0}^{N_s-1} e^{i\theta_q(j-l)} = \delta_{jl} \tag{13}$$

provided that $|j|, |l| \leq N_s$. Therefore the sum over k gives the exact value of the integral if $N_s \geq 2n+1$.

By comparison of Eq. (2) with Eq. (10) we then see that the subset sum is equivalent to the projection onto the $q=0$ canonical determinant, that is

$$\frac{1}{N_s}\sum_{k=0}^{N_s-1} d(\mu,\theta_k) = D_0. \tag{14}$$

This is the physical explanation of what the subset is.

Since $Z_{q=0} = Z$ (the $q=0$ part makes up the entire partition function because it is independent of μ) the subset method gives the full result. Moreover, as the subset sum for a given configuration is equivalent to the canonical determinant with $q=0$, it is clear that the subset sum is necessarily real and positive: as can be seen explicitly from Eq. (9), we have that $D_{q=0}$ is independent of μ, and for $\mu=0$ all determinants in the subset sum are real and positive. This is the physical explanation of why the subset method works, see also [7, 8].

For the variant of the chiral random matrix partition function used in [7, 8] the interpretation of the subset is analogous, see Appendix A. The original argument for why the subset method works given in [7, 8] is also related to the argument given above.

In general the QCD partition function will of course depend on the chemical potential and hence in QCD one will need to evaluate all D_q. For the evaluation of D_q it is also possible to turn the integral into a sum. In this case the maximum order of the polynomial in $e^{\pm i\theta}$ is $2n + |q|$, and therefore the subset sum evaluates the integral exactly for $N_s \geq 2n + |q| + 1$. Note, however, that the D_q with $q \neq 0$ are not real and positive so we do not have a weight to perform Monte Carlo Simulations (even if we can do these integrals exactly). This is in exact analogy with the observations of [15] in lattice QCD.

The argument given above also applies if Φ is unitary rather than complex. More generally, for unitary lattice gauge theories where the chemical potential is introduced into the temporal links by [16]

$$\begin{aligned} U_t &\to e^{\mu} U_t, \\ U_t^\dagger &\to e^{-\mu} U_t^\dagger. \end{aligned} \tag{15}$$

the partition function is μ-independent and equal to the charge zero canonical partition function. The subset method then applies in exactly the same way as in the random matrix model discussed above.

III. CONCLUSIONS

The subset solution to the sign problem in chiral random matrix theory has been shown to be equivalent to the projection, configuration by configuration, onto the zero quark number canonical determinants. Since the chiral random matrix partition function is independent of the chemical potential, the canonical partition function makes up the full grand canonical partition function. This gives the physical reason how the subset construction works. The same argument applies to unitary lattice gauge theories at nonzero chemical potential.

The vanishing value of the canonical partition functions in chiral random matrix theory for nonzero quark number is the result of detailed cancellations: the canonical determinants with nonzero quark number take complex values and only the average value is zero. The projection onto the canonical determinants with nonzero quark number can also be obtained from a subset sum, however, it remains a challenge to devise a numerical method to control the cancellations in the average. Such a method would potentially have direct application to full QCD where partition functions with $q \neq 0$ are nonvanishing. It may also be able to cast further light on the special nature of the noise [17, 18] related to the sign problem.

Despite the μ-independence of the chiral random matrix partition function the random matrix theory gives a plethora of nontrivial results for the spectral correlation functions of the Dirac operator and for the fluctuations of the fermion determinant. The reason for this is that the generating functionals for such partially quenched observables have a highly nontrivial dependence on the chemical potential. It would be most interesting if one would be able to extend the subset method to these partially quenched observables.

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Appendix A. EQUIVALENCE OF THE CHIRAL RANDOM MATRIX FORMULATIONS

The form of the chiral random matrix theory used in [7, 8] was

$$Z_B(m,\mu_B) = \int d\Phi_1 d\Phi_2 \det \begin{pmatrix} m & i\Phi_1+\mu_B\Phi_2 \\ i\Phi_1^\dagger+\mu_B\Phi_2^\dagger & m \end{pmatrix} e^{-n\mathrm{Tr}(\Phi_1\Phi_1^\dagger+\Phi_2\Phi_2^\dagger)}. \tag{16}$$

This partition function depends on μ_B for finite n [11]. Because of the μ_B-dependence of the partition function $Z_B(m,\mu_B)$, the subset sum is not equal to the canonical partition function for $q_B=0$ and the corresponding canonical partition functions for $q_B\neq 0$ are nonvanishing. The μ_B-dependence is, however, of a form where the partition function at non-zero μ_B is trivially related to the one at $\mu_B=0$ [11]

$$Z_B(m,\mu_B) = (1-\mu_B^2)^n Z_B(\frac{m}{\sqrt{1-\mu_B^2}},0). \tag{17}$$

In [8] it was shown that the subset sum for each configuration realizes this relation. When $\mu_B<1$ both the prefactor $(1-\mu_B^2)^n$ and the rescaled quark mass are real and positive thus, as originally argued in [7, 8], the subset sum for the right hand side is always real and positive. The relation, Eq. (17), is the analogue of the μ-independence of the chiral random matrix theory used in this paper, and the fact that subsets realizes this relation configuration by configuration is the analogue of the projection onto the canonical determinant with zero quark charge.

The form of the chiral random matrix theory adopted in Eq. (1) is related to the form, Eq. (16), used in [7, 8] by a μ dependent rescaling of the mass and a trivial overall factor. If we start from

$$Z(m,\tilde{\mu}) = \frac{1}{(1-\tilde{\mu}^2)^n}\int d\Phi_1 d\Phi_2 \det\begin{pmatrix} m\sqrt{1-\tilde{\mu}^2} & i\Phi_1+\tilde{\mu}\Phi_2 \\ i\Phi_1^\dagger+\tilde{\mu}\Phi_2^\dagger & m\sqrt{1-\tilde{\mu}^2}\end{pmatrix} e^{-n\mathrm{Tr}(\Phi_1\Phi_1^\dagger+\Phi_2\Phi_2^\dagger)}, \quad (18)$$

then it is clear from Eq. (17) that $Z(m,\tilde{\mu})$ is independent of $\tilde{\mu}$. Moreover, with $\tilde{\mu}$ given by

$$\tanh(\mu) = \tilde{\mu}, \quad (19)$$

then this partition function is identical to the one of Eq. (1). In order to see this first note that $\cosh(\mu) = 1/\sqrt{1-\tilde{\mu}^2}$ and $\sinh(\mu) = \tilde{\mu}/\sqrt{1-\tilde{\mu}^2}$ and then use this to express the determinant in terms of μ

$$\begin{aligned} &\det\begin{pmatrix} m/\cosh(\mu) & 1/\cosh(\mu)(i\cosh(\mu)\Phi_1+\sinh(\mu)\Phi_2) \\ 1/\cosh(\mu)(i\cosh(\mu)\Phi_1^\dagger+\sinh(\mu)\Phi_2^\dagger) & m/\cosh(\mu)\end{pmatrix} \\ &= 1/\cosh^{2n}(\mu)\det\begin{pmatrix} m & i\cosh(\mu)\Phi_1+\sinh(\mu)\Phi_2 \\ i\cosh(\mu)\Phi_1^\dagger+\sinh(\mu)\Phi_2^\dagger & m\end{pmatrix}. \end{aligned} \quad (20)$$

The factor $1/\cosh^{2n}(\mu)$ cancels against the prefactor $1/(1-\tilde{\mu}^2)^n$ in the partition function of Eq. (18). After choosing

$$\Phi_1' = \frac{i}{2}(\Phi_1 - i\Phi_2), \qquad \Phi_2' = \frac{i}{2}(\Phi_1^\dagger - i\Phi_2^\dagger) \quad (21)$$

as new integration variables, we recover the form given in Eq. (1).

The subsets defined in [7, 8] consist of rotated matrices

$$\Phi_1 \to \cos\theta_k\Phi_1 + \sin\theta_k\Phi_2, \qquad \Phi_2 \to -\sin\theta_k\Phi_1 + \cos\theta_k\Phi_2 \quad (22)$$

which translates into

$$\Phi_{1,2}' \to e^{i\theta_k}\Phi_{1,2}', \quad (23)$$

as in Eq. (2).

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