Complex Probability Distributions: A Solution for the Long-Standing Problem of QCD at Finite Density

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ABSTRACT

We show how the prescription of taking the absolute value of the fermion determinant in the integration measure of QCD at finite density, forgetting its phase, reproduces the correct thermodynamical limit. This prescription, which applies also to other gauge theories with non-positive-definite integration measure, also has the advantage of killing finite size effects due to extremely small mean values of the cosine of the phase of the fermion determinant. We also give an explanation for the pathological behaviour of quenched QCD at finite density.

1. Introduction

Non-perturbative investigations of QCD at finite temperature and density have received much attention in the last years. The aim of these investigations is to find the matter conditions in the early Universe and to get a clear insight into experimental signatures in the heavy-ion collision experiments. Even if considerable progress has been achieved in the investigations of QCD at finite temperature and zero chemical potential using the lattice approach, the present situation of the field at finite density is not so satisfactory. As is well known, the complex nature of the determinant of the Dirac operator at finite chemical potential, which makes it impossible to use standard simulation algorithms based on positive-definite probability distribution functions, has much delayed investigations on the full theory with dynamical fermions. On the other hand the quenched approximation, which has been extensively and successfully used in simulations of QCD at zero chemical potential, seems to have some pathological behaviour when applied to QCD at finite density [1, 2].

I want to show in this article how one of the main technical difficulties in simulating QCD at finite density, the complex fermion determinant, can be easily surmounted. In fact I will demonstrate that it is enough, in order to get the correct thermodynamical limit to take the absolute value of the fermion determinant in the integration measure, forgetting completely the contribution of its phase. I will also show how not only do we get the correct thermodynamical limit in this way but also that it is an efficient way to kill finite size effects present in the exact simulations and related to very small expectation values of the cosine of the fermion determinant phase [3].

This result, which applies also to more general cases such as non-positive-definite fermion determinants in gauge theories with Wilson fermions [4], agrees with a recent finding of Stephanov [5] in the random matrix model approximation. In fact QCD at finite chemical potential and with n flavours can be seen as a theory with $\frac{n}{2}$ quarks with original action and $\frac{n}{2}$ with conjugate action. This notwithstanding, the zero flavour limit of the model corresponds precisely to standard quenched QCD at finite density. The anomalous behaviour of the quenched model observed in the numerical simulations remains therefore unclear yet. We will give in this paper an explanation for the pathological behaviour of the quenched model in the forbidden region, a region of the chemical potential μ characterized by wild fluctuations [6].

2. Complex Distributions

Let me fix here the standard notation in gauge theories with dynamical fermions, even if the results I am going to discuss apply to every equilibrium statistical mechanics system with a complex "Boltzmann weight". The starting point is the following partition function

$$Z = \int [dU] e^{-\beta S_G(U)} \det \Delta(U, m, \mu) \tag{1}$$

where U are the gauge variables (elements of $SU(3)$ in the QCD case), β the inverse gauge coupling, $S_G(U)$ the pure gauge action and $\Delta(U, m, \mu)$ the lattice Dirac operator at fermion mass m and chemical potential μ.

There are several physically interesting cases in which the determinant of the Dirac operator $\Delta(U)$ for a generic gauge configuration U is either not positive-definite (gauge theories with Wilson fermions) or even a complex number (QCD at finite density). In all these cases, standard simulation algorithms based on the interpretation of the fermion determinant as a probability distribution function $(p.d.f.)$ to be multiplied by the pure gauge probability distribution $e^{-\beta S_G(U)}$ fail. The standard way to overcome this problem is to take the absolute value of the fermion determinant in the $p.d.f.$ of the path integral. The integration measure becomes

$$[dU] e^{-\beta S_G(U)} \left| \det \Delta(U, m, \mu) \right|. \tag{2}$$

The vacuum expectation value of any operator $O(U)$ with the previous prescription now becomes

$$\langle O(U) \rangle = \frac{\langle O(U) e^{i\phi_\Delta} \rangle_{||}}{\langle e^{i\phi_\Delta} \rangle_{||}} \tag{3}$$

where $\phi_\Delta(U, m, \mu)$ is the phase of the determinant of the Dirac operator and $\langle \ \rangle_{||}$ in (3) represents the mean value computed with the $p.d.f.$ (2).

In QCD at finite chemical potential and due to the symmetries of the action, the numerator and denominator of (3) are real numbers. However simulations of this model show that the real part of the denominator of (3) in the physically interesting region of the chemical potential becomes extremely small and impossible to measure numerically [3]. As I will show, this kind of measurements are not necessary since in the thermodynamic limit we get the following factorization:

$$\langle O(U) e^{i\phi_\Delta} \rangle_{||} = \langle O(U) \rangle_{||} \langle e^{i\phi_\Delta} \rangle_{||} \tag{4}$$

for any intensive operator $O(U)$. Equation (4) implies that by taking the absolute value prescription in the integration measure instead of the fermion determinant we get the correct thermodynamical limit, i.e.

$$\lim_{V\to\infty} \langle O(U) \rangle = \langle O(U) \rangle_{||}. \tag{5}$$

To show the correctness of equation (5) let me consider the partition function (1) and write it as

$$Z = \langle e^{i\phi_\Delta} \rangle_{||} \int [dU] e^{-\beta S_G(U)} \left| \det \Delta(U, m, \mu) \right|. \tag{6}$$

The vacuum expectation value of any thermodynamical quantity, the chiral condensate for instance, can be written as

$$\langle \bar{\psi}\psi \rangle = \lim_{V\to\infty} \frac{1}{V} Z^{-1} \frac{\partial Z}{\partial m}$$

$$= \lim_{V\to\infty} \frac{1}{V} \left(Z_{||}^{-1} \frac{\partial Z_{||}}{\partial m} + \langle e^{i\phi_\Delta} \rangle_{||}^{-1} \frac{\partial \langle e^{i\phi_\Delta} \rangle_{||}}{\partial m} \right) \tag{7}$$

with

$$Z_{||} = \int [dU] e^{-\beta S_G(U)} \left| \det \Delta(U, m, \mu) \right|. \tag{8}$$

Since $\langle e^{i\phi_\Delta} \rangle_{||}$ is a bounded function of the system's parameters for every lattice volume, it takes a finite value in the infinite volume limit. Therefore the second contribution to the expectation value of equation (7) will vanish in the thermodynamical limit except, at most, in some isolated points. It gives only non-vanishing values at finite volume. These are pure finite size effects but they can significantly distort the results on finite lattices in regions of the parameters where this term could be large [3].

These results apply for any thermodynamical quantity. The general rule is therefore to take $Z_{||}(\beta, m, \mu)$ as the generating partition function, the logarithmic derivatives of which will give us the right vacuum expectation values. Notice also that the practical rule of taking the absolute value of the fermion determinant works also for any intensive operator, like correlation functions, which can be obtained as a derivative of the partition function with external sources.

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3. The Quenched QCD Puzzle

The results of the preceding section tell us that the fermionic contribution to the integration measure of QCD at finite chemical potential can be written as $(\det \Delta \det \Delta^+)^{1/2}$, i.e. QCD with n dynamical flavours is a theory with $\frac{n}{2}$ quarks with original action and $\frac{n}{2}$ quarks with conjugate action [5]. The zero flavour limit of this model is however standard quenched QCD. I will show here, with the help of the fermion effective action formalism [7], that quenched QCD at small but finite chemical potential actually breaks dynamically chiral symmetry. Furthermore the chiral transition at finite μ is second order in the quenched model, a fact that is most likely to be a pathology of the quenched approximation and which will be removed with the inclusion of dynamical fermions. The very large fluctuations observed in quenched simulations [6] should be a manifestation of the second-order character of the phase transition. If the inclusion of dynamical fermions makes the phase transition of first order, as expected, fluctuations will decrease due to a strong selection in the relevant configuration sample caused by the inclusion of the fermion determinant in the integration measure.

The effective fermion action formalism is based on the definition of an effective fermion action, which depends on the gauge energy density E, bare fermion mass m and chemical potential μ. This can be done by including in expression (8) a δ function $\delta(\frac{1}{6V}S_G - E)$ and a integral over the gauge energy density E [7]. This allows us to write the partition function (8) as a one-dimensional integral:

$$Z = \int dE N(E) e^{-6\beta V E} \langle |\det \Delta(U, m, \mu)| \rangle_E. \tag{9}$$

$N(E)$ is the density of states of fixed energy E and $\langle \rangle_E$ the mean value computed over gauge configurations of fixed energy density E. The normalized fermion effective action $S_{eff}^F(E, m, \mu)$ is then defined as

$$S_{eff}^F(E, m, \mu) = -\frac{1}{V} \log \langle |\det \Delta(U, m, \mu)| \rangle_E. \tag{10}$$

The thermodynamics of this system can be solved in the infinite volume limit by the saddle point technique. The chiral condensate $\langle \bar{\psi}\psi \rangle$ and number density $\langle J_0 \rangle$ will be respectively given by

$$\langle \bar{\psi}\psi \rangle = -\frac{\partial S_{eff}^F}{\partial m} \qquad \langle J_0 \rangle = -\frac{\partial S_{eff}^F}{\partial \mu}, \tag{11}$$

both expressions evaluated at the energy $E(\beta, m, \mu)$ which satisfies the saddle point equation. In the quenched approximation the fermion effective action

does not appear in the integration measure. The saddle point solution for the plaquette energy E depends only on the inverse gauge coupling β in this approximation; therefore, it does not change by changing the fermion mass m or the chemical potential μ. The fact that also in the quenched approximation the chiral condensate and number density are finite numbers for any value of the gauge coupling β tells us that the fermion effective action must be a continuous function of m and μ for every value of E and with finite first derivatives. Simple mathematics shows that also $\frac{\partial S_{eff}^F}{\partial m}$ and $\frac{\partial S_{eff}^F}{\partial \mu}$ will then be continuous functions of μ and m, respectively. Taking now into account that $\frac{\partial S_{eff}^F}{\partial m}$ is the chiral condensate and that by changing μ the energy E does not change in the quenched approximation, we get as a result that the chiral condensate is a continuous function of μ for every value of m in this approximation. Since chiral symmetry is dynamically broken at $\mu = 0$ it must be broken also at small μ. Even more, the chiral transition at finite μ must be continuous. The only way to get a discontinuous transition is to have a two-minimum structure in the full effective action (9). The compact $U(1)$ model has a first order chiral transition in the quenched approximation, since the pure gauge action has a two-minimum structure. Since the pure gauge $SU(3)$ model has no first order transitions at zero temperature, only the inclusion of dynamical fermions can produce such a structure in the full effective action. In such a case and for some selected values of the model parameters, the plaquette energy, which verifies the saddle point equation, will jump between two different values as well as the other thermodynamical quantities.

4. Summary

I have shown here how the difficulty in applying standard simulation algorithms to QCD at finite density, due to the complex nature of the fermion determinant, can be easily surmounted by taking the absolute value in the integration measure. This prescription not only gives the properly behaved thermodynamical limit but also has the advantage to kill unwanted finite size effects. I have also shown that the solution to the quenched QCD puzzle is on the line pointed out in [6], i.e. chiral symmetry is spontaneously broken at small μ. The only pathology of the quenched approximation, which is most likely to change with the inclusion of dynamical fermions, is the continuous character of the chiral transition; this allows us to understand the large fluctuations observed in quenched simulations.

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