Rigorous arguments against current wisdoms in finite density QCD

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ABSTRACT

QCD at finite chemical potential is analytically investigated in the region of large bare fermion masses. We show that, contrary to the general wisdom, the phase of the fermion determinant is irrelevant at zero temperature. However if the system is put at finite temperature, the contribution of the phase is finite. We also discuss on the quenched approximation and suggest that the origin of the failure of this approximation in finite density QCD could relay on the fundamental role that Pauli exclusion principle plays in this case.
Numerical simulations of QCD at finite chemical potential $\mu$ are plagued by technical difficulties which, as well known, have delayed progress in this field. The non positivity of the determinant of the Dirac operator, together with indications coming from random matrix models, suggests that the phase of the determinant can not be neglected in the thermodynamical limit of the model. The present situation is therefore rather pessimistic; it seems that there is no reliable hope to get important improvements in the knowledge of QCD at finite density from first principles.

Having in mind these limitations, our aim here is to improve our knowledge of this field by analyzing QCD at finite $\mu$ in a limiting case which, even if far from the continuum limit of the model, allows one to do analytical manipulations forbidden in full QCD. The hope is that what is learned here can be of interest for the progress in this subject.

We are going to take the large bare fermion mass limit; the main simplification that follows is that all the temporal chains in the determinant of the Dirac operator decouple and the determinant can be written as a product of $V_s$ chains for every gauge configuration, $V_s$ being the number of space-like lattice points.

We analyze QCD in this limit and will derive its phase diagram. We will show that, at $T = 0$, the phase of the fermion determinant in the infinite volume limit does not contribute to the free energy, a result against the general wisdom. The contrary happens at finite temperature. Lastly, we show that, even at $T = 0$, the Grand Canonical Partition Function approach leads to numerically uncorrect results, not being able to reproduce the exact
analytical features.

1 Analytic results

The Dirac-Kogut-Susskind operator of QCD at finite chemical potential can be written as

\[ 2\Delta = 2mI + e^{\mu}G + e^{-\mu}G^\dagger + V \]  

where \( G (G^+) \) contains all forward (backward) temporal links and \( V \) all space-like links.

The determinant of \( \Delta \) in the integration measure can be replaced, at large fermion masses \( m \), by

\[ \det \Delta = m^{3V_s L_t} \det \left(I + \frac{e^{\mu}}{2m}G\right) \]  

If the fugacity \( e^{\mu} \) is much smaller than \( 2m \), the second factor of (2) can be replaced by 1 and the theory is independent of the chemical potential. Therefore, in order to get a non trivial \( \mu \) dependence, we need to go to a region of large chemical potential in which the fugacity is of the order of \( 2m \).

Since all space-like links have disappeared in equation (2), the determinant of \( \Delta \) factorizes as a product of \( V_s \) determinants for the single temporal chains. A straightforward calculation allow us to write

\[ \det \Delta = e^{3V_s L_t \mu} \prod_{i=1}^{V_s} \det(c + L_i) \]
with \( c = (\frac{2m}{e\mu})^{Lt} \), \( L_t \) is the lattice temporal extent and \( L_i \) the SU(3) variable representing the forward straight Polyakov loop starting from the spatial site \( i \) and circling once the lattice in the temporal direction. The determinants in (3) are gauge invariant quantities which can therefore be written as functions of the trace and the determinant of \( L_i \). Since the gauge group is a unitary group, \( \det(L_i) = 1 \) and therefore the only contributions depending on the gauge configuration will be functions of \( Tr(L_i) \). In fact simple algebra allows to write

\[
\det(c + L_i) = c^3 + c^2 Tr(L_i) + c Tr(L_i^*) + 1 \tag{4}
\]

In the infinite gauge coupling limit, the integration over the gauge group is trivial since we get factorization \[2\]. The final result for the partition function at \( \beta = 0 \) is

\[
Z = V_G e^{3V_s (2m/e\mu)^{3L_t} + 1} \tag{5}
\]

where \( V_G \) is a constant irrelevant factor diverging exponentially with the lattice volume which accounts for the gauge group volume. Equation (5) gives for the free energy density \( f = \frac{1}{3V_s L_t} \log Z \)

\[
f = \mu + \frac{1}{3L_t} \log \left( (\frac{2m}{e\mu})^{3L_t} + 1 \right) \tag{6}
\]

The first contribution in (6) is an analytical function of \( \mu \). The second contribution has, in the limit of infinite temporal lattice extent, a non analyticity at \( \mu_c = \log(2m) \) which induces in the number density a step jump,
indication of a saturation transition of first order at the value of $\mu_c$ previously given.

This is an expected result on physical grounds. In fact in the infinite fermion mass limit baryons are point-like particles, and pion exchange interaction vanishes, since pions are also very heavy. Therefore we are dealing with a system of very heavy free fermions (baryons) and by increasing the baryon density in such a system we expect an onset at $\mu_c = \frac{1}{3} m_b$, i.e., $\mu_c = \log(2m)$ since $3 \log(2m)$ is the baryon mass at $\beta = 0$ for large $m$ \[3\].

Let us now discuss the relevance of the phase of the fermion determinant at $\beta = 0$. The standard wisdom based on random matrix model results is that the phase of the fermion determinant plays a fundamental role in the thermodynamics of QCD at finite baryon density \[4\] and that if the theory is simulated by replacing the determinant by its absolute value, one neglects a contribution to the free energy density which could be fundamental in order to understand the critical behavior of this model. We are going to show now that, contrary to this wisdom, the phase of the determinant can be neglected in the large $m$ limit at $T = 0$.

Equations (3) and (4) imply that an upper bound for the absolute value of the fermion determinant is given by the determinant of the free gauge configuration. Therefore the mean value of the phase factor in the theory defined taking the absolute value of the determinant

$$\langle e^{i\phi} \rangle \parallel = \frac{\int [dU] e^{-\beta S_G(U)} \det \Delta}{\int [dU] e^{-\beta S_G(U)} |\det \Delta|}$$

(7)

is, at $\beta = 0$, bounded from below by the ratio
At zero temperature \((L_t = L, V_s = L^3)\), and letting \(L \to \infty\), it is straightforward to verify that the ratio (8) goes to 1 except at \(\mu_c = \log(2m)\) (at \(\mu = \mu_c\) the ratio goes to zero but it is bounded from below by \((1/4)^{V_s}\)). Therefore the mean value of the cosine of the phase in the theory where the fermion determinant is replaced by its absolute value gives zero contribution.

At \(T \neq 0\), i.e. taking the infinite \(V_s\) limit by keeping fixed \(L_t\), the lower bound (8) for the mean value of the phase factor (7) goes to zero exponentially with the spatial lattice volume \(V_s\). This suggests that the phase will contribute in finite temperature \(QCD\). In fact, it is easy to convince oneself that expression (7), at \(\beta = 0\), vanishes also exponentially with the lattice spatial volume at finite temperature (see fig. 1). The contribution of the phase is therefore non zero (in the limit considered here) in simulations of \(QCD\) at finite temperature.

The free energy density at finite temperature (equation (6)) is an analytic function of the fermion mass and chemical potential. It develops a singularity only in the limit of zero temperature \((T = \frac{1}{t_t})\). Therefore \(QCD\) at large \(m\) and finite temperature does not show phase transition in the chemical potential but a crossover at \(\mu = \log(2m)\) which becomes a true first order phase transition at \(T = 0\).

The standard way to define the theory at zero temperature is to consider symmetric lattices. However a more natural way to define the theory at
\( T = 0 \) is to take the limit of finite temperature QCD when the physical temperature \( T \to 0 \). In other words, we should take first the infinite spatial volume limit and then the infinite temporal extent limit. We will show here that, as expected, physical results are independent of the procedure chosen.

The free energy density of the model can be written as the sum of two contributions \( f = f_1 + f_2 \). The first contribution \( f_1 \) is the free energy density of the theory where the fermion determinant in the integration measure is replaced by its absolute value. The second contribution \( f_2 \), which comes from the phase of the fermion determinant, can be written as

\[
f_2 = \frac{1}{V_s L_t} \log \left\langle e^{i\phi} \right\rangle. \tag{9}\]

Since the mean value of the phase factor (7) is less or equal than 1, \( f_2 \) is bounded from above by zero and from below by

\[
\frac{1}{L_t} \log \left( \left( \frac{2m}{e^\mu} \right)^{3L_t} + 1 \right) \tag{10}\]

When \( L_t \) goes to infinity, expression (10) goes to zero for all the values of \( \mu \) and therefore the only contribution to the free energy density which survives in the zero temperature limit is \( f_1 \). Again, we conclude that zero temperature QCD in the strong coupling limit at finite chemical potential and for large fermion masses is well described by the theory obtained by replacing the fermion determinant by its absolute value.

These results are not surprising as follows from the fact that at \( \beta = 0 \) and for large \( m \) the system factorizes as a product of \( V_s \) noninteracting \( 0+1 \)
dimensional QCD’s and from the relevance (irrelevance) of the phase of the fermion determinant in 0 + 1 QCD at finite (zero) “temperature” \([5]\). More surprising maybe is that, as we will see in the following, some of these results do not change when we put a finite gauge coupling.

The inclusion of a non trivial pure gauge Boltzmann factor in the integration measure of the partition function breaks the factorization property. The effect of a finite gauge coupling is to induce correlations between the different temporal chains of the determinant of the Dirac operator. The partition function is given by

\[
Z = \int [dU] e^{-\beta S_G(U)} \prod_{i=1}^{V_s} (c^3 + 1 + c \text{Tr}(L_i^+ + c^2 \text{Tr}(L_i)))
\]

and can be written as

\[
Z(\beta, \mu) = Z_{pg} \cdot Z(\beta = 0, \mu) \cdot R(\beta, \mu)
\]

where \(Z_{pg}\) is the pure gauge partition function, \(Z(\beta = 0, \mu)\) the strong coupling partition function (equation (5)) and \(R(\beta, \mu)\) is given by

\[
R(\beta, \mu) = \frac{\int [dU] e^{-\beta S_G(U)} \prod_{i=1}^{V_s} \left(1 + \frac{c \text{Tr}(L_i) + c^2 \text{Tr}(L_i^+)}{c^3 + 1}\right)}{\int [dU] e^{-\beta S_G(U)}}
\]

In the zero temperature limit (\(L_t = L, L_s = L^3, L \rightarrow \infty\)) the productory in the numerator of (13) goes to 1 independently of the gauge configuration. In fact each single factor has an absolute value equal to 1 up to corrections which vanish exponentially with the lattice size \(L\) and a phase which vanishes also exponentially with \(L\). Since the total number of factors is \(L^3\), the
productory goes to 1 and therefore $R = 1$ in the zero temperature limit.

The contribution of $R$ to the free energy density vanishes therefore in the infinite volume limit at zero temperature. In such a case, the free energy density is the sum of the free energy density of the pure gauge $SU(3)$ theory plus the free energy density of the model at $\beta = 0$ (equation (6)). The first order phase transition found at $\beta = 0$ is also present at any $\beta$ and its location and properties do not depend on $\beta$ since all $\beta$ dependence in the partition function factorizes in the pure gauge contribution. Again at finite gauge coupling the phase of the fermion determinant is irrelevant at zero temperature.

At finite temperature and finite gauge coupling the first order phase transition induced by the contribution (6) to the free energy density at zero temperature disappears and becomes a crossover. Furthermore expression (13) gives also a non vanishing contribution to the free energy density if $L_t$ is finite.

The common physical interpretation for the theory with the absolute value of the fermion determinant is that it possesses quarks in the $3$ and $3^*$ representations of $SU(3)$, having baryonic states made up of two quarks which would give account for the physical differences respect to real QCD. We have proven analytically (at $\beta = 0$) that the relation between modulus and real QCD is temperature dependent, i.e. they are different only at $T \neq 0$, a feature that does not support the above interpretation.
2 Numerical results

From the point of view of simulations, work has been done by several groups mainly to develop numerical algorithms capable to overcome the non positivity of the fermionic determinant. The most promising of these algorithms [6], [7] are based on the GCPF formalism and try to calculate extensive quantities (the canonical partition functions at fixed baryon number). Usually they measure quantities that, with actual statistics, do not converge.

In a previous paper [8] we have given arguments to conclude that, if the phase is relevant, a statistics exponentially increasing with the system volume is necessary to appreciate its contribution to the observables (see also [9]).

What happens if we consider a case where the phase is not relevant (i.e. the large mass limit of QCD at zero temperature, as discussed in the previous section)?

To answer this question we have reformulated the GCPF formalism by writing the partition function as a polynomial in $c$ and studied the convergence properties of the coefficients at $\beta = 0$ using an ensemble of (several thousands) random configurations. This has been done as in standard numerical simulations (i.e. without using the factorization property) for lattices $4^4$ (fig. 2a), $4^3 \times 20$ (fig. 2b), $10^3 \times 4$ (fig. 2c) [2] and the results compared with the analytical predictions [3] (solid lines in the figures).

From these plots we can see that, unless we consider a large lattice temporal extension, our averaged coefficients in the infinite coupling limit still suffer from sign ambiguities i.e. not all of them are positive. For large $L_t$ the sign
problem tends to disappear because the determinant of the one dimensional system (4) becomes an almost real quantity for each gauge configuration and obviously the same happens to the determinant of the Dirac operator (3) in the four dimensional lattice. It is also interesting to note that the sign of the averaged coefficients is very stable and a different set of random configurations produces almost the same shape.

However, the sign of the determinant is not the only problem: in fact, as one can read from fig. 2, even considering the modulus of the averaged coefficients we do not get the correct result. We used the same configurations to calculate the average of the modulus of the coefficients. We expect this quantity to be larger than the analytic results reported in fig. 2. The data, however, contrast with this scenario: the averages of the modulus are always smaller (on a logarithmic scale) than the analytic results from formula (5). In fact these averages are indistinguishable from the absolute values of the numerical results reported in fig. 2.

In conclusion, even if the phase of the fermion determinant is irrelevant in QCD at finite density (T = 0 and heavy quarks) the numerical evaluation of the Grand Canonical Partition Function still suffers from sampling problems.

A last interesting feature which can be discussed on the light of our results concerns the validity of the quenched approximation in finite density QCD. An important amount of experience in this field [10] suggests that contrary to what happens in QCD at finite and zero temperature, the quenched approximation does not give correct results in QCD at finite chemical potential. Even if the zero flavour limit of the theory with the absolute value of the
fermion determinant and of actual QCD are the same (quenched approximation), the failure of this approximation has been assigned in the past [4] to the fact that it corresponds to the zero flavour limit of the theory with $n$ quarks in the fundamental and $n$ quarks in the complex representation of the gauge group. In fig. 3 we have plotted the number density at $\beta = 0$ and for heavy quarks in three interesting cases: actual QCD, the theory with the absolute value of the fermion determinant and quenched QCD. It is obvious that the quenched approximation produces results far from those of actual QCD but also far from those of QCD with the modulus of the determinant of the Dirac operator. The former results are furthermore very near to those of actual QCD. In other words, even if the phase is relevant at finite temperature, its contribution to the number density is almost negligible.

It seems unplausible on the light of these results to assign the failure of the quenched approximation to the feature previously discussed [4]. It seems more natural to speculate that it fails because does not incorporate correctly in the path integral the Fermi-Dirac statistics and we do expect that Pauli exclusion principle play, by far, a more relevant role in finite density QCD than in finite temperature QCD.

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References
[1] T. Blum, J.E. Hetrick and D. Toussaint, Phys. Rev. Lett. 76 (1996) 1019.

[2] R. Aloisio, V. Azcoiti, G. Di Carlo, A. Galante and A.F. Grillo, hep-lat 9809186, to appear in the proceedings of the Conference "Lattice 98", Denver July 1998.

[3] H. Kluberg-Stern, A. Morel and B. Peterson, Nucl. Phys. B215 [FS7] (1983) 527.

[4] M.A. Stephanov, Phys. Rev. Lett. 76 (1996) 4472.

[5] R. Aloisio, V. Azcoiti, G. Di Carlo, A. Galante and A.F. Grillo, Nucl. Phys. (Proc. Suppl.) 63 (1998) 442.

[6] I.M. Barbour, S.E. Morrison, E.G. Klepfish, J.B. Kogut, M.P. Lombardo, Phys. Rev D56 (1997) 7063.

[7] R. Aloisio, V. Azcoiti, G. Di Carlo, A. Galante, A.F. Grillo, Phys. Lett. B428 (1998) 166.

[8] R. Aloisio, V. Azcoiti, G. Di Carlo, A. Galante, A.F. Grillo, Phys. Lett. B435 (1998) 175.

[9] I.M. Barbour, to appear in the proceedings of the conference “QCD at finite baryon density”, Bielefeld, April 1998.

[10] J.B. Kogut, M.P. Lombardo, D.K. Sinclair, Phys. Rev. D51 (1995) 1282, Phys. Rev. D54 (1996) 2303.
Figure 1: Inverse temperature in lattice units times the contribution to the free energy density coming from the phase. This quantity is evaluated in the strong coupling limit and plotted as a function of $c^{-1}$; it is invariant under the transformation $c \to c^{-1}$. 


Figure 2: Logarithm of the modulus of the GCPF coefficients times the sign of the coefficients. $V = 4^4 \times 4$ (a), $4^3 \times 20$ (b), $10^3 \times 4$ (c); the uppermost continuous curve are the analytic results.
Figure 3: Baryonic density $n$ as a function of $c^{-1}$ for the complete theory (continuous line), the theory defined using the modulus (dashed line) and the quenched theory (dotted-dashed line). All the results reported in this figure have been obtained analytically (we can use the relation $n(c) = 1 - n(1/c)$ to reconstruct the whole curves).