

Frustration in Finite Density QCD

R. Aloisio^{a,d}, V. Azcoiti^b, G. Di Carlo^c, A. Galante^{a,c} and A.F. Grillo^d

^a *Dipartimento di Fisica dell'Università dell'Aquila, L'Aquila 67100 (Italy).*

^b *Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza (Spain).*

^c *Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, P.O.B. 13 - Frascati 00044 (Italy).*

^d *Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali del Gran Sasso, Assergi (L'Aquila) 67010 (Italy).*

ABSTRACT

We present a detailed analysis of the QCD partition function in the Grand Canonical formalism. Using the fugacity expansion we find evidence for numerical instabilities in the standard evaluation of its coefficients. We discuss the origin of this problem and propose an issue to it. The correct analysis shows no evidence for a discontinuity in the baryonic density in the strong coupling limit. The moderate optimism that was inspired by the Grand Canonical Partition Function calculations in the last years has to be considered ill-founded.

Non perturbative investigations of finite density QCD have received a growing attention in the last years. Concerning the most powerful non perturbative approach, numerical simulations on a lattice, there is some evidence that the long standing problem of dealing with a complex valued determinant can be overcome using non standard numerical approaches based on the calculation of the Grand Canonical Partition Function (GCPF). This technique has attracted much attention since, once evaluated the coefficients in the fugacity expansion, it allows free mobility in the chemical potential μ at negligible computer cost.

The strong coupling limit is by far the most investigated since it is possible to check numerical results with analytical predictions [1] and monomer-dimer simulations [2]. Using the Glasgow algorithm evidence for a first order phase transition at a value of the chemical potential in good agreement with the old results of the monomer-dimer simulations was found [3].

In a previous paper [4] we have performed simulations with a Microcanonical Fermion Average (MFA) [5] inspired method, using the modulus of the fermionic determinant to define a real and positive definite effective action. Concerning the baryon density, we have found essential agreement with the results of [3]. In that work we have completely diagonalized the propagator matrix P [6] and the eigenvalues have been used to calculate the coefficients of the fugacity expansion through a standard recursion method. We found evidence for a first order phase transition at zero and non zero masses up to $m \sim 0.7$ and vanishing of such a signal for larger masses. The critical chemical potential μ_c was in good agreement with the one of Karsch and Mütter [2] for small and intermediate masses. The lacking of the transition at larger masses is, on physical grounds, an unexpected result, previously reported also in [3].

In addition to the diagonalization of the quark propagator matrix, we also performed in [4] a direct diagonalization of the Dirac operator (Δ) in a 4^4 lattice. At large values of m the results were in contradiction. The latter method allowed a clear determination of a first order transition with a critical chemical potential μ in agreement with an extrapolation of the data of [2] and with quenched simulations [7], whereas the former approach, based on the calculation of the coefficients in the fugacity expansion, did not produce any signal of first order transition.

These contradictory results point to the existence of numerical problems in the evaluation of thermodynamical quantities. Three are the possible sources for numerical troubles: i) the evaluation of the eigenvalues of the fermion matrix (Δ), ii) the diagonalization of the propagator matrix (P) and

iii) the determination of the fugacity expansion coefficients.

We used a standard NAG library routine to perform the diagonalization of Δ and P . At $\mu = 0$, we found a perfect agreement between the Δ eigenvalues computed with this routine with the ones obtained using a standard Lanczos algorithm. Using the two sets of eigenvalues, we have also verified the relation [6]

$$\left(\frac{1}{2}\right)^{3V} e^{3V\mu} \det(P - e^{-\mu}) = \det \Delta. \quad (1)$$

in the whole range considered for the chemical potential μ and quark mass m . We conclude that the diagonalization procedure is stable for any value of the mass and the chemical potential and that the numerical problems can only be due to the manipulations necessary to go from the P eigenvalues to the Grand Canonical expansion coefficients a_n

$$e^{3V\mu} \det(P - e^{-\mu}) = \sum_{n=-3V_s}^{3V_s} a_n e^{-n\mu}. \quad (2)$$

This conclusion was indeed corroborated by the numerical results at large fermion masses in 4^4 and $6^3 \times 4$ lattices. The numerical results in this region of masses, when computed from the eigenvalues of Δ or from the eigenvalues of P , without making use of the fugacity coefficients, are in perfect agreement and show a clear signal for a first order phase transition, as discussed below. This signal was absent in the numerical results obtained from the fugacity coefficients.

The single configuration analysis

Having localized the source of numerical troubles in the determination of the fugacity coefficients and in order to get some insight of these numerical difficulties, we will first focus on a single random configuration of a $6^3 \times 4$ lattice. A property of the effective action which can be used to check the numerical calculations of the Grand Canonical expansion coefficients is the parity under the transformation $\mu \rightarrow -\mu$ since, as well known, the real part of the determinant must be an even function of the chemical potential. In fig 1 we report the asymmetry $\log |Re(\det \Delta(\mu))| - \log |Re(\det \Delta(-\mu))|$ against the chemical potential μ at $m = 0.1$. This quantity has been computed using the left and right hand sides of expression (2) with a 128 bit arithmetic. It is evident that the coefficients do not respect the symmetry $a_{-n} = a_n^*$ while the determinant, directly evaluated through (1), behaves as expected. These results hold in the chiral limit as well as for masses up to 1.5.

Again this analysis suggests the existence of perverse effects in the code used to determine the fugacity coefficients. Therefore it is important to realize how these problems origin and how can be overcome to get full advantage of the Grand Canonical formalism.

To this end, and inspired by the strong coupling results [2], we have analysed a simple case. In the strong coupling limit we expect a first order saturation transition in the number density $n(\mu)$ which can be approximated by a Heaviside θ function. To check our ideas we have considered a particular distribution of the P eigenvalues that reproduces the number density with the expected behaviour. In the infinite volume limit the radial distribution of the eigenvalues is related to the first derivative of the number density with respect to the chemical potential. To mimic a first order saturation transition separating a phase where $n(\mu) = 0$ for $\mu < \mu_c$ from another phase where $n(\mu) = 1$ for $\mu > \mu_c$ we have considered the eigenvalue distribution $\lambda_i^\pm = e^{\pm\mu_c} e^{\pm i\theta_i}$, where the phases θ_i are uniformly distributed in $(-\pi, \pi)$.

The a_n coefficients for this set of eigenvalues have been calculated with the same algorithm used for real data. This has been done either with input eigenvalues ordered respect to their phases or randomly ordered. In fig 2 we report the number density obtained in both cases. It is evident that the former case leads to wrong results while the latter reproduces the correct ones.

The origin of numerical instabilities in this model can be easily understood. If we consider $2N$ eigenvalues uniformly distributed on two circles of radius ρ and ρ^{-1} the polynomial in the fugacity contains only three non vanishing terms: $a_{\pm N} = 1$ and $a_0 = \rho^N + \rho^{-N}$. If we calculate the coefficients with the standard recursion method we use the first n eigenvalues to calculate the coefficients of a polynomial P_n of degree n :

$$a_k^n = a_{k-1}^{n-1} - \lambda_n a_k^{n-1} \quad k \geq 1 \quad (3)$$

where a_k^n is the coefficient of order k of P_n . If the eigenvalues are phase-ordered, at any intermediate step we calculate the coefficients of a polynomial whose zeros lay on an arc of circle of increasing length. These coefficients are non zero and of order $O(\rho^n)$. Once their logarithm is bigger than $q \log_{10} 2$, where q are the bits of the mantissa in the floating point representation number ($q = 113$ for 128 bits arithmetic), rounding propagation prevents to obtain the correct answer. This happens already for relatively small N and forbids the symmetries to be realized in the final results (see [8] for a similar effect in a different context). Randomly ordered eigenvalues modify this scenario since the symmetries are (almost) enforced at each intermediate

step as well as in the final result. The coefficients of P_n never grow too much and rounding effects are better under control.

We have noticed that, for real simulations, the output of our diagonalization routine has part of the eigenvalues with almost ordered phases. If we shuffle them before starting the computation of the coefficients, we recover the μ , $-\mu$ symmetry for each gauge configuration and the results are indistinguishable from the ones obtained computing the determinant of the quark propagator matrix without making use of the coefficients. Therefore we expect that the anomalous behaviour observed in the naive Heaviside model is not peculiar of its (ad hoc) eigenvalue distribution but will remain valid also for the P eigenvalues of actual simulations. A good way to cure the perverse effects, induced by the rounding in the routine which computes the fugacity coefficients, is to shuffle the full set of eigenvalues before starting the computation of the coefficients.

Strong coupling results

We have reanalyzed our $\beta = 0$ data in $6^3 \times 4$ lattices with different methods. The coefficients have been evaluated using for each configuration a random ordering of its eigenvalues. In order to define a real and positive partition function we have considered the modulus of the fermionic determinant as in [4], or we set equal to zero the coefficients with negative real part [3] (Glasgow approach). The results for the number density have been checked computing the same quantity without the coefficients and are shown in figures 3 and 4.

Figure 3 contains the results for $m=1.5$, the value of the fermion mass at which contradictory results were found in [4]. The diamonds stand for the results obtained through the use of the fugacity coefficients computed in the standard way ($6^3 \times 4$ lattice), to be compared with the results obtained from the coefficients computed from the randomized set of eigenvalues (solid line, $6^3 \times 4$ lattice), and with the ones corresponding to a direct diagonalization of the Dirac matrix Δ (4^4 lattice). We see how, after introducing the randomization procedure in the computation of the fugacity coefficients, the contradiction reported in [4] disappears and the numerical results for the baryon density, showing a clear first order phase transition, are in good agreement with those reported in [2] and also with the quenched results [7]. We want to remark also that if we do not take the absolute value of the fermion determinant and compute the coefficients of the Grand Canonical Partition Function as in [3] but using the randomization procedure, we get results indistinguishable from the solid line in Fig. 3. These are encouraging

results since they solve a contradiction and agree with other reliable results and with physical expectations.

In figures 4-a and 4-b we plot the same quantity as in Fig. 3 but for $m = 0.1$. Fig. 4-a contains the results for the baryon density obtained using the logarithm of the absolute value of the fermion determinant as effective action [4], whereas in Fig. 4-b the analysis has been done without taking the absolute value of the fermion determinant and setting to zero all negative averaged coefficients in the fugacity expansion [3]. In both figures the diamonds stand for the results obtained from the fugacity coefficients computed with the standard procedure. The solid lines in Figs. 4-a, 4-b correspond to the number density obtained from the fugacity coefficients computed using the randomized procedure previously described. Computing the modulus of the determinant directly from the eigenvalues of the quark propagator matrix P (1), we obtain numerical results for the number density indistinguishable from the solid line in Fig. 4-a.

A very unpleasant consequence of the analysis reported in Fig. 4 is that the numerical data, if correctly analysed, show no evidence for a first order phase transition, contrary to what previously reported [3], [4] (diamonds in Figs 4-a, 4-b). The perverse effects detected in the standard computation of the fugacity coefficients are relevant not only at large values of the fermion masses but also at $m=0.1$ and in the chiral limit. Preliminary results in a $8^3 \times 4$ lattice at $m = 0$ confirm this scenario.

After we have removed all the possible numerical artifacts some comments are necessary to evidenciate the physical meaning of the results. The first observation concerns the distribution of the phase of the determinant. When we reach the onset μ and up to the saturation point it becomes (within the errors) indistinguishable from a flat distribution (in the $-\pi, \pi$ range). The same flat distribution is observed for all the coefficients except for the first, the last and the central one that are constrained to be real from the eigenvalues symmetries. With available statistics we have found no correlation between the phase and the modulus of the determinant. The consequence is that the averaged determinant is no longer a real and positive quantity as it should be. The same happens for each averaged coefficient whose sign is completely indeterminate. This can be easily checked splitting the configurations set in two or more subsets and calculating independent averages: the phases of different averages have again a flat distribution while the modulus converge reasonably well. We can conclude that the averaged determinant and coefficients have not converged and we can not rely on the results for finite density QCD. This can explain the discrepancies between the data

obtained from the Grand Canonical Partition Function and the Monomer-Dymer-Polymer algorithm [2].

A second comment is in order, to explain why the Glasgow approach [3] and the modulus of the determinant give the same results. To address this point it is important to note that the partition function of finite density $SU(3)$ can be written as [4]

$$\mathcal{Z} = \mathcal{Z}_{||} \langle e^{i\phi_\Delta} \rangle_{||} \quad (4)$$

where $\mathcal{Z}_{||}$ is defined using the modulus of the determinant, ϕ_Δ is the phase of the determinant and $\langle \rangle_{||}$ is the average defined using $|\det \Delta|$ as weight. The same formula is valid for the coefficients (that are partition function at fixed number density) once we substitute $\det \Delta$ with a_n and ϕ_{a_n} to ϕ_Δ . The difference between \mathcal{Z} and $\mathcal{Z}_{||}$ (or between $\langle a_n \rangle$ and $\langle |a_n| \rangle$) is significant only if the contribution of the phase is a quantity proportional to e^{-V} [4]. Such contribution (if present) can be appreciated only if we reduce the statistical error to $O(e^{-V})$ and to this aim we need a number of independent measurements of the order of the exponential of lattice volume. The data of phase distributions suggest that this is the scenario for finite density QCD. Without $O(e^V)$ configurations the results will never be significantly different from the ones obtained using the modulus of the determinant. A recent simulation of a 2^4 lattice in the strong coupling limit shows clearly how $O(10^6)$ configurations are needed to reproduce the expected mean field results [9]. We can use the Glasgow approach or whatever else but the result will never be different from $\mathcal{Z}_{||}$ with reasonable statistics on larger lattices.

This can also clarify the behaviour of the onset μ observed using the GCPF formalism: it goes to zero when $m \rightarrow 0$ in a way that seems to be consistent with one half the pion mass [3], [4]. This is what we expect from the theory defined through the modulus of the determinant where baryons of vanishing mass should be present in the chiral limit [10].

The main conclusion which follows from this work is rather pessimistic and frustrating. Neither the Glasgow method [3] nor our absolute value of the fermion determinant based approach [4] are able to reproduce the reliable results of Karsch and Mütter in the strong coupling limit [2]. The moderate optimism that was inspired by the Grand Canonical Partition Function calculations in the last years has to be considered ill-founded.

Preliminary analysis at larger values of β give indications that the infinite gauge coupling limit is the worst situation. In fact many of the coefficients in the fugacity expansion, which are negative with finite statistics at $\beta = 0$, become positive at larger values of β , as they should be. There is still some

hope that these approaches work better in the physically interesting region of larger β and it is therefore worthwhile to check if this is the case.

This work has been partly supported through a CICYT (Spain) - INFN (Italy) collaboration.

References

- [1] I.M. Barbour, N.E. Behilil, E. Dagotto, F. Karsch, A. Moreo, M. Stone, H.W. Wyld, Nucl. Phys. **B275** (1986) 296.
- [2] F. Karsch, K.H. Mütter, Nucl. Phys. **B313** (1989) 541.
- [3] I.M. Barbour, S.E. Morrison, E.G. Klepfish, J.B. Kogut, M.P. Lombardo, Phys. Rev **D56** (1997) 7063.
- [4] R. Aloisio, V. Azcoiti, G. Di Carlo, A. Galante, A.F. Grillo, hep-lat **9802004** (1998).
- [5] V. Azcoiti, G. Di Carlo, A.F. Grillo, Phys. Rev. Lett. **65** (1990) 2239; V. Azcoiti, A. Cruz, G. Di Carlo, A.F. Grillo and A. Vladikas, Phys. Rev. **D43** (1991) 3487; V. Azcoiti, G. Di Carlo, L.A. Fernandez, A. Galante, A.F. Grillo, V. Laliena, X.Q. Luo, C.E. Piedrafita and A. Vladikas, Phys. Rev. **D48** (1993) 402; V. Azcoiti, G. Di Carlo, A. Galante, A.F. Grillo, V. Laliena, Phys. Rev. **D50** (1994) 6994.
- [6] P.E. Gibbs, Phys. Lett. **B172** (1986) 53.
- [7] J.B. Kogut, M.P. Lombardo, D.K. Sinclair, Phys. Rev. **D51** (1995) 1282.
- [8] M. Karliner, S.R. Sharpe, Y.F. Chang, Nucl. Phys. **B302** (1988) 204.
- [9] I.M. Barbour, to appear in the proceedings of the Conference "QCD at finite baryon density", Bielefeld April 1998.
- [10] C.T.H. Davies, E.G. Klepfish, Phys. Lett. **B256** (1991) 68.

Figure Captions

- Fig. 1: Difference between $\log|\Delta(\mu)|$ and $\log|\Delta(-\mu)|$ vs μ for a single gauge configuration obtained using the coefficients calculated in the standard way (a), and from the eigenvalues of the propagator matrix (b).
- Fig. 2: Number density in the naive Heaviside model computed with phase ordered eigenvalues (diamonds) and with shuffled ones (solid line).
- Fig. 3: Number density in a $6^3 \times 4$ lattice at $\beta = 0$ and $m = 1.5$ obtained using the coefficients calculated in the standard way (diamonds) and with the shuffled eigenvalues (solid line); the same quantity for a 4^4 lattice, computed from the eigenvalues of Δ (squares).
- Fig. 4: Number density in a $6^3 \times 4$ lattice at $\beta = 0$ and $m = 0.1$ obtained using the coefficients computed in the standard way (diamonds) and with the shuffled eigenvalues (solid line); fermionic effective action as in the Glasgow method (a) and from the modulus of the fermion determinant (b).