Three and Two Colours Finite Density QCD at Strong Coupling: 
A New Look

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ABSTRACT

Simulations in finite density, $\beta = 0$ lattice QCD by means of the Monomer-Dimer-Polymer algorithm show a signal of first order transition at finite temporal size. This behaviour agrees with predictions of the mean field approximation, but is difficult to reconcile with infinite mass analytical solution. The MDP simulations are considered in detail and severe convergence problems are found for the SU(3) gauge group, in a wide region of chemical potential. Simulations of SU(2) model show discrepancies with MDP results as well.
The present scenario of finite density QCD is quite disappointing. Ideas concerning new phases of SU($N$) gauge theories at high density have been recently proposed and tested using phenomenological models, but a direct (theoretical) confirmation is, at present, still lacking. In the last fifteen years several first principle calculations of finite density QCD have been tried. The well-known sign problem in these simulations has prevented in most cases any success and, until now, no solution is at sight.

The only exceptions in this scenario are the Monomer-Dimer-Polymer (MDP) simulations. Even if the main limitation of this algorithm is that it is effective uniquely in the strong coupling limit, it has been able to provide reasonable results in the case of SU(3) gauge group, in the sense that they are not affected from early onset and are in qualitative agreement with mean field calculations. For these reasons they are considered a non trivial test for any newly proposed algorithms in finite density QCD.

More recently, $\beta = 0$ QCD has been exactly solved in the limit of infinite mass and chemical potential. In this limit unexpected results have been obtained concerning the relevance of the phase as well as the role of quenched approximation.

In the next section we are mainly concerned in discussing the compatibility of MDP results with the infinite mass solution for SU(3). Indeed we have found difficult to reconcile the numerical and analytical predictions. This led us to reconsider the MDP algorithm more carefully, and we found evidences of severe convergence problems in a wide region of chemical potential.

Lastly we considered the SU(2) case where simulations are not affected by the sign problem. Results using the Grand Canonical Partition Function formalism turn out to be in very good agreement with Hybrid Montecarlo calculations while, once again, MDP results are inaccurate in the critical region.

We conclude that, in both cases, the MDP algorithm is unable to reproduce correctly the physics in the more interesting region of chemical potential.

1 SU(3) at infinite coupling

The analytical results available for SU(3) are essentially the mean field predictions and the exact computation of QCD partition function in the infinite mass limit. While the former predicts a first order saturation transition at a value of $\mu$ smaller than 1/3 of the baryon mass the latter shows
a richer scenario. Let us recall the main features of infinite mass $QCD$ [3]:

i) at zero temperature ($L_t \to \infty$) the system undergoes a first order saturation transition. In this case the phase of the Dirac determinant is not relevant (simulations using the modulus of the determinant are exact in the thermodynamic limit);

ii) at non zero temperature the phase is relevant but its contribution to the free energy density is small (simulations using the modulus of the determinant are almost exact);

iii) the quenched approximation is very bad, failing to reproduce not only quantitatively but also qualitatively the true results. It is a much worse approximation than modulus $QCD$.

Even if the infinite mass model can not provide physical insights for the most interesting cases we may still use it as a test for numerical algorithms in the strong coupling and large mass regime. In a previous paper we used the (analytically calculable) canonical partition functions to check the Gran Canonical Partition Function simulations for various lattice sizes [3]. We saw that overlap problems are present and, as expected, they are more and more severe for larger lattices. Here we want to use the infinite mass model as a check for the MDP approach [2], up to now the only algorithm that has been able to handle the sign problem of finite density calculations and has provided results in very good qualitative agreement with mean field predictions. Even if the applicability of the MDP algorithm is restricted to the strong coupling regime the strong first order signal observed for $L_t = 4$ is the only evidence we have that the mean field approximation has been able to catch some relevant aspects of finite density physics.

The MDP results [2] are somehow puzzling if considered in the light of the infinite mass solution. In the original work Karsch and Mutter saw a strong first order transition for $L_t = 4$ (with spatial extent $L_s = 4$ and 8) and $0.1 < m < 0.7$ while for $m \to \infty$ [3] the number density is a smooth function of $\mu$ for any non vanishing lattice temperature. If we assume the MDP result for granted we have to conclude that, at finite $L_t$, the transition disappears at some large bare mass $\bar{m}$. This possibility seems very unnatural since it would imply the existence of a (large) physical scale where something dramatic should happen, changing completely the system behaviour and washing out the transition.
To solve this puzzle we have tried to use the MDP algorithm \cite{8} directly in the large mass regime in order to have data more easily comparable with the analytic predictions.

The authors of the MDP code noticed in their original paper that for small masses the algorithm becomes ineffective. When we tried to use the code for $m > 1.0$ we saw something similar: even if the acceptance rate in the Metropolis update was reasonable ($\approx 10\%$) in the low density phase, whatever large the value of $\mu$ the system never moved into the saturated phase.

The same degradation in performances has been observed for increasing lattice size. This is not surprising for an algorithm based on a global accept/reject step. What is more surprising is that the degradation seems to be related only to the value of $L_t$: simulations for lattices $8^3 \times 4$ are feasible but not for the smaller volume $4^3 \times 8$. We have not been able to simulate any $L_t > 4$ lattice. This behaviour indicates severe slowing down problems at least for some choices of the parameters.

The behaviour of MDP code prevented us from completing our original program. Any direct comparison of MDP at large masses (and various $L_t$) with the infinite mass model was impossible: a severe quantitative test for the algorithm could not be performed.

Given the impossibility to obtain MDP results for values of the parameters different from the ones used in the original paper, we have repeated the simulations with these same parameters, i.e. $m = 0.1$ and $V = 4^4$.

We used start configurations with zero density as well as saturated configurations and $O(10^6)$ Montecarlo steps for each value of $\mu$. The first observation was a very clear signal of hysteresis in the data: while runs with zero density start undergo a strong saturation transition at $\mu = 0.69$ (the published result), runs with saturated start jump into the zero density phase for $\mu = 0.58$ (fig. 1). This result casts some doubts on the determination of the critical point and may well reconcile the MDP results with mean field predictions (the mean field prediction for this mass, $\mu_{c,F} = 0.61$, lies inside the hysteresis region).

If this behaviour signals a first order transition the width of the region should shrink with increasing statistics, and one should observe a two peak structure in the probability distribution of the number density, i.e. observe several flip-flops in the Montecarlo history.

We considered runs of up to $O(10^9)$ accepted configurations (see fig. 2) for $\mu$ inside the hysteresys region, observing the following typical pattern. Starting from a zero density configuration $n(\mu)$ remains zero until $\mu \sim 0.69$. 

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At this point the system typically goes in the saturated phase. Once the system is in the saturated phase it never goes back. The same behaviour has been observed (near $\mu \sim 0.58$) for the saturated start: once in the zero density region the system never comes back. Changing the quark mass we only move the position of the hysteresis cycle unless we reach too small ($m < 0.1$) or too large ($m > 1.0$) masses where simulations can not be performed any more.

Even if we have physical as well as numerical indications that the present scenario of MDP results implies a pathological behaviour of the algorithm, we cannot discard the possibility of a strong first order transition at small mass and finite $L_t$. To explain the observed Montecarlo data this transition should be characterized, at finite volume ($4^4$), by a huge energy barrier between the two equilibrium states thus suppressing considerably the possibility of transitions among them. In such a case, a first order signal should survive at smaller lattices too, where an exact simulation is possible.

To overcome the sign problem, the only possibility consists in measuring observables on an unbiased ensemble (i.e. the ensemble corresponding to $\mu = 0$) of random generated configurations. Due to overlap problems, this technique allows to compute observables for any value of $\mu$ only if the generated ensemble contains a number of configurations of the order of the exponential of the volume $[^9, ^{10}]$. From a practical point of view this limits its applicability to a very small volume, in our case $V = 2^4$. Clearly this lattice is definitely not suitable for real physics but we are simply interested in verifying the presence of any first order transition signal.

We have simulated a $2^4$ lattice at mass $m = 0.1$ diagonalising the propagator matrix $[^{11}]$ and calculating the coefficients of the Gran Canonical Partition Function. From these coefficients we can calculate $Z$ and its derivatives for any value of $\mu$. In figs. 3 we plot the logarithm of the modulus and the phase of an averaged coefficient as a function of the statistics. It is clear that, after $O(10^5)$ configurations, this coefficient has reached a constant and almost real value. All the other coefficients converge to a real and positive quantity with equal or smaller statistics and we considered $10^6$ configurations sufficient to avoid any overlap problem in our reconstructed partition function.

We calculated the number density and no evidence of coexistence of two phases was present (figure 4). Therefore, the MDP results at $L_t = 4$ are not supported by $L_t = 2$ simulations at $m = 0.1$.

We conclude that the MDP results for $SU(3)$ have to be reconsidered. They are difficult to reconcile with the infinite mass solution and, from a numerical point of view, they seem not self consistent in the most interesting
region of $\mu$. The exact determination of the critical point and the much more interesting issue of the order of the transition can not be addressed with the MDP technique.

2 \textbf{SU(2) at infinite coupling}

In the previous section we have shown quite convincing evidences of convergence problems for the MDP algorithm applied to finite baryon density simulations in SU(3); we now address the same issue in the case of SU(2) as gauge group.

The motivation is twofold: firstly, to investigate if the problems of the MDP approach present in the SU(3) case are universal and independent of the gauge group; moreover, the SU(2) gauge group offers us the possibility of performing direct simulations using other algorithms, not only for the smallest possible lattice as in SU(3). In fact since quarks and antiquarks belong to the same (real) representation the fermion determinant is real and positive also for non zero chemical potential, and we can recover the meaning of Boltzmann weight for the exponential of minus the action.

In order to have a complete set of results, with $\mu$ varying continuously in a finite range of values, we used the Gran Canonical Partition Function (GCPF) scheme. In the SU(2) case it is possible to test the (non)occurrence of the severe drawbacks observed in SU(3). In fact, there exist results of SU(2) theory in the strong coupling limit at $\mu \neq 0$, obtained using the HMC (Hybrid Monte Carlo) algorithm in a $4^3 \times 4$ lattice; this approach, even if not convenient from a computer resources point of view (the simulation has to be repeated for each value of $\mu$ considered), is a good workbench for our GCPF simulations, being the fermion determinant explicitly included in the integration measure. We have therefore tested our results with those in [4].

We have performed simulations in the strong coupling limit at lattice volumes $4^3 \times 4$, $6^3 \times 4$ and $8^3 \times 4$ at three different values of the quark mass ($m = 0.1; 0.2; 0.4$) measuring the number density and the chiral condensate as functions of the chemical potential $\mu$.

In these simulations we have diagonalised, for each quark mass value, $O(1000)$ gauge configurations generated randomly (e.g. only with the Haar measure of the group) and then reconstructed iteratively the coefficients of the fugacity expansion of the partition function (GCPF coefficients). Rounding effects in the determination of the coefficients for these relatively large lattices have been kept under control using the same procedure developed
for the SU(3) case \[9\] \[12\]. At this point a numerical evaluation of the
derivatives of free energy allows the calculation of the observables we are
interested in.

In figure 5 we report the number density and chiral condensate as ob-
tained in our simulations (continuous line) compared with the HMC results
of \[4\] (diamonds). From these figures it is evident that our simulations repro-
duce the HMC results quite accurately. The agreement obtained in SU(2)
between the GCPF and HMC schemes suggests that sampling problems are
not present in this case, at least for the lattices and operators we used.

As a further check of the goodness of GCPF results we have com-puted
the pion mass in a $6^3 \times 12$ lattice at the quark mass values we used in our
simulations. In fact simplified models predict a phase transition (at least at
small temperature) at chemical potential coinciding, in SU(2), to half of the
mass of the lightest baryon of the theory (degenerate with the pion at $\mu = 0$).

To extract the critical value of the chemical potential we have used the
following criterium. The number density appears, with increasing volume,
to be almost zero up to the critical point, with a linear rise beyond it and
flat at large $\mu$ (saturation). To identify the critical point we have computed
$\partial n(\mu)/\partial \mu$ for two volumes and defined $\mu_c$ as the position of the first crossing
of the curves. In the infinite volume limit this definition correctly identifies
the value of $\mu$ where the linear behaviour starts. In the table we report our
critical chemical potential and half the pion mass for different values of $m$.

| $m$ | $\mu_c$    | $\frac{m_\pi}{2}$ |
|-----|------------|--------------------|
| 0.1 | 0.340(4)   | 0.3408(7)          |
| 0.2 | 0.485(5)   | 0.4840(6)          |
| 0.4 | 0.693(5)   | 0.6889(5)          |

We can conclude from these data that our predicted critical chemical
potential equals $m_\pi/2$ and moves with quark mass in the expected way, and
this behaviour increases the confidence on our numerical results.

We now compare the GCPF results with MDP ones. The published
results for SU(2) in the MDP scheme \[5\] are obtained in simulations of $4^3 \times 4$
and $8^3 \times 4$ lattices; from these simulations we will compare the number density
and chiral condensate with ours.

In fig. 6 we report the number density as function of the chemical po-
tential computed at $m = 0.2$ for $L_t = 4$ for the three different lattice spatial
volumes. Superimposed to our data we report the number density obtained
with the MDP algorithm (from figure 6 of \[4\]), at the same quark mass in
a $8^3 \times 4$ lattice. It is evident a marked difference between MDP results and
those by our simulations, again limited around the critical chemical potential as in the $SU(3)$ case. In particular our critical chemical potential is significantly smaller than the one reported in [5].

The largest part of published MDP results concerns the chiral condensate; in [5] there are results for different volumes, thus allowing a more detailed comparison with our results. We have computed this observable at the same value of the quark mass as in [5] ($m = 0.2$) in three lattices: $4^3 \times 4$, $6^3 \times 4$ and $8^3 \times 4$. In figure 7 we report our and MDP results (from figure 2 of [5]).

It is evident that for the smaller lattice (i.e. $4^3 \times 4$) the MDP data are in good agreement with ours; MDP results in $8^3 \times 4$ still agree with ours except at $\mu = 0.6$ (the critical point derived in [5]). The strong finite volume effect noticed by the authors of [5] seems unlikely on the chiral condensate at infinite coupling, at least this far from the chiral limit.

In the case of $SU(3)$ gauge group, as seen before, we have found severe slowing down for the MDP scheme. For $SU(2)$ gauge group Klaetle and Mutter, as reported in [5], have tested the independence of their results on the initial configuration only for the $4^3 \times 4$ lattice. In this case the results agree at a good level with ours. In our opinion the observed discrepancy has to be ascribed to convergence problems of the MDP algorithm, although they arise at volumes larger than in the $SU(3)$ case. Once again there are serious doubts on the accuracy that the MDP algorithm can achieve near the critical region.

### 3 Conclusions

The strong first order signal seen using the MDP code for $L_t = 4$ is difficult to reconcile with i) the absence of a phase transition at finite temperature and infinite mass and ii) the (reliable) numerical results on $2^4$ lattice. To solve this discrepancy we tried to repeat the MDP simulations at larger masses. This turned out to be impossible due to a dramatic drop in performances at large ($m > 1$) masses. We had the same evidence trying to change $L_t$ from 4 to larger values. We repeated the simulations at small mass and $L_t = 4$ finding unexpected huge hysteresis signal but not a direct evidence of two state coexistence.

The peculiar behaviour of the MDP algorithm seems not confined to the $SU(3)$ case. Indeed MDP $SU(2)$ simulations agree well with HMC and GCPF results except in the critical region and the discrepancies are more
severe with the system volume.

From these evidences we conclude that the MDP algorithm (for two and tree colours) is not reliable in the most interesting region of $\mu$ where the number density varies rapidly and no conclusion on the presence of a phase transition can be achieved using this technique.

More in general, we conclude that even the infinite coupling limit of finite density QCD, in principle easier to be studied, is still awaiting an efficient simulation scheme.
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Figure 1: Number density for a $4^4$ lattice and $m = 0.1$ computed using the MDP algorithm. Zero density starts (squares) and saturated starts (diamonds).
Figure 2: Montecarlo history for the number density in a MDP simulation at $\mu = 0.69$. 
Figure 3: Plots of the averaged Gran Canonical coefficient of order 72 ($\langle c_{72} \rangle = \rho e^{i\theta}$) as a function of the statistics in a $2^4$ lattice at $m = 0.1$: the logarithm of the modulus and the phase.
Figure 4: Number density at $m = 0.1$ evaluated using $10^6$ configurations on a $2^4$ lattice (continuous line) and in a $4^4$ lattice from the MDP code as reported in [2] (symbols).
Figure 5: Number density and chiral condensate at $m = 0.2$ in a $4^3 \times 4$ lattice from GCPF (continuous line, the errorbars are reported at some values of $\mu$) and from HMC algorithm (diamonds).
Figure 6: Number density computed at $m = 0.2$ in the three lattices $4^3 \times 4$ (dotted), $6^3 \times 4$ (dashed) and $8^3 \times 4$ (continuous) and from the MDP algorithm (diamonds) in a $8^3 \times 4$. 
Figure 7: Chiral condensate computed at $m = 0.2$ in the three lattices $4^3 \times 4$ (dotted), $6^3 \times 4$ (dashed) and $8^3 \times 4$ (continuous). Errorbars are reported at some values of $\mu$. The same quantity for the MDP algorithm in the $4^3 \times 4$ lattice (diamonds) and in the $8^3 \times 4$ lattice (squares).