QCD at small baryon number

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We consider the difficulties of finite density QCD from the canonical formalism. We present results for small baryon numbers, where the sign problem can be controlled, in particular by supplementing the $\mu=0$ sampling with imaginary $\mu$ ensembles. We initiate the thermodynamic study of few-nucleon systems, starting with the measurement of the free energy of a few baryons in the confined and deconfined phase. We present a simple model for the phase transition, whose results are in good agreement with the literature, but extend to lower temperatures.

1. INTRODUCTION

QCD at finite density is of great physical interest, but numerically challenging: the usual Monte Carlo sampling weight becomes complex, causing a sign problem. Recently, progress has been made using different approaches [1,2,3,4]. However all these methods have severe limitations which are already being reached, with little prospect for further progress.

Therefore, we propose yet another method - in a canonical formalism. Physically, we are interested in the study of systems consisting of a few baryons, for example the formation of nuclear matter or the binding of Deuteron. Here, we measure the free energy of sectors with small baryon number, and present a simple model for the QCD deconfinement phase transition. Numerically, our method has severe limitations which are in good agreement with the literature, but extend to lower temperatures.

However, for imaginary $\mu = i \mu_I$, $\text{det} M(U; i \mu_I)$ remains real. Moreover, $Z_{GC}(i \mu_I)$ is even and $2\pi T/3$-periodic in $\mu_I$ [5].

The canonical partition function with fixed quark number $Q$ can be obtained from the grand canonical one using a Fourier transform,

$$Z_C(Q) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\left(\frac{\mu_I}{T}\right) e^{-iQ S} Z_{GC}(\mu = i \mu_I).$$

The $2\pi T/3$-periodicity of $Z_{GC}(i \mu_I)$ implies that $Z_C(Q \neq 0 \mod 3) = 0$. Hence, we only deal with integer baryon number $B \equiv Q/3$.

Knowing the canonical partition functions, $Z_{GC}(\mu)$ can then be calculated for arbitrary chemical potential using the fugacity expansion (Laplace transformation):

$$Z_{GC}(\mu) = \sum_{B=-\infty}^{\infty} e^{-3B S} Z_C(B).$$

3. THE METHOD

Our main observable is the free energy per baryon, $F(B)$, defined by $Z_C(B)/Z_C(B=0) \equiv e^{-\frac{1}{T} F(B)}$.

We obtain $Z_C(B)$ by following the approach in \cite{7}, which samples $Z_{GC}(i \mu_I)$ at fixed $\mu_I$'s, then Fourier transforms each $\text{det} (U; i \mu_I)$ (all the $\mu_I$-dependency is in the determinant),

$$\text{det} M(U; i \mu_I) = \sum_{B=V}^{B=E-V} Z_C(U; B) e^{-i3B S}.$$ Substituting into Eq. (1) then into Eq. (2) gives

$$Z_C(B) = \int [DU] \tilde{Z}_C(U; B) e^{-S_h[U]}.$$
We sample the grand-canonical ensemble at couplings \( \beta \) and \( i\mu_I \), hence the observables we measure are ratios of partition functions,

\[
\frac{Z_C(\beta, B)}{Z_{MC}(\beta, i\mu_I)} = \left( \frac{\hat{Z}_C(B,U)}{\det M(U;i\mu_I)} \right)_{\beta,\mu_I}.
\]

In [1], the idea of the existence of a particular \( \mu_I(B) \) to extract \( Z_C(\beta, B) \) optimally has been formulated. Here, in order to improve the accuracy on the \( Z_C(\beta, B) \)'s, we simply combine results from several \( (\beta, \mu_I) \)-ensembles by Ferrenberg-Swendsen reweighting [3]. This requires knowing the determinant for different \( \mu_I \)'s. This information comes as a by-product of our determination of the \( \hat{Z}_C(B) \) in Eq. [4]. In the temporal gauge \( U_s(x,t) = 1 \) except for \( t = N_t - 1 \), the staggered fermion matrix \( M \) can be written as

\[
M = \begin{pmatrix}
B_0 & 1 & 0 & \ldots & 0 & U_{N_t-1}^{g-a}N_l \\
-1 & B_1 & 1 & \ldots & 0 & 0 \\
0 & -1 & B_2 & 1 & 0 & \ldots \\
- U_{N_t-1}e^{aN_l} & 0 & \ldots & 0 & -1 & B_{N_t-1}
\end{pmatrix}
\]

Following [10], we define a fermionic transition matrix

\[
P = \prod_{j=0}^{N_t-1} \begin{pmatrix}
B_j & 1 \\
1 & 0
\end{pmatrix} U_{N_t-1}
\]

with eigenvalues \( \lambda_1, \ldots, \lambda_{6V} \). We obtain the \( \hat{Z}_C(U; B) \) using Eq. [4] and the equality

\[
det M(U; \mu) = e^{3V\frac{\mu}{B}} \prod_{i=1}^{6V} \left( \lambda_i + e^{-\frac{\mu}{B}} \right).
\]

4. RESULTS

Since this is a feasibility study, we consider a small \( (4^4) \) lattice with volume \( V \sim (1.2 \text{ fm})^3 \). We use four flavours of staggered quarks with mass \( m = 0.05a^{-1} \). This theory is expected to have a first-order phase transition in the whole \((T,\mu)\) plane. With Hybrid Monte Carlo, we generate 55 ensembles of 4000–16000 configurations, at 11 temperatures \( T/T_c \in [0.8, \ldots, 1.1] \), each at five imaginary chemical potentials.

In the-high-temperature phase \( T > T_c \), we observe the characteristics of a system of free, relatively light quarks: the free energy \( F(\mu) \) is proportional to \( \mu^2 \) for small \( \mu \) [8], so that the free energy \( F(B) \sim B^2 \) for small \( B \) (\( \mu \) is conjugate to \( B \)). Furthermore, \( F(B) \) is almost independent of temperature in this regime. In Fig. 1, we show \( T^{-1}F(B)/B \) as a function of \( \beta \) for various \( B \), and indeed observe almost equidistant, \( \beta \)-independent levels \( (F(B)/B \sim B) \). For entropy reasons, we expect \( F(B = 1) \) to vanish in the thermodynamic limit. Deviations from these expectations are caused by finite size effects.

As \( T \) approaches \( T_c \) from below, the free energy drops dramatically. This is caused by an increase in the number of thermally accessible states, which triggers an entropic catastrophe à la Hagedorn. This collective phenomenon (of gluons) is visible even in the 1-baryon sector.

In the low-temperature phase \( T < T_c \), our results are consistent with a simple model of weakly interacting heavy baryons at rest \( (\rho_{min} = 24a^{-1} \Rightarrow T = \frac{4}{a}a^{-1}) \). At fixed temperature, \( F(B)/B \) stays constant over a whole range of \( B \geq 2 \), so that the free energy grows linearly with \( |B| \) as sketched in Fig. 2. The interaction is repulsive: \( F(B)/B - F(B = 1) \approx 0.1a^{-1} \sim 60 \text{ MeV per baryon} \), see Fig. 1. In the presence of a (real) quark chemical potential \( \mu \), the free energy acquires an additional term \( 3\mu B \), which tilts the free energy in Fig. 2. The free energy minimum jumps away from \( B = 0 \), and a first-order transition to a finite density occurs, when

\[
\mu_c = \frac{F(B)}{3B}|_{\text{plateau}}.
\]

The phase diagram resulting from our simple model is shown in Fig. 3. The agreement with other methods for \( \mu \lesssim 0.35a^{-1} \) is very good, except at low \( \mu \), where our method suffers from finite size effects. In the thermodynamic limit, \( F(B = 1) \) will develop a singularity exactly at the
$T = T_c, \mu = 0$ transition. Moreover, in the limit $T \to 0$, $F(B = 1) = m_N$, yielding via Eq. 5
$\mu_c = m_N / 3$, which already is a good approximation of the true phase transition. Therefore, we
expect Eq. 5 to give a good estimate of the critical chemical potential in the whole $(T, \mu)$ plane.
On our small lattice, a plateau for $F(B)/B$ is already reached for $B = 2$. The resulting phase
boundary is shown in Fig. 3. Note the bending down for $\mu/T > 1$, where the reliability of other
methods may be questioned.

5. CONCLUSION

In 4-flavor QCD, we have observed that the free energy grows linearly with the baryon number,
for small densities at $T < T_c$. This behavior is consistent with a first-order transition from
weakly interacting heavy baryons to light, quasi-free quarks. The corresponding phase boundary agrees with the literature for moderate $\mu/T$, then bends downward.

The same information could, in principle, be obtained by reconstructing the full grand-canonical partition function Eq. 3. However, the sectors with large baryon number, which we did not consider, bring in little information but a lot of noise. This is why our approach works better.

Since the sign problem is moderate, we can increase the volume and lower the temperature. As we do so, we expect the weak Pauli repulsion among baryons to be overcome by nuclear attraction, leading to the formation of nuclear matter.

Figure 2. Sketch of the free energy $F(B)$ in the two phases, for increasing (real) chemical potential. For $T < T_c$, the free energy minimum jumps to a non-zero density at a critical $\mu_c$.

Figure 3. The $(\mu, T)$ phase diagram. An approximation of the phase boundary is given by $F(1)/3$, where we neglect the baryonic interactions. $F(2)/6$ already gives the plateau-value in Eq. 5. Also shown are [1] and [4], which use the same simulation parameters. Agreement is very good for $\mu \lesssim 0.35a^{-1}$. Ch. Schmidt recently obtained one point [13] using the factorization method [14].

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