

Heavy-dense QCD at fixed baryon number without a sign problem

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QCD at fixed baryon number can be formulated in terms of transfer matrices explicitly defined in the canonical sectors. In the heavy-dense limit, the fermionic contributions to the canonical partition functions in terms of Polyakov loops and quark occupation numbers turn out to be completely factorized in space. At low temperatures and infinitely strong coupling the sign problem is reduced by orders of magnitude for any baryon number as compared to the corresponding grand-canonical ensemble. In the canonical formulation it is straightforward to integrate out the Polyakov loops in the fermionic weights yielding the partition function as a sum of only baryon occupation numbers in which the sign problem is absent. Using an effective form of the gauge action valid for small values of the gauge coupling, the same can be achieved away from the strong coupling limit in terms of quark occupation numbers and fluxes which couple the quarks with each other. The emerging clusters suggest the construction of algorithms which circumvent the sign problem in the heavy-dense limit including the full gauge action for any value of the gauge coupling.

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1. Motivation

Let us briefly summarize our motivation for investigating the canonical formulation instead of the commonly used grand-canonical one. Consider the grand-canonical partition function in terms of the Hamiltonian \mathcal{H} at finite chemical potential μ and temperature T ,

$$Z_{\text{GC}}(\mu) = \text{Tr} \left[e^{-\mathcal{H}(\mu)/T} \right] = \text{Tr} \prod_t \mathcal{T}_t(\mu).$$

The calculation of the trace may suffer from a sign problem depending on the choice of the basis states over which the trace is taken. The sign problem manifests itself in cancellations between different states: while all states are present for any values of μ and T , different states need to cancel out for different values of μ and T . In QCD, for example, at high temperatures the states describing deconfined quarks are highly relevant and provide the dominant contributions to the partition function, while in the confined phase at low temperatures those contributions need to cancel out. In the canonical formulation, the partition function reads

$$Z_{\text{C}}(N_q) = \text{Tr}_{N_q} \left[e^{-\mathcal{H}/T} \right] = \text{Tr}_{N_q} \mathcal{T} = \text{Tr} \prod_t \mathcal{T}_t^{(N_q)},$$

where the sum is now restricted to the states with a fixed number of fermions or quarks N_q . Therefore, it is clear that the dimension of the Fock space is tremendously reduced and much less cancellations are necessary. As an example, consider again QCD where in the canonical formulation it is explicit that $Z_{\text{C}}^{SU(N_c)}(N_q) = 0$ for $N_q \neq 0 \bmod N_c$ with the obvious implications, while in the grand-canonical formulation the corresponding physical principle is achieved only through implicit cancellations of unphysical states involving quark numbers $N_q \neq 0 \bmod N_c$. Another example concerns the Schwinger model where it is explicit that $Z_{\text{C}}^{U(1)}(N_q) = 0$ for $N_q \neq 0$, i.e., only noncharged states are physical, while in the grand-canonical ensemble the same physical property emerges only after the cancellation of the contributions from all charged states. Finally, we point out that the so-called "Silver Blaze" phenomenon is realised automatically in the canonical formulation, in contrast to the grand-canonical one.

In the expressions above we have indicated that the trace is taken over a product of transfer matrices $\mathcal{T} = \prod_t \mathcal{T}_t$. The conservation of fermion number manifests itself in the fact that the transfer matrices are block diagonal where the block matrices are the canonical transfer matrices $\mathcal{T}_t^{(N_q)}$. It turns out that these transfer matrices and their product are known in closed form and can be calculated explicitly in terms of the dimensionally reduced matrices [1]. The connection between the canonical and grand-canonical ensemble is given by the fugacity expansion

$$\det M[\mathcal{U}; \mu] = \sum_{N_q} e^{-N_q \mu/T} \cdot \det_{N_q} M[\mathcal{U}]$$

where $M[\mathcal{U}; \mu]$ denotes the fermion matrix depending on the gauge field U and the chemical potential μ . The expansion relates the grand-canonical fermion determinant to the canonical ones. Each canonical determinant $\det_{N_q} M[\mathcal{U}]$ can be expressed as the trace over the minor matrix \mathcal{M}_{N_q} of order N_q of the dimensionally reduced transfer matrix \mathcal{T} at zero chemical potential

$$\det_{N_q} M[\mathcal{U}] = \sum_{|J|=N_q} \det \mathcal{T}^{JJ}[\mathcal{U}] = \text{Tr} \prod_t \mathcal{T}_t^{(N_q)} = \text{Tr} \mathcal{M}_{N_q}.$$

While this connection is completely general, in the following we apply it to QCD with Wilson fermions in the heavy-dense limit.

2. Heavy-dense limit of QCD

The heavy-dense approximation of QCD consists in general of taking the hopping parameter of the Wilson fermion $\kappa \equiv (2m + 8)^{-1} \rightarrow 0$ and the chemical potential $\mu \rightarrow \infty$, while keeping the combination $\kappa e^{+\mu}$ fixed [2, 3]. This procedure has the property that only the static quarks are kept as degrees of freedom, while the static antiquarks are removed from the system. Another slightly different approximation consists in distinguishing the spatial and temporal hopping of the fermions, dropping only the spatial hopping terms and keeping the forward and backward hopping in time. This procedure has the advantage that one retains a relativistic system of static quarks and antiquarks which is closer to real-world QCD.

In the grand-canonical formulation, the heavy-dense limit, as described above, leads to a three-dimensional fermion action in terms of Polyakov loops P and anti-Polyakov loops P^\dagger with the fermion determinant

$$\det M_{GC}^{HD} = \prod_{\bar{x}} \det [\mathbb{I} - (2\kappa e^{+\mu})^{N_t} P_{\bar{x}}]^2 \det [\mathbb{I} - (2\kappa e^{-\mu})^{N_t} P_{\bar{x}}^\dagger]^2, \quad (1)$$

where N_t is the number of time slices and \bar{x} denotes the spatial lattice sites. As described in the previous section, in the canonical ensemble the canonical determinants are given by the trace over the minor matrix \mathcal{M}_{N_q} ,

$$\det_{N_q} M^{HD} = (2\kappa)^{2N_c L_s^3 N_t} \cdot \text{Tr} \mathcal{M}_{N_q} [((2\kappa)^{+N_t} \cdot P_+ \mathcal{P} + (2\kappa)^{-N_t} \cdot P_- \mathcal{P})],$$

where $P_\pm = 1/2(\mathbb{I} \mp \gamma_4)$ are Dirac projectors and \mathcal{P} denotes the collection of Polyakov loops $P_{\bar{x}}$ in the matrix $\mathcal{P}_{\bar{x}, \bar{y}} = \mathbb{I}_{4 \times 4} \otimes P_{\bar{x}} \cdot \delta_{\bar{x}, \bar{y}}$ taking into account the degeneracy with respect to the Dirac structure. The matrix in square brackets has a simple block diagonal structure and essentially corresponds to the dimensionally reduced product of transfer matrices $\mathcal{T} = \prod_t \mathcal{T}_t$ before the explicit projection onto the canonical sectors. This latter step is achieved by constructing the minor matrix \mathcal{M}_{N_q} .

From the structure of the minor matrix \mathcal{M}_{N_q} , or rather the matrix \mathcal{T} in the square bracket, it is immediately clear that the canonical determinants transform as $\det_{N_q} M^{HD} \rightarrow z_k^{N_q} \cdot \det_{N_q} M^{HD}$ under a global $z_k \in \mathbb{Z}_{N_c}$ transformation. Consequently, one finds that

$$\det_{N_q} M = 0 \quad \text{for } N_q \neq 0 \pmod{N_c}$$

which reflects the explicit and exact cancellation of the contributions from many states in the canonical setup, which is not evident in the grand-canonical one.

Instead of providing explicit expressions for the canonical determinants, we just point out that they are simple polynomials of $\text{Tr} P_{\bar{x}}$ and $\text{Tr} P_{\bar{x}}^\dagger$ where all terms have triality $N_q \pmod{N_c}$ with respect to a \mathbb{Z}_{N_c} transformation. For example, for the canonical determinants with $N_q = 0$ (and $N_c = 3$) one finds terms proportional to $\text{Tr} P_{\bar{x}}^\dagger \text{Tr} P_{\bar{y}}$ and $\text{Tr} P_{\bar{x}} \text{Tr} P_{\bar{y}} \text{Tr} P_{\bar{z}}$, and so on, which are invariant under global \mathbb{Z}_3 transformations, as discussed above. The terms can be interpreted as contributions from the propagation of quarks and antiquarks forming mesons and baryons. As

a consequence, the contributions can be described in terms of quark and antiquark occupation numbers $n_{\bar{x}} \in \{-2N_c, \dots, 2N_c\}$.

It turns out that the system suffers from a severe sign problem, which, however, is avoided in two cases. Firstly, if all Polyakov loops $P_{\bar{x}}$ align along one of the three center elements, which is the case in the deconfined phase, the contributions from all Polyakov loops add up coherently and yield a positive contribution. Secondly, if the global \mathbb{Z}_{N_c} symmetry can be promoted to a local one, as is the case in the strong coupling limit, only those contributions survive that satisfy the triality condition locally, i.e., $n_{\bar{x}} = 0 \pmod{N_c}$.

3. Heavy-dense strong coupling limit of QCD

As mentioned above, in the strong coupling limit the global \mathbb{Z}_{N_c} transformations are promoted to local ones in the canonical formulation. This means that since the canonical fermion determinants transform covariantly under a \mathbb{Z}_{N_c} transformation, integrating locally over all \mathbb{Z}_{N_c} -transformed gauge fields makes all of them vanish except when $n_{\bar{x}} = 0 \pmod{N_c}$, i.e., the remaining, nonvanishing contributions are invariant under a local \mathbb{Z}_{N_c} transformation. This is in contrast to the grand-canonical setup, where the fermionic contribution Eq. (1) does not transform covariantly and is not \mathbb{Z}_{N_c} -invariant in the strong coupling limit. As a consequence, the partition function becomes a summation over all baryon configurations $\{n_B(\bar{x})\}$ with (essentially) positive contributions. More precisely, the partition function reads

$$Z_C(N_B) = (2\kappa)^{2N_c N_t L_s^3} \cdot \sum_{\{n_B\}, |n_B|=N_B} \int \mathcal{D}U \prod_{\bar{x}} \det \mathcal{M}_{n_B(\bar{x})}^{HDSS} [\text{Tr } P_{\bar{x}}], \quad (2)$$

where the fermionic weight is completely factorised in space and $\det \mathcal{M}_{n_B(\bar{x})}^{HDSS} [\text{Tr } P_{\bar{x}}]$ are the single-site fermion weights. They are simple polynomials of $\text{Tr } P_{\bar{x}}$ and $\text{Tr } P_{\bar{x}}^\dagger$ with coefficients depending on $(2\kappa)^{N_t} = \exp(-m/T)$ which parameterizes the temperature.

It is now very easy to analytically integrate out the remaining gauge field degrees of freedom. This leads to a system where the local baryon occupation numbers are the only degrees of freedom and where all weights are positive, i.e., the sign problem at fixed baryon number is solved in the strong coupling limit. For small system sizes the remaining summation over the baryon occupation numbers can be done analytically, while for larger systems one needs to resort to a stochastic summation. However, it turns out that in the strong coupling limit, the finite size effects are rather mild and observables typically saturate already on small systems.

As an example of such a calculation we show in Figure 1 the local baryon number fluct-

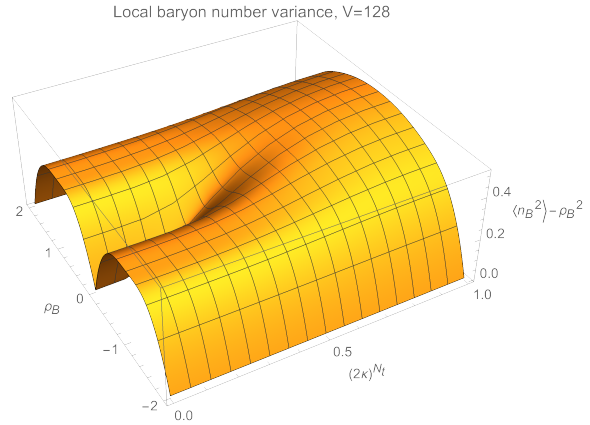


Figure 1: Local baryon number susceptibility as a function of the baryon density ρ_B and the temperature expressed as $\exp(-m/T) = (2\kappa)^{N_t}$.

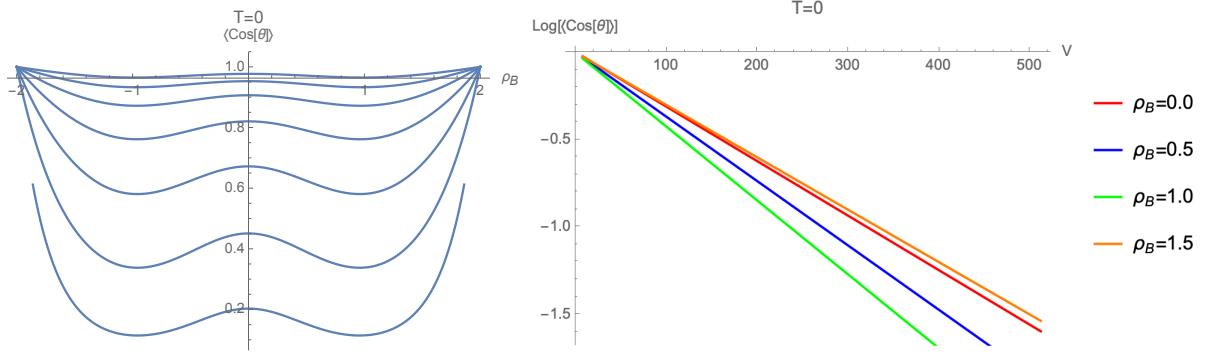


Figure 2: *Left:* Average sign as a function of the baryon density ρ_B for a range of system sizes. *Right:* Logarithm of the average sign as a function of the system size V for various baryon densities.

tuations $\chi_{n_B} = \langle n_B^2 \rangle - \rho_B^2$, where $\rho_B = N_B/V$ is the baryon density, as a function of ρ_B and $\exp(-m/T) = (2\kappa)^{N_t}$. It is clear that the fluctuations are symmetric w.r.t. an interchange of baryons and antibaryons and it would suffice to show only the positive density part. At zero density and low temperatures, the fluctuations are essentially zero, but cross over to larger values with growing temperature. At zero temperature one finds a steep increase of χ_{n_B} with growing baryon density, reaching a plateau around half-filling. When the density is further increased towards saturation, the fluctuations tend to zero regardless of the temperature.

Of course it is also possible (and instructive) to simulate the combined system of baryon occupation numbers and the gauge fields, i.e., the system in Eq. (2), in order to assess the severity of the sign problem. In Figure 2 we show the average sign $Z_C(N_B)_{|\cdot|}/Z_C(N_B) = \langle \cos \theta \rangle_{|\cdot|}$ measured in a phase-quenched simulation. The left plot shows the average sign as a function of ρ_B for a range of volumes at zero temperature. While for small system sizes the sign problem is barely noticeable, it becomes more severe with the growing size of the system. The right plot in Figure 2 shows the logarithm of the average sign as a function of the volume V for a few selected baryon densities, still at zero temperature. The exponential decay of the average sign with growing volume indicates that the sign problem is indeed severe. The severity can be quantified by determining the free energy density difference between the phase quenched and the full canonical partition functions,

$$Z_C(N_B)_{|\cdot|}/Z_C(N_B) = \exp[-\sigma \cdot V] \quad \text{with} \quad \sigma = \Delta f/T. \quad (3)$$

The full anatomy of the sign problem can be uncovered by repeating this exercise for all temperatures and baryon densities yielding the left plot in Figure 3. The sign problem is most severe at high temperature and half-filling. This can be understood from the fact that the single-site weight with $n_q = 3$ is the only one that can give negative contributions. However, even there the sign problem is so mild that simulations on rather large lattices are still practical. It is interesting to compare this situation to the one in the grand-canonical ensemble shown in the right plot of Figure 3 which shows a rather different behaviour. In particular, at low temperatures the sign problem quickly becomes severe for increasing μ_B , but at μ_B/m_B , which corresponds to half-filling $\rho_B = 1$, it vanishes — a curious observation that has already been made before [4]. The less favourable behaviour in the grand-canonical ensemble (note the different scale on the σ -axis) suggests that at

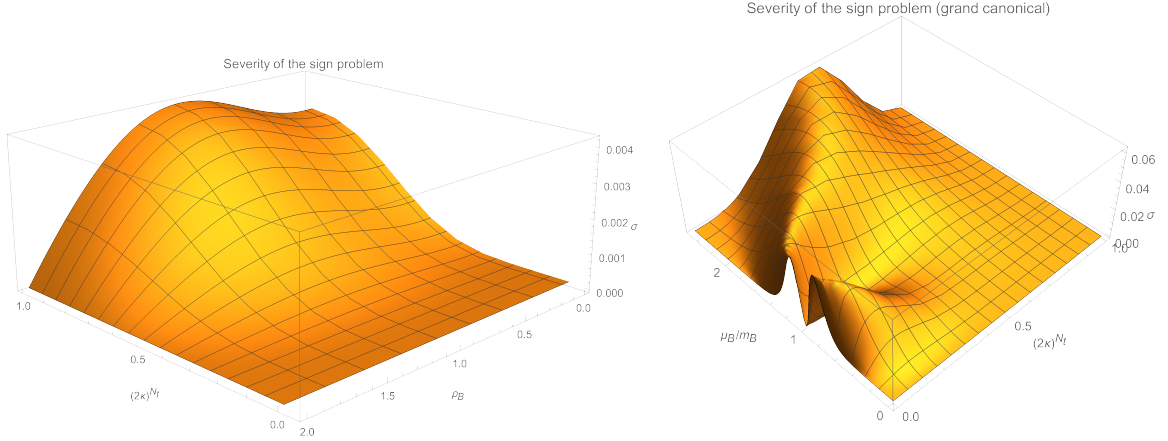


Figure 3: Severity of the sign problem as a function of temperature and baryon density or baryon chemical potential. *Left:* Canonical ensemble. *Right:* Grand-canonical ensemble.

finite density (except maybe at half-filling) and especially at low temperatures, it is preferable to perform simulations in the canonical ensemble.

4. Heavy-dense limit of QCD beyond strong coupling

Trying to go beyond strong coupling and just naively switching on the gauge coupling ends in complete disaster. For any nonzero gauge coupling, however small, the sign problem becomes so severe that Monte Carlo simulations are no longer practical, not even on small systems. This is due to the fact that as soon as the gauge coupling is finite, quarks and antiquarks are no longer confined into mesons and baryons localized on a single site. Instead, they can move away from each other generating weights with nonzero triality which are no longer guaranteed to vanish by the local \mathbb{Z}_{N_c} symmetry. In order to get the local \mathbb{Z}_{N_c} symmetry back into action, we employ the effective gauge action introduced in [5],

$$\exp(-S_{\text{eff}}[\mathcal{U}]) = \prod_{\langle \bar{x}\bar{y} \rangle} (1 + 2\lambda \text{Re Tr } P_{\bar{x}} \text{Tr } P_{\bar{y}}^\dagger).$$

It introduces a nearest-neighbour interaction between Polyakov loops and can be derived in a systematic way from the original plaquette gauge action in the heavy-dense limit. As a consequence, the effective gauge coupling λ is in fact a function of the original gauge coupling and the hopping parameter κ , and for small λ the effective action provides a good description of the full heavy-dense limit of QCD close to the strong coupling limit.

On a practical level, since the canonical fermion weights are factorized in space, it is straightforward to “dualize” the effective nearest-neighbour interaction by introducing fluxes on the bonds connecting two neighbouring sites. The flux can either be 0 or ± 1 and when present on a bond, it induces an additional weight factor λ and additional (anti-)Polyakov loops P and P^\dagger at the ends of the bond which modify the corresponding fermion site weights. Integrating the gauge fields locally over the elements of \mathbb{Z}_3 induces a local constraint which requires that the local net flux plus the number of quarks on that site is zero modulo 3. That is, quarks and antiquarks, which

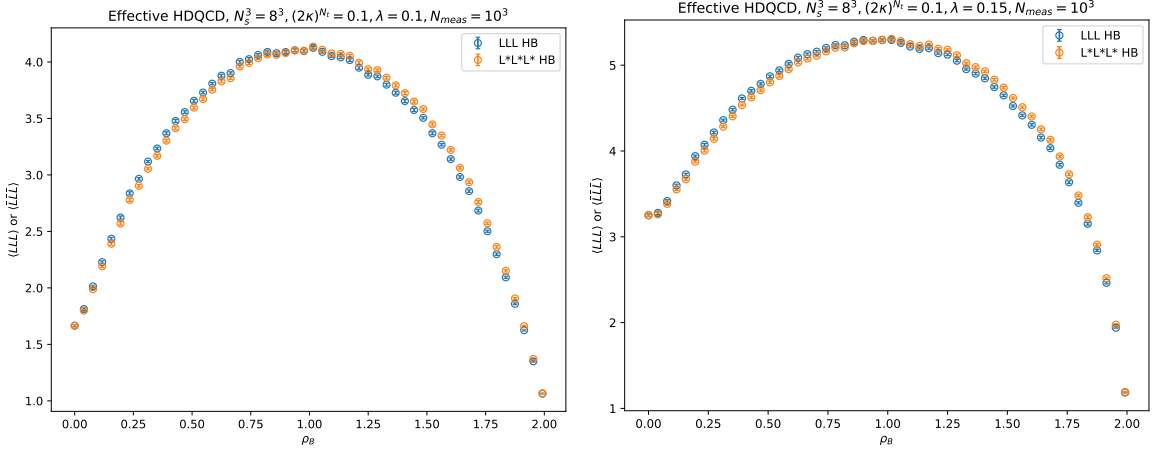


Figure 4: Expectation value of a static baryon or antibaryon in the background of finite baryon density for canonical effective heavy-dense QCD at two different values of the effective gauge coupling, $\lambda = 0.1$ (left plot) and 0.15 (right plot).

act as sources and sinks for the \mathbb{Z}_3 flux, can now separate from each other, as long as they are connected by a corresponding flux. This is essentially a realization of the flux model proposed and elaborated in [6, 7], now derived in a controlled way from the underlying theory of QCD with Wilson fermions. Finally, the gauge fields can now be integrated out analytically yielding a system which is described in terms of integer quark occupation numbers $n_{\bar{x}} \in [-6, \dots, 6]$ and bond occupation numbers $n_b \in [-1, 0, +1]$ with weights that are positive. Hence, the sign problem is solved beyond strong coupling and Monte Carlo simulations respecting the local constraints on the integer occupation numbers are straightforward.

In the following we present a few results as examples of what can be calculated in this setup. In Figure 4 we show the expectation value of a static baryon or antibaryon in the background of increasing finite baryon density. Interpreting the expectation value in terms of the free energy for an additional baryon or antibaryon, the results demonstrate that it is slightly more favourable to add an antibaryon to a system with finite baryon density than it is for a baryon. This is simply due to the fact that an antibaryon can be screened more easily by the already present baryons and can therefore more easily be accommodated. Maybe more surprising is the fact that this situation is reversed once the baryon density goes beyond half filling $\rho_B > 1$.

It is noteworthy that for low densities there is a pronounced change when going from smaller to larger effective coupling λ . In the left plot of Figure 5 we investigate this in more detail and show the expectation value of a static baryon at zero density and low temperatures as a function of the effective coupling λ . Note that even at zero density, the vacuum is full of baryon and antibaryons. The temperature is parameterized by $(2\kappa)^{N_t} = \exp(-m/T)$ and as we lower it, the transition becomes more pronounced.

Finally, in the right plot of Figure 5 we show an example of the determination of the baryon chemical potential as a function of the baryon density. The chemical potential is calculated from the free energy difference between two systems with N_B and $N_B + 1$ baryons. As can be seen from comparing the results at two different volumes, finite size effects are completely negligible for these parameters. More importantly, the plot demonstrates nicely how the canonical formulation

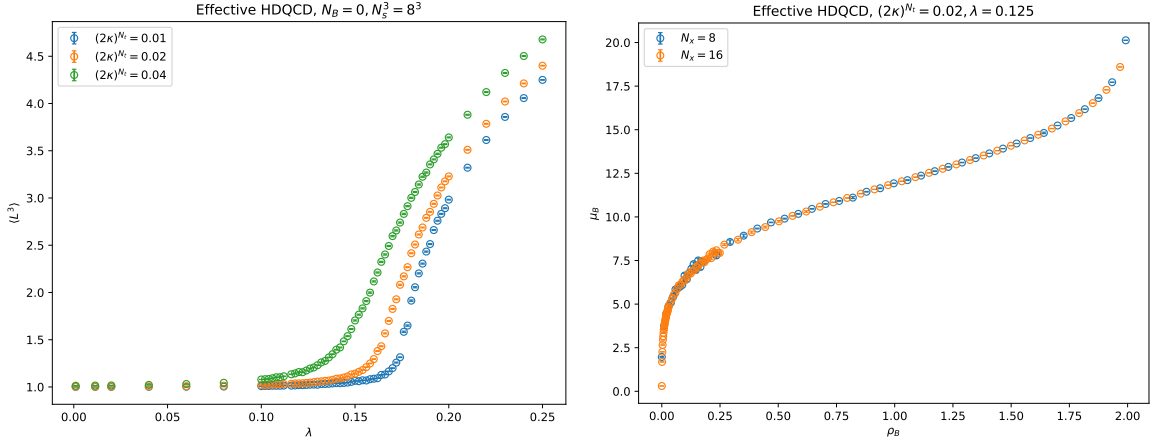


Figure 5: *Left:* Expectation value of a static baryon at zero baryon density as a function of the effective gauge coupling for three different temperatures parameterized by $(2\kappa)^{N_t} = \exp(-m/T)$. *Right:* Baryon chemical potential as a function of baryon density at low temperature and for two different volumes.

provides a picture complementary to the grand-canonical one, in the sense that the intensive chemical potential parameter is determined as an observable depending on the extensive number of baryons, in contrast to what is done in the grand-canonical formulation. As such, the determination of the chemical potential in the various baryon sectors is equivalent to a determination of the energies of multi-baryon states.

5. Summary and outlook

In these proceedings we reported on the progress in simulating heavy-dense QCD at fixed baryon number without a sign problem. Starting from the generic construction of transfer matrices with fixed fermion numbers applied to the heavy-dense limit of QCD, we derive an effective Polyakov loop model directly from the underlying QCD Wilson fermion matrix. In contrast to the grand-canonical formulation, in the canonical one the \mathbb{Z}_3 symmetry is manifest. This in turn leads to a straightforward solution of the sign problem in the strong coupling limit. After the gauge fields are integrated out, the only degrees of freedom are configurations of baryon occupation numbers which need to be summed over. In order to assess potential advantages of simulations including the gauge field degrees of freedom in the canonical ensemble compared to the grand-canonical one, we investigated the anatomy of the sign problem in both cases. It turns out that the sign problem is less severe in the canonical formulation by at least an order of magnitude, in particular at low temperatures the sign problem is so mild that simulations on very large volumes would be feasible. Finally we presented some selected results beyond the strong coupling limit. Using an effective gauge action derived from the usual plaquette action, the sign problem can also be solved in this case. It is instructive to see how this is achieved: the effective gauge action induces fluxes between separated quarks and antiquarks, which binds them together into clusters. Only clusters with zero triality have nonvanishing weights which turn out to be positive. Not surprisingly, this is the same mechanism that is also at work in the Potts model at fixed fermion number [8]. It also suggests a way forward to a possible solution for heavy-dense QCD using the standard plaquette

action. While in that case the cluster algorithms are in general not efficient at temperatures close to the deconfinement transition, they might be sufficiently efficient at low temperatures where the constructed clusters remain small.

In the canonical formulation one has explicit control over the spatial positions of the baryons, which allows us to calculate, e.g., the static baryon potential, or properties of nuclear matter along the lines of [9]. Another interesting application could be the calculation of the energies of multi-baryon states, and of course the determination of the phase diagram as a function of the effective coupling, the temperature and the baryon density.

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