

Finite density lattice QCD without extrapolation: Bulk thermodynamics with physical quark masses from the canonical ensemble

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Quantum chromodynamics (QCD) at finite density is most often formulated on the lattice as a grand canonical ensemble. Since lattice QCD has a complex action problem at finite baryo-chemical potential (μ_B), its results at finite density are indirect: e.g. in the form of a set of expansion coefficients. In contrast, the canonical formulation offers direct results for integer-valued net-baryon number. In this work we present for the first time results in the canonical formulation with physical quark masses. To this end we use a high statistics finite-volume lattice ($16^3 \times 8$) dataset that we generated at $\mu_B = 0$ with our 4HEX staggered action. We extend the canonical ensemble to noninteger net-baryon number and connect the results back to the grand canonical ensemble. Unlike reweighing to real μ_B , this method can also be used with rooted staggered quarks. For densities where the sign problem can be overcome by brute force computing power, this scheme provides lattice QCD results (e.g., for pressure, baryon density) directly, without relying on any extrapolation in the baryo-chemical potential. In this work we chart the phase diagram by studying bulk thermodynamic observables, which we show to be feasible up to $\mu_B \approx 500$ MeV.

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I. INTRODUCTION

Through the gravitational wave observations we gained access to the densest and hottest matter that our Universe presents, merging neutron stars. Laboratory experiments of colliding nuclei interpolate between these conditions and those in the much hotter Early universe with almost vanishing net-baryon density. Most notably, the Large Hadron Collider (LHC) at CERN and the Relativistic Heavy Ion Collider (RHIC) at BNL, have recently explored a broad range of the phase boundary between the high temperature quark gluon plasma and the colder hadronic phase. The thermodynamical parameters of the cooling plasma at the instant of the last inelastic scattering, the

chemical freeze-out, was argued to give accurate estimates on the phase boundary itself, at least for high collision energies [1].

Theoretical solutions to the underlying theory, quantum chromodynamics (QCD), later confirmed the good agreement between the chemical freeze-out and the chiral crossover. Most prominently, lattice QCD was able to establish the fact that the transition is a crossover [2], its temperature at zero density [3–6], and the crossover line on the plane of temperature (T) and baryo-chemical potential (μ_B) [7–10]. Other theoretical tools, too, have been successfully employed to compute the crossover line, e.g. in the Dyson-Schwinger formalism [11–13] or with the functional renormalization group [14].

The interest in hot and dense QCD matter is further fuelled by the prospect of the discovery of a critical point on the chiral crossover line [15]. Several effective models support the existence of such a critical point, e.g. random matrix, quark-meson model or Nambu-Jona-Lasino, including their extensions with the Polyakov loop. Quite interestingly, first principles functional methods, too, give

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predictions to the location of this conjectured point [12–14], all in the ballpark of $\mu_B \approx 650$ MeV, $T \approx 100$ MeV. See Ref. [16] for a recent summary.

Lattice QCD can access this range only indirectly. In the standard formulation, the quark degrees of freedom are integrated out to form the so-called quark determinant. The latter depends on the quark mass, the chemical potential and the background gauge field, which is then sampled with the weight given by the gauge action and this determinant. Unfortunately, unless the chemical potential is either zero or purely imaginary, the determinant becomes a complex number, unsuitable for a probability to be used in importance sampling. Perhaps the most successful indirect methods are the Taylor expansion, where derivatives of the grand potential and other observables are computed at $\mu_B = 0$ [17,18], and the analytical continuation from imaginary chemical potential [19–21]. Both methods depend on favorable analytical features of the grand potential. Physics results at finite density are obtained in form of truncated extrapolation formulas with lattice data as input. By today continuum extrapolated results are available up to second [22–24], fourth [25,26], sixth [27,28] order of the μ_B expansion and even eighth [28–30] and tenth orders [31] at finite lattice spacing. While the Taylor coefficients are computed at $\mu_B = 0$, thus, free from the complex action problem, they are hit by a cancellation (or sign) problem, with exponentially increasing severity with volume and order [31].

The idea of reweighting from $\mu_B = 0$ to the physical $\mu_B > 0$ parameter space was a natural suggestion [32]. This, however, introduces a sign problem and an overlap problem. The latter could be mitigated using multiparameter reweighting [33,34] or a density-of-states approach [35]. In a more advanced setup with finer lattices the overlap problem was surprisingly mild in small volumes [36]. Let us point out, that the Taylor coefficients, when computed from a single $\mu_B = 0$ ensemble, are equivalent to those of the reweighted ensemble. In this viewpoint, the Taylor expanded finite density results are mere approximations of what a full reweighting would give, and inherit a sign problem and an overlap problem of the same magnitude.

The sign problem is only one aspect of the difficulties with reweighting. Even if the additional overlap problem is treated e.g. by employing sign quenched simulations [36–38], and we own sufficient computer resources to control the sign problem, there is a further obstacle. The overwhelming majority of lattice thermodynamics results is simulated in the staggered formulation, especially so for physical quark masses. The rooting procedure at finite chemical potential is ambiguous, leading to severe lattice artefacts [39] including a fake transition at $\mu_B \approx m_\pi 3/2$ [40,41]. This paper offers a solution to the rooting problem through a detour to the canonical formalism.

The canonical ensemble does not easily lend itself for simulation on the lattice. While it is well known how to

introduce a baryo-chemical potential such that it respects the underlying $U(1)_V$ symmetry [42], one cannot associate a baryon number (N) to a given gauge configuration, once the quark degrees of freedom are integrated out. Each configuration contributes to every baryon number N with some complex weight [43]. Specifically the $N = 0$ sector can and has been simulated without a sign problem [44]. The $N > 0$ ensembles can be obtained e.g. by reweighting from the grand canonical $\mu_B = 0$ ensemble [45]. Importance sampling at finite density was introduced in Refs. [46,47] in a sign-quenched setup. Early studies demonstrate that the easily accessible canonical observable $\mu_B(N)$ marks the first order finite density transition with an unambiguous S-shape pattern [45,48] from which a strategy to locate the critical endpoint can be derived [49].

Since the severity of the finite density sign problem is strongly linked to the pion mass [43], reaching the physical point, or any realistic lattice spacing has not been feasible, previously. Yet, many technical issues could be discussed in detail, e.g. the deterministic [45,50] computation of the complex weight associated with N baryon numbers, the so-called canonical determinant, or its numerically stable construction through a winding number expansion [48,51].

A further challenge posed by fixed- N canonical data is the extraction of grand canonical information, such as the fluctuations of conserved charges [52]. At finite μ_B each Z_N sector contributes with the weight $e^{N\mu_B}$. Thus, grand canonical observables, such as moments of N are the results of an infinite sum in N . The inevitable truncation in N leads to systematic errors especially for higher moments of N . This is unfortunate near the physical point, where one quickly loses control for higher N sectors.

The aim of this work is twofold. With simulations at the physical point on a finite lattice we demonstrate the practical feasibility of the canonical approach. We will work with a physical system size of $LT = 2$. In this volume (ca. 20 fm³ at $T = 145$ MeV) the sign problem can be addressed with high statistics ensembles up to $\mu_B \lesssim 500$ MeV in the crossover range. We can relate the phenomenological findings to the expected Skellam distribution of a noninteracting hadron gas. We briefly discuss how the strangeness number can be added to the formalism.

The second aim of this work is to give a somewhat technical discussion on how the partition function is obtained from a single $\mu_B = 0$ ensemble, including all center sectors, and how the staggered rooting problem is circumvented at the same time. The method to recover grand canonical results from canonical lattice data without performing a truncated sum in N is a further novelty in this work. The final results on the QCD pressure and chemical potential as a function of the baryon density are analogous to the would-be outcome of reweighting, as if the complex rooting problem of Refs. [39,41] did not exist.

The exciting feature of these results is the absence of an extrapolation in μ_B . The phenomenological results and

theoretical arguments of this work then suggest an optimistic prospect: lattice QCD is no longer a mere tool to provide extrapolation coefficients, but it can also give actual truncation-free finite density results. The sign problem itself can be dealt with, thanks to today's computer power, up to a certain density. Thus, finite density simulations are indeed possible, even with physical parameters and with a lattice resolution ($N_\tau = 8$) that is suitable for phenomenological studies, covering much of the parameter space accessible to the RHIC Beam Energy Scan program.

In Fig. 1 we give an example on what is possible with our methodological improvements. We show the results of our high statistics lattice simulations as contours of fixed baryon density on the $T - \mu_B$ plane of the QCD phase diagram. At present, we can follow these up to a chemical potential of ca. 500 MeV. These lines will be tangential to the transition line in the case of a true transition. In the infinite volume limit these lines collapse to the same line, that of the transition. The knowledge of these lines also implies that the equation of state is known at finite density.

This paper starts with revisiting the canonical formalism in Sec. II. The basic concepts are illustrated with the example of a noninteracting hadron gas (see Appendix). In Sec. III we propose new algorithmic ingredients that optimize the numerical procedure. The first phenomenological results in the canonical formalism are presented in Sec. IV, mostly focusing on the pressure and chemical potential as observables. Here, the direct results at fixed (canonical) baryon number are specific to the system volume. We generalize the discussion to an arbitrary volume and connect back to the grand canonical ensemble in Sec. V. We conclude with a discussion on future directions in Sec. VI.

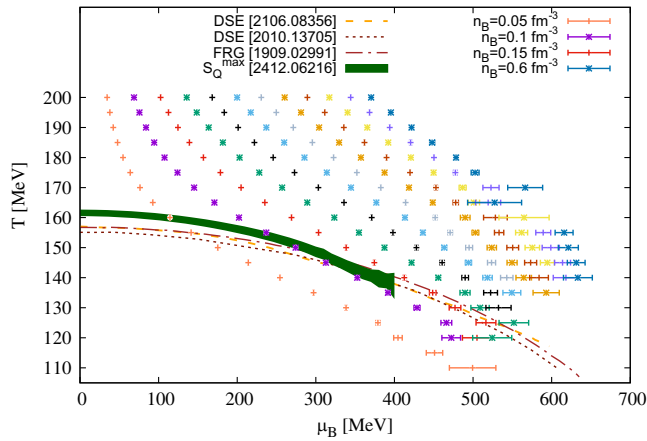


FIG. 1. Contours of constant net-baryon density on the QCD phase diagram. Each color represents a fixed density, from left to right $n_B = 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35, 0.40, 0.45, 0.50, 0.55, 0.60 \text{ fm}^{-3}$. For clarity reasons, not all the densities are explicitly labeled in the plot. To help the reader: the densities 0.05, 0.15, 0.25, 0.35, 0.45, 0.55 are labeled with a cross. The densities 0.10, 0.20, 0.30, 0.40, 0.50, 0.60 are labeled with a star. The errors are statistical.

II. THE CANONICAL FORMALISM

A. Generic thermodynamics

At the energy scale of the QCD transition the theory features three exactly conserved charges, which can be seen as the net quark number for each of the up, down and strange flavors, or equivalently the baryon number B , electric charge Q and strangeness S . For the purpose of this paper we do not consider heavier quarks, hence our dynamical lattice simulations will be performed with $N_f = 2 + 1$ flavors, and we introduce the quark chemical potentials in the standard exponential form [42]. We focus on two of said conserved charges, namely the net baryon number N_B and the net strangeness N_S .

In textbooks one can find a simple relation between the canonical (Z_C) and grand canonical partition functions (Z_{GC}):

$$Z_{GC}(T, V, \mu) = \sum_{N=-\infty}^{\infty} e^{\mu N} Z_C(T, V, N). \quad (1)$$

For simplicity, here and in the following discussions we use generic μ and N as conjugate variables, standing for chemical potential and net particle number. Note that Eq. (1) features a summation over integer-valued N , as in fact there is no state in any finite box with a fractional baryon number (or strangeness). This remains true in lattice QCD, also with rooted staggered quarks, since this feature is protected by the unbroken center symmetry $\mathbb{Z}_3$ of the gauge group $SU(3)$. A consequence of this symmetry is the periodicity in the imaginary-valued chemical potential $\mu/T = i\varphi$, which is evident from the relation

$$Z_{GC}(T, V, i\varphi T) = \sum_{N=-\infty}^{\infty} e^{i\varphi N} Z_C(T, V, N). \quad (2)$$

A more practical, equivalent form of Eq. (2) can be obtained by inverting the Fourier series as

$$Z_C(T, V, N) = \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i\varphi N} Z_{GC}(T, V, i\varphi T), \quad (3)$$

or in terms of the grand potential (Ω) and the Helmholtz free energy (F)

$$\Omega(T, V, \mu) = -T \log Z_{GC}(T, V, \mu), \quad (4)$$

$$F(T, V, N) = -T \log Z_C(T, V, N), \quad (5)$$

which inserting Eq. (2) yields

$$F(T, V, N) = -T \log \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i\varphi N - \frac{1}{T} \Omega(T, V, i\varphi T)}. \quad (6)$$

The right-hand side of Eq. (6) can be directly implemented in lattice QCD, since only imaginary-valued chemical

potentials are used. Note that the canonical free energy (F) of Eq. (6) is defined only at integer values of N .

Another route from $\Omega(T, V, \mu)$ to $F(T, V, N)$ employs the Legendre transform

$$F_{LT}(T, V, \langle N \rangle) = \Omega(T, V, \mu) + \mu \langle N \rangle, \quad (7)$$

with $\langle N \rangle = -\frac{\partial \Omega}{\partial \mu}$

and a function F_{LT} (LT stands for Legendre transform) depending on the unconstrained particle number $\langle N \rangle$, expected to agree with $F(T, V, N)$ only in the thermodynamic limit.

For the purpose of the paper it is instructive to derive the relation between $F(T, V, N)$ and $F_{LT}(T, V, \langle N \rangle)$. For this we will suppress some of the function arguments. Let us imagine that the system described by $\Omega(\mu)$ is replicated α times. The replicas together are described by the total thermodynamic potential, volume and particle number of $\alpha\Omega$, αV and αN . The total baryon number $N_\alpha = \alpha N$ we require to be an integer, so that we can define the total Helmholtz free energy. F_α is $1/\alpha$ times this total free energy.

$$F_\alpha(T, V, N = N_\alpha/\alpha) = -\frac{T}{\alpha} \log \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i\varphi N_\alpha - \frac{\alpha}{T} \Omega(i\varphi T)} \quad (8)$$

F_α stands for the canonical free energy averaged over the replicas, which together account for $N_\alpha = \alpha N$ particles. The Fourier transform in Eq. (8) requires that the replicas have N_α particles among themselves, but the distribution among the replicas is unspecified. Therefore $N = N_\alpha/\alpha$ does not need to be an integer. Moreover, F_α can be defined through Eq. (8) even for noninteger valued α .

In the following derivation we demonstrate that the Legendre transformed free energy can be obtained in the following limit:

$$F_\alpha(T, V, \langle N \rangle) = F_{LT}(T, V, \langle N \rangle) - \frac{T}{\alpha} \log \frac{1}{2\pi\sqrt{\alpha}} \int_{-\pi\sqrt{\alpha}}^{\pi\sqrt{\alpha}} dx \exp \left[-VT^3 \sum_{n=2}^{\infty} \frac{\chi_n(\varphi^*)}{n! \alpha^{n/2-1}} (x - \sqrt{\alpha} i \text{Im } \varphi^*)^n \right] \quad (13)$$

Since this definite Gaussian integral converges to $\int_{-\infty}^{\infty} dx$ faster than any power as $\alpha \rightarrow \infty$, being interested in the leading asymptotic behavior we can safely extend the integral limits. This then allows us to shift the integration contour via $z = x - i\sqrt{\alpha} \text{Im } \varphi^*$. At this point the leading Gaussian integral asymptotically gives $\sqrt{\frac{2\pi}{VT^3 \chi_2(\varphi^*)}}$, while the subleading terms can be further expanded in $1/\sqrt{\alpha}$ as

$$\int_{-\infty}^{\infty} dz e^{-\frac{VT^3 \chi_2}{2} z^2} \prod_{n=3}^{\infty} \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{z}{\sqrt{\alpha}} \right)^{nk} \left[\frac{-VT^3 \alpha \chi_n}{n!} \right]^k.$$

$$F_{LT}(T, V, \langle N \rangle) = F_\alpha(T, V, \langle N \rangle) + \frac{T}{2} \alpha^{-1} \log \alpha^{-1} + \mathcal{O}\left(\frac{1}{\alpha}\right) \quad (9)$$

In this limit procedure α can take only values where $\langle N \rangle \alpha$ is integer valued.

Let us denote with μ^* the chemical potential solving the equation

$$\langle N \rangle = -\frac{\partial \Omega}{\partial \mu} \Big|_{\mu=\mu^*}. \quad (10)$$

In this case, at $i\varphi^* = \mu^*/T$ the φ -derivative of the exponent in Eq. (8) is zero: in other words, φ^* defines a saddle point. Note that, a real $\langle N \rangle$ will result an imaginary valued φ^* . We will, nevertheless, consider a generic complex φ^* . First adjusting the boundaries of the periodic integral, then expanding around the saddle point φ^* one finds

$$F_\alpha(T, V, \langle N \rangle) = -\frac{T}{\alpha} \log \int_{\text{Re } \varphi^* - \pi}^{\text{Re } \varphi^* + \pi} \frac{d\varphi}{2\pi} e^{-i\varphi^* \alpha \langle N \rangle - \frac{\alpha}{T} \Omega(i\varphi^* T)} \cdot e^{-\alpha VT^3 \sum_{n=2}^{\infty} \frac{\chi_n(\varphi^*)}{n!} (\varphi - \varphi^*)^n}, \quad (11)$$

where we introduced the standard notation for the generalized (baryon) susceptibilities:

$$\chi_n = \frac{1}{VT^3} \frac{\partial^n \log Z_{GC}}{\partial (\mu/T)^n}. \quad (12)$$

Now, in the first exponent of Eq. (11) we recognize $-\frac{\alpha}{T} F_{LT}(T, V, \langle N \rangle)$, which is independent of the integration variable φ and can be pulled out. After the substitution $x = \sqrt{\alpha}(\varphi - \text{Re } \varphi^*)$ we get

Here, odd terms in $\sqrt{\alpha}$ will evaluate to zero, hence the leading correction will be of order $1/\alpha$ [one term is $\sim (\chi_3)^2$ and one is $\sim \chi_4$]. For this derivation we assumed that $\Omega(\mu)$ is an analytic function, allowing the shifting of the integration contour and the use of the Taylor expansion.

In conclusion, we can express the Legendre-transformed F_{LT} as a limit with known asymptotic behavior [53]

$$F_\alpha(T, V, \langle N \rangle) = F_{LT}(T, V, \langle N \rangle) + \frac{T}{2\alpha} \log (2\pi \alpha \chi_2(\mu^*) VT^3) \times (1 + \mathcal{O}(\alpha^{-1})), \quad (14)$$

as announced in Eq. (9). The $\alpha^{-1} \log \alpha^{-1}$ term also converges to zero in the infinite α limit, and drops out from the V and N derivatives. In Sec. V we will use Eq. (9) with several α values to numerically perform the $\alpha \rightarrow \infty$ extrapolation and recover F .

In this paper we will focus on the charting of the QCD phase diagram, and in particular on bulk observables like the chemical potential μ , the pressure and its derivatives with respect to μ itself. The chemical potential is easily found in the Legendre transform formalism via

$$\mu(T, V, \langle N \rangle) = \frac{\partial F_{LT}(T, V, \langle N \rangle)}{\partial \langle N \rangle}. \quad (15)$$

In the case of $F(T, V, N)$ with integer-valued N this is usually understood as a discrete derivative of the form

$$\mu^f = F(T, V, N+1) - F(T, V, N), \quad (16)$$

$$\mu^b = F(T, V, N) - F(T, V, N-1), \quad (17)$$

where the indices f and b stand for forward and backward derivatives. Some authors in the lattice community prefer μ^f [46,49], some use μ^b [45], but in a sufficiently large volume ($V \rightarrow \infty$ with constant density N/V) both derivatives approach $\mu(T, V, N)$ as $1/V$, as one can easily see from Eq. (15). This is under the assumption that the volume asymptotics in the grand canonical $\Omega(T, V, \mu)$ is faster than $1/\alpha$. In fact, in the absence of a massless degree of freedom, one expects an exponential approach to the thermodynamic limit.

To define the grand canonical pressure it is common to make the assumption of perfect homogeneity, i.e.,

$$p_{GC} = -\frac{\partial \Omega}{\partial V} \approx -\frac{\Omega}{V} = \frac{T}{V} \log Z_{GC}, \quad (18)$$

and the volume derivative for the pressure in the canonical setup can only be performed under the same assumption, that is

$$\Omega(T, cV, \mu) = c\Omega(T, V, \mu), \quad (19)$$

$$F(T, cV, N) = -T \log \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i\varphi N - cT^{-1}\Omega(T, V, i\varphi T)}. \quad (20)$$

With this volume dependence the canonical pressure reads

$$\begin{aligned} p_C(T, V, N) &= -\left(\frac{\partial F(T, V, N)}{\partial V} \right)_{T, N} = -\frac{1}{V} \frac{dF(T, cV, N)}{dc} \Big|_{c=1} \\ &= -\frac{T}{V} \frac{\int_0^{2\pi} \frac{d\varphi}{2\pi} \Omega(i\varphi T) e^{-i\varphi N - T^{-1}\Omega(T, V, i\varphi T)}}{\int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i\varphi N - T^{-1}\Omega(T, V, i\varphi T)}}. \end{aligned} \quad (21)$$

So far we have not fixed the normalization of Z_{GC} and Z_C . What we will actually compute in Sec. III is the ratio

$$Z_{GCR}(\varphi) = Z_{GC}(\mu = i\varphi T) / Z_{GC}(\mu = 0) \quad (22)$$

(GCR stands for grand canonical ratio). Then, on the level of Eq. (6) we will actually have $\log Z_C(N) - \log Z_{GC}(\mu = 0)$ as the logarithm of the Fourier transform of Eq. (22). This means that this formalism computes the QCD pressure relative to the grand canonical $\mu = 0$ result, i.e.

$$\begin{aligned} \Delta p_C(T, V, N) &= p_C(T, V, N) - p_{GC}(T, V, \mu = 0) \\ &= \frac{T}{V} \frac{\int_0^{2\pi} \frac{d\varphi}{2\pi} Z_{GCR}(\varphi) \log Z_{GCR}(\varphi) e^{-i\varphi N}}{\int_0^{2\pi} \frac{d\varphi}{2\pi} Z_{GCR}(\varphi) e^{-i\varphi N}} \end{aligned} \quad (23)$$

This last equation is convenient for lattice implementation, and we will show our corresponding results in Sec. IV. Note that at $N = 0$ this is negative and proportional to $\sim 1/V$.

Another quantity of great interest in the study of the QCD phase diagram is the fluctuation of N (the net baryon number), which is a grand canonical observable (χ_2). Yet, it is possible to extract this from F_{LT} as

$$\frac{\partial^2}{\partial \langle N \rangle^2} F_{LT}(T, V, \langle N \rangle) = \frac{T}{(VT^3)\chi_2}, \quad (24)$$

or, starting from F and with integer N

$$\begin{aligned} \frac{1}{\chi_2} &= VT^2 (F(T, V, N+1) - 2F(T, V, N) \\ &\quad + F(T, V, N-1)) + \mathcal{O}(V^{-1}), \end{aligned} \quad (25)$$

where the asymptotic form is valid at fixed density.

For the interested reader we present a detailed account on the noninteracting hadron gas in the Appendix. There we actually derive the leading volume effects and show how the thermodynamic limit is reached. It turns out that in the hadronic phase the finite volume corrections to the backward derivative approximately cancel, and so it reproduces the grand canonical μ already with very small N . Of course, the range where this model gives an adequate description of lattice data is limited to $T < T_c$. Nevertheless, we will use the backward derivative μ^b of Eq. (17), motivated by this model, consistently at all temperatures.

III. OPTIMIZED REWEIGHTING TO THE CANONICAL ENSEMBLE

We include all technical details on our lattice analysis in this section. Section III A summarizes the main ingredients to go from the original $\mu_B = 0$ ensembles to observables at fixed N_B . We will also discuss the staggered rooting here. Section III B proposes an optimized reweighting scheme for the correct sampling of the center sectors. Without this step the errors would be dramatically larger. Readers not interested in these technical details can safely skip this section.

A. Construction of the canonical determinants

The starting point for our study is a set of grand canonical ensembles at $\mu_B = 0$ on a $16^3 \times 8$ lattice with physical pion masses, namely one ensemble per temperature in the range $T = 110 \dots 200$ MeV. Each ensemble was simulated in $\mathcal{O}(100)$ streams with ca. 300k trajectories in every RHMC stream. The employed 4HEX staggered action and earlier stages of these simulations have already been documented in Refs. [27,54]. The statistics is given in Table I.

There are several approaches in the literature to create a canonical ensemble. Our approach is most similar to Refs. [45,52], in the sense that these works also start with $\mu_B = 0$ ensembles.

The grand canonical path integral at imaginary baryochemical potential $\mu_B/T = i\varphi$ in QCD with N_f degenerate flavors reads

$$Z_{GCR}(\varphi) = \frac{1}{Z_{GC}(\mu=0)} \int \mathcal{D}U (\det M(U, \varphi/3))^{N_f} e^{-\beta S_G(U)} \quad (26)$$

where S_G is the gauge action, and $\det M$ stands for the quark determinant. Its argument $\varphi/3$ refers to the (imaginary) quark chemical potential. We work in the staggered

TABLE I. Statistics of the $\mu_B = 0$ ensembles on the $16^3 \times 8$ lattice. On each configuration the full eigenvalue problems of both the strange and light determinants were solved. We also give the percentage of the gauge configurations per center sector as defined in Sec. III B.

T [MeV]	Statistics	Center sector distribution [%]		
		0	$+2\pi/3$	$-2\pi/3$
110	410816	87.7	6.1	6.2
115	1054391	90.8	4.6	4.6
120	1080583	93.3	3.4	3.3
125	1512103	95.4	2.3	2.3
130	2129599	96.9	1.5	1.5
135	1216275	98.0	1.0	1.0
140	4002298	98.8	0.6	0.6
145	2277535	99.3	0.35	0.34
150	1496094	99.6	0.19	0.19
155	1622365	99.8	0.93	0.94
160	2226025	99.9	0.045	0.044
165	1649108	100.0	0.019	0.02
170	1166291	100.0	0.0083	0.0086
175	1599122	100.0	0.0027	0.0036
180	1240882	100.0	0.0015	0.0012
185	851014	100.0	0.00071	0.00035
190	317898	100.0	0.00031	0.0
195	361870	100.0	0.00028	0.0
200	323969	100.0	0.0	0.0

formulation with degenerate light flavors and a heavier strange flavor. In this (physical) setup we introduce two phases, φ_B and φ_S for the baryon and strange chemical potentials, respectively.

$$Z_{GCR}(\varphi_B, \varphi_S) = \frac{1}{Z_{GC}(\mu=0)} \int \mathcal{D}U (\det M_{KS}(U, m_{ud}, \varphi_B/3))^{1/2} \times (\det M_{KS}(U, m_s, \varphi_B/3 - \varphi_S))^{1/4} e^{-\beta S_G(U)}. \quad (27)$$

We wrote the mass arguments (m_{ud} and m_s) of the Kogut-Susskind quark determinants explicitly for clarity.

A crucial feature of Eq. (27) is that all determinants are real and positive for real φ_B, φ_S . This means that no ambiguous rooting is performed on complex numbers. Z_{GCR} will only ever be evaluated at such real phases. Once the path integral (or in other words: ensemble average) is taken, we will introduce real densities in the canonical formalism.

A second important feature of the path integral in Eq. (27) is its periodicity both in φ_B and in φ_S :

$$Z_{GCR}(\varphi_B, \varphi_S) = Z_{GCR}(\varphi_B, \varphi_S + 2\pi) \quad (28)$$

$$Z_{GCR}(\varphi_B, \varphi_S) = Z_{GCR}(\varphi_B + 2\pi, \varphi_S). \quad (29)$$

This was pointed out first in Ref. [55]. Its direct consequence is the Roberge-Weiss transition at $\mu_B = i\pi T$ at high temperature. The periodicity is the consequence of two statements:

(a) An imaginary quark chemical potential φ_q can be interpreted as a phase factor $e^{i\varphi_q}$ introduced in the periodic Euclidean temporal boundary condition for the quark fields. Since this factor is just 1 for $\varphi_q = 2\pi$, this immediately explains Eq. (28).

(b) The unbroken center symmetry of the gauge action and the Haar measure allows the simultaneous transformation of the gauge fields on a single time slice by an element of the center group $\mathbb{Z}_3$: $e^{-i2\pi/3}$. The determinants will maintain their value if all quark chemical potentials are set forward by $2\pi/3$ at the same time. This amounts to a change $\varphi_B \rightarrow \varphi_B + 2\pi$. From (a) and (b) follows that the parameter space we need to cover is $0, \dots, 2\pi$ in both φ_B and φ_S .

Let us now exploit charge conjugation ($\mathcal{C}$) symmetry. It applies for φ_B and φ_S together, implying

$$Z_{GCR}(\varphi_B, \varphi_S) = Z_{GCR}(-\varphi_B, -\varphi_S) = Z_{GCR}(2\pi - \varphi_B, 2\pi - \varphi_S). \quad (30)$$

This means, that $\mathcal{C}$ -symmetry connects each (φ_B, φ_S) point with its mirror image with respect to $(\pi/2, \pi/2)$. This further shrinks the parameter space by a factor two. We choose to half the space as $\varphi_B = 0, \dots, \pi$ and $\varphi_S = 0, \dots, 2\pi$, though

other halving prescriptions are also possible. This two dimensional range was explored in Ref. [56] through a 2D mesh of simulation points in an effort to compute the fugacity expansion of $Z_{GCR}(\varphi_B, \varphi_S)$. Here, instead, we compute this ratio by means of reweighting from zero to imaginary chemical potential. It may sound unnecessary to reweight to a point in the parameter space, where simulations are easily possible. However, reweighting has some clear advantages. First, one can evaluate the determinants at any chemical potential, thus $Z_{GCR}(\varphi_B, \varphi_S)$ will be available as a continuous function in both arguments. Second, the statistical correlations between nearby (and also distant) parameters are fully kept. Without the first feature some modeling of the data would be necessary, this is precisely what we wish to avoid in this work. Without the second feature the higher modes in the Fourier transform of Z_{GCR} would be lost in the noise.

The computation of the quark determinants is a numerical challenge. We use the reduced matrix formalism for staggered quarks [50], whereby the quark determinant are represented by a set of $6N_x \times N_z \times N_y$ eigenvalues ξ_i

$$\frac{\det M_{KS}(U, m, \varphi)}{\det M_{KS}(U, m, 0)} = \prod_{i=1}^{6N_x} \frac{\xi_i(m, U) - e^{i\varphi}}{\xi_i(m, U) - 1}. \quad (31)$$

This determinant is manifestly real, thanks to the γ_5 -Hermiticity. This implies that every ξ_i eigenvalue has a pair ξ_j with $\xi_i = 1/\xi_j^*$. This can be also exploited to maintain numerical stability. The resulting reweighted partition function can then be written as an ensemble average

$$Z_{GCR}(\varphi_B, \varphi_S) = \left\langle \left(\frac{\det M_{KS}(U, m_{ud}, \varphi_B/3)}{\det M_{KS}(U, m_{ud}, 0)} \right)^{1/2} \times \left(\frac{\det M_{KS}(U, m_s, \varphi_B/3 - \varphi_S)}{\det M_{KS}(U, m_s, 0)} \right)^{1/4} \right\rangle \quad (32)$$

The practical usefulness of this formula depends on the knowledge of the $\xi_i(U, m)$ eigenvalues. Our lattice simulation code computes the reduced matrix, which is 24576×24576 for our $16^3 \times 8$ staggered lattices. The 4HEX smearing is applied before the construction of the matrix, and we do this computation and the subsequent call to QR-algorithm (and the preparatory transformation to upper Hessenberg form) separately for the two masses. For the dense linear algebra we use the MAGMA linear algebra package [57]. The main part of the computer resources used for this project is spent in the MAGMA library. We carried out these steps for all the configurations listed in Table I. We refer to Ref. [58] for further technical details.

Once we know the 2×24576 eigenvalues for each of the $\mathcal{O}(10^6)$ configurations, the computation of Eq. (32) is straightforward and requires the computational power of a

modern workstation. We computed $Z_{GCR}(\varphi_B, \varphi_S)$ on a grid of 33×64 parameters [mapped to $[0, \pi] \times [0, 2\pi]$]. Refining the grid did not bring noticeable changes in the result. Before taking the ensemble averages two manifestly positive determinant functions were precalculated at 192 imaginary quark chemicals each, amounting to 384 real numbers per configuration:

$$D_q(\varphi_q) = \left(\frac{\det M_{KS}(U, m_{ud}, \varphi_q)}{\det M_{KS}(U, m_{ud}, 0)} \right)^{1/2} \times \left(\frac{\det M_{KS}(U, m_s, \varphi_q)}{\det M_{KS}(U, m_s, 0)} \right)^{1/4}, \quad (33)$$

$$D_s(\varphi_s) = \left(\frac{\det M_{KS}(U, m_s, \varphi_s)}{\det M_{KS}(U, m_s, 0)} \right)^{1/4}. \quad (34)$$

The average in Eq. (32) is finally transformed to a canonical partition function via

$$Z_C(N_B, N_S) = \int_0^{2\pi} \frac{d\varphi_B}{2\pi} e^{-i\varphi_B N_B} \times \int_0^{2\pi} \frac{d\varphi_S}{2\pi} e^{-i\varphi_S N_S} Z_{GCR}(\varphi_B, \varphi_S). \quad (35)$$

While our data and this formalism allow two conserved charges, N_B and N_S , in the present work we will focus on the N_B dependence only. The study of the role played by strangeness is deferred to future work. Some preliminary results in N_B and N_S together were shown in [59]. Hence, we study the baryo-canonical ensemble

$$Z_C(N_B) = \int_0^{2\pi} \frac{d\varphi_B}{2\pi} e^{-i\varphi_B N_B} Z_{GCR}(\varphi_B, \varphi_S = 0) \quad (36)$$

which was also the focus of existing literature.

Notice that we deferred the Fourier transform to after the ensemble average. Contrary to other works in the literature, we did not introduce a canonical determinant. For the simple $\varphi_S = 0$ case this is a complex sequence $\tilde{D}_N$ for every configuration

$$\tilde{D}_N(U) = \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i\varphi N} D_q(\varphi/3). \quad (37)$$

Since the ensemble average in Eq. (32) is linear, it is our freedom, to choose the order: we either Fourier transform each determinant function separately [obtaining $\tilde{D}_N(U)$] and average these, or averaging $Z_{GCR}(\varphi)$ and transforming the average once. Our choice for the latter is motivated not merely to save the costs of several million Fourier transforms, but it will also give us the freedom to introduce the α replica parameter of Eq. (8), that will play an important role in Sec. V.

Here we mention a promising sampling algorithm that is based on canonical determinants [46]. Although the

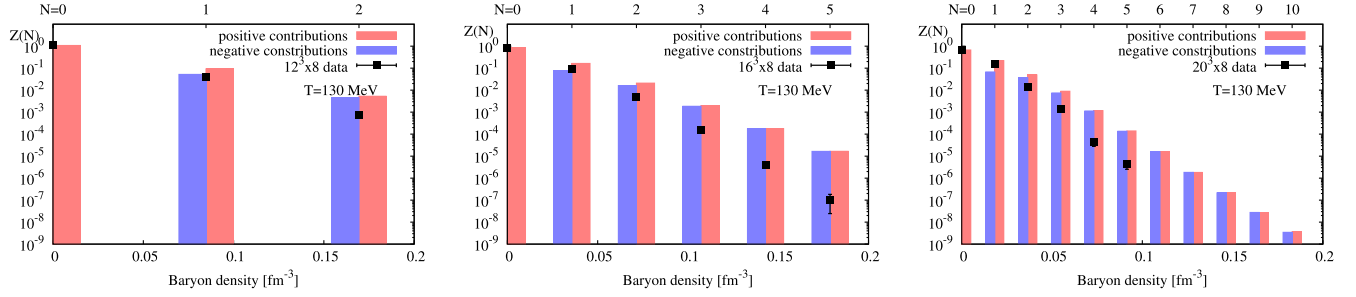


FIG. 2. We show the canonical partition function as a function of baryon density for three volumes at a fixed temperature $T = 130$ MeV. The black symbols are the result of the cancellation of positive and negative contributions, shown as red and blue bars, respectively. The set of plots illustrates the growing severity of the sign problem as the density or the volume is increased.

canonical determinants are complex numbers, $Z_C(N)$ is real, as the imaginary parts exactly cancel between configuration U and its conjugate U^* . The real part of $\tilde{D}_N(U)$ is not positive, though. If it was, a straightforward importance sampling could be implemented. The Kentucky algorithm [46,48] simulates a canonical ensemble with fixed N . It takes $|\text{Re}\tilde{D}_N(U)|$ instead of $\text{Re}\tilde{D}_N(U)$ as the simulation weight, in a procedure called sign quenching. In a second step the missing sign is reintroduced by means of reweighting, which is where the sign problem hits. An analogous procedure was applied to finite μ_B in Refs. [37,38]. For staggered fermions the canonical sign quenching has one advantage over its grand canonical analog: the staggered rooting is performed on real determinants, which become complex only after the rooting through the Fourier transform. The Kentucky algorithm comes with the high costs of computing $\tilde{D}_N(U)$ at every update, unlike the approach followed in this work, where we save every 20th configuration and thus calculate $D_q(\varphi)$ on a much smaller set.

The sign problem in the canonical ensemble can be illustrated by displaying the resulting $Z_C(N)$ together with its positive and negative contributions (see Fig. 2). The distance between the top edge of the red bar and the black data point on the logarithmic scale can be interpreted as the severity of the cancellations for a given particle number. Although both $Z(N)$ and the sum of the positive-only contributions drop near-exponentially with increasing N , the rates differ, resulting in an exponential sign problem.

B. Algorithmic support for the restoration of center symmetry

Dynamical grand canonical simulations break the $\mathbb{Z}_3$ center symmetry through the temporal boundary condition, even at $\mu_B = 0$. If the simulation volume is large, this can mean that only a single sector is sampled. Remarkably, all three center sectors contribute equally to the canonical ensemble. The employed lattice algorithm must then ensure the even sampling of the sectors. This is clearly not

automatically achieved in a grand canonical simulation. For example, with the moderate volume used here ($16^3 \times 8$ lattice), only a small minority of the configurations belong to either of the two disfavored center sectors. See Table I for the empirical distribution between center sectors.

The $D_q(\varphi_q)$ of Eq. (33) can be computed without difficulty, and has a period of 2π by construction. Upon building an ensemble average $\langle D_q(\varphi_q) \rangle = Z_{GCR}(\varphi_q/3)$ has a period of $2\pi/3$, as required by the center symmetry. It was already noticed in the earliest canonical work [50] that the naive average $\langle D_q(\varphi_q) \rangle$ contradicts this symmetry principle. We illustrate this in Fig. 3. As Ref. [50] notes, only very good statistics simulations can recover the correct periodic behavior, shown here in red. We see in this example that ten-folding the statistics two times in a row has only made the errors larger, while a precise periodic $\langle D_q(\varphi_q) \rangle$ could not be obtained even in the moderate volume and with the high statistics used in this study. Reference [50] could identify the “outliers” (shown as sector 1,2 example in the right panel of Fig. 3). Reference [50] also introduces the idea of using the geometric mean of rotated versions of the determinant, as a remedy. This, however, would be equivalent to simulating at an imaginary isospin chemical potential, known to lead to a first order transition [60,61].

In the canonical update algorithms of Refs. [44,46] an extra sector-changing update is performed ($U \rightarrow U'$), by rotating the temporal link variables on one fixed time-slices with the center element of the gauge group. Since the phase on the last time-slice is just how the imaginary-valued chemical is defined, this also means

$$U \xrightarrow{e^{-i2\pi/3}} U': D_q(U, \varphi_q) \rightarrow D_q(U, \varphi_q + 2\pi/3) = D_q(U', \varphi_q) \quad (38)$$

In a canonical ensemble U and the center rotated U' and U'' configurations have exactly equal weight, given by the

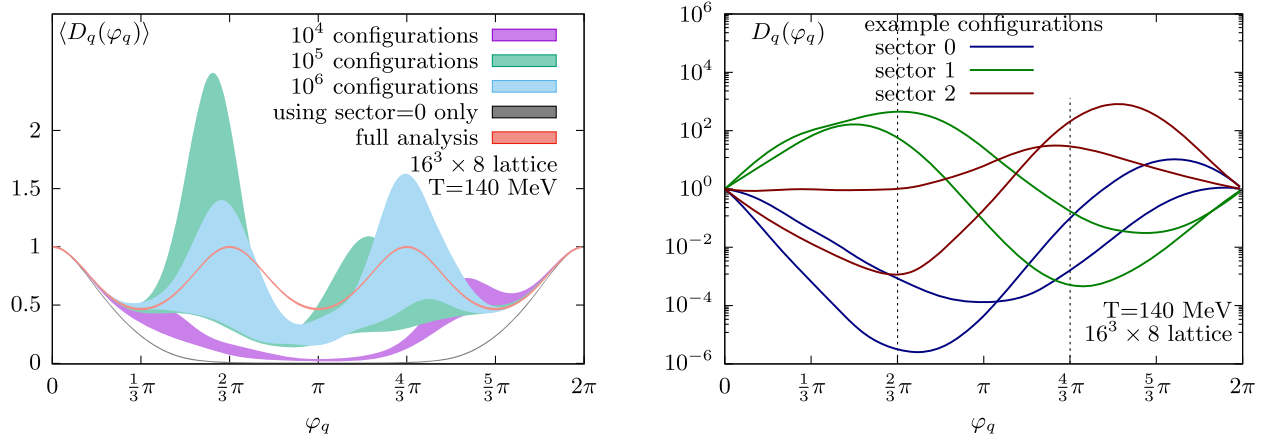


FIG. 3. Illustrations of the quark determinant in Eq. (33) and our strategy to compute its ensemble average. Left panel: while the period of $D_q(\varphi_q)$ is $2\pi/3$, this is very difficult to see even in a high statistics ensemble. With 10^4 configurations we get a clearly wrong answer, but even ten or hundredfold statistics does not bring us much closer to the true result, either. The solution is the partitioning of the configuration space into three equivalent center sectors, the zero sector's result is shown in black [$\langle D_q(\varphi_q) \rangle_{S0}$]. The red curve is the sum of the black curve and its two possible shifted forms with an additional normalization [see Eq. (46)]. Right panel: we show an example configuration for each sector from our pool of configurations.

arithmetic (not geometric) mean of rotated and not rotated determinants [44].

$$w(U', \varphi_q - 2\pi/3) = w(U, \varphi_q) = \frac{1}{3} (D_q(\varphi_q) + D_q(\varphi_q + 2\pi/3) + D_q(\varphi_q - 2\pi/3)). \quad (39)$$

Then, our task is to compute $\langle w(U, \varphi) \rangle$ starting from a $\mu_B = 0$ ensemble. The key principle for doing so is a partitioning of the configuration space into three disjoint center sectors. It is then necessary that (i) this is well defined for any given configuration, (ii) a center transformation of an individual configuration steps through the sectors, and (iii) a center transformation does not change the weight [$w(U, \varphi_q)$] in the canonical ensemble. A suboptimal partitioning adhering to these axioms could be given in terms of the phase of the Polyakov loop, for the optimal method we ask for the reader's patience.

We will write the ensemble average of an observable $\mathcal{O}$ restricted to one sector, e.g., sector 1 as

$$\langle \mathcal{O} \rangle_{S1} = \frac{\int DU|_{\text{Sector1}} e^{-S_{\text{eff}}(U)} \mathcal{O}(U)}{\int DU|_{\text{Sector1}} e^{-S_{\text{eff}}(U)}} \quad (40)$$

where S_{eff} is the effective action after integrating out the quarks at zero chemical potential, where the simulation was run. Clearly, the normalization of this path integral differs from that of the unrestricted integral, because their ratio is not $1/3$ due to the $\mu_B = 0$ ensemble breaking center symmetry.

Calling the restricted partition functions Z_{S0} , Z_{S1} and Z_{S2} for the three sectors, the full expectation value of an arbitrary operator can be expressed as

$$\langle \mathcal{O} \rangle = \frac{Z_{S0} \langle \mathcal{O} \rangle_{S0} + Z_{S1} \langle \mathcal{O} \rangle_{S1} + Z_{S2} \langle \mathcal{O} \rangle_{S2}}{Z_{S0} + Z_{S1} + Z_{S2}} \quad (41)$$

Let us now substitute $D_q(\varphi_q)$ for $\mathcal{O}$. The unbroken center symmetry is manifest in Eq. (41), and we only need the range $-\pi/3 \leq \varphi_q \leq \pi/3$ for a full result.

$$\langle D_q(\varphi_q) \rangle = \frac{Z_{S0} \langle D_q(\varphi_q) \rangle_{S0} + Z_{S1} \langle D_q(\varphi_q) \rangle_{S1} + Z_{S2} \langle D_q(\varphi_q) \rangle_{S2}}{Z_{S0} + Z_{S1} + Z_{S2}} \quad (42)$$

We exploit that the center transformation ($\varphi_q \rightarrow \varphi_q + 2\pi/3$) steps into the next sector, e.g.

$$\begin{aligned}
Z_{S1} \langle D_q(\varphi_q) \rangle_{S1} &= \int DU|_{\text{Sector}1} e^{-S_{\text{eff}}(U)} D_q(\varphi_q) \\
&= \int DU|_{\text{Sector}0} e^{-S_{\text{eff}}(U)} D_q(\varphi_q + 2\pi/3) = Z_{S0} \langle D_q(\varphi_q + 2\pi/3) \rangle_{S0}
\end{aligned} \tag{43}$$

$$\langle D_q(\varphi_q) \rangle = \frac{Z_{S0} \langle D_q(\varphi_q) \rangle_{S0} + Z_{S0} \langle D_q(\varphi_q + 2\pi/3) \rangle_{S0} + Z_{S0} \langle D_q(\varphi_q - 2\pi/3) \rangle_{S0}}{Z_{S0} + Z_{S1} + Z_{S2}} \tag{44}$$

Using Eq. (43) also to relate Z_{S0} , Z_{S1} and Z_{S2} as

$$\frac{Z_{S1,S2}}{Z_{S0}} = \langle D_q(\pm 2\pi/3) \rangle_{S0} \tag{45}$$

we finally write the desired expectation value solely employing sector 0 configurations:

$$\langle D_q(\varphi_q) \rangle = \frac{\langle D_q(\varphi_q) \rangle_{S0} + \langle D_q(\varphi_q + 2\pi/3) \rangle_{S0} + \langle D_q(\varphi_q - 2\pi/3) \rangle_{S0}}{\langle D_q(0) \rangle_{S0} + \langle D_q(+2\pi/3) \rangle_{S0} + \langle D_q(-2\pi/3) \rangle_{S0}}. \tag{46}$$

For an optimal partitioning of the configuration space into center sectors we should have a second look at Fig. 3. What makes the naive averaging of $D_q(\varphi_q)$ difficult between $\pi/3$ and $5\pi/3$ is the dynamical range of the determinants. The six random examples in Fig. 3 spread across nine orders of magnitude, which would be even more in a larger volume. The true expectation value of $\langle D_q(2\pi/3) \rangle = 1$ is realized as an average including some extremely rare $[\mathcal{O}(10^{-3})]$ configurations in sectors 1 and 2 with a contribution of $[\mathcal{O}(10^{+3})]$.

Every configuration can be sampled by either of the three ensembles, defined at $\mu_q/T = i\phi_q \in \{0, i2\pi/3, -i2\pi/3\}$, though with different probability. It is the determinant ratio $D_q(U, \varphi_q)$ itself that tells this relative probability: a configuration U will be generated in an ensemble at $\mu_q/T = i2\pi/3$ with a factor $D_q(U, 2\pi/3)/D_q(U, 0)$ larger probability in comparison to the ensemble at $\mu_q = 0$. Our partitioning is based on the chemical potential (one of $\{0, i2\pi/3, -i2\pi/3\}$) where a given configuration has the highest probability to appear. In other words, whichever of the three positive (rooted) determinants is the largest,

$$D_q(U, 0), \quad D_q(U, 2\pi/3), \quad D_q(U, -2\pi/3) \tag{47}$$

specifies the sector to be S0, S1 or S2, respectively. This criterion trivially fulfills the axioms required above and is optimal in the sense that it keeps only those configurations from the $\mu_B = 0$ ensemble, that would not have been better sampled by other ensembles, such as $\mu_q = \pm i2\pi/3$. With this selection rule, Eq. (46) gives a very precise result. We show this in red in Fig. 3. The percentage of the configurations that contribute to the final average, and the discarded ones in sector 1 and 2 are listed in Table I.

IV. THERMODYNAMICS AT FINITE DENSITY

The observable that we directly computed on the lattice in the previous section is $Z_{GCR}(T, V, \varphi)$, which gives the canonical partition function $Z_C(T, V, N)$ through a Fourier transform in φ as written in Eq. (3). The limiting factor of how large an N we can extract with this Fourier transform is the statistical error.

An example of the resulting $Z_C(T, V, N)$ is shown in Fig. 4 at $T = 140$ MeV, which is the temperature with the highest statistics (see Table I). Sitting below the pseudocritical temperature, we expect $Z_C(N)$ to follow the Skellam

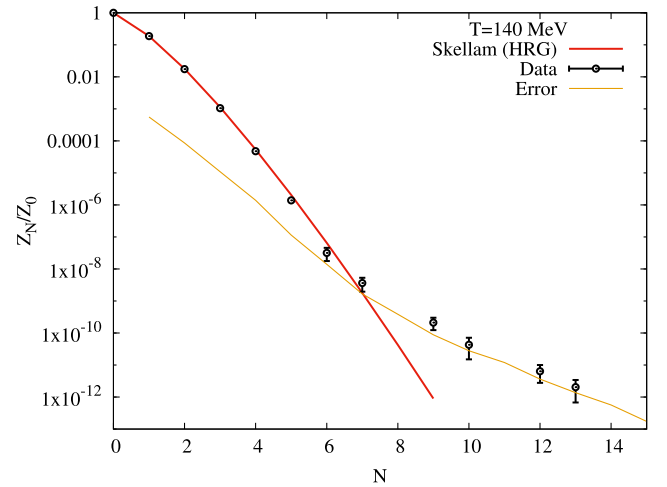


FIG. 4. The canonical partition sum Z_C for the example of $T = 140$ MeV. For the lowest particle numbers we find good agreement with the Skellam distribution. The level of the statistical error is shown as an orange line. From $N = 6$ on the statistical error is 100%. The magnitude of Z_N then simply follows the error as a function of N .

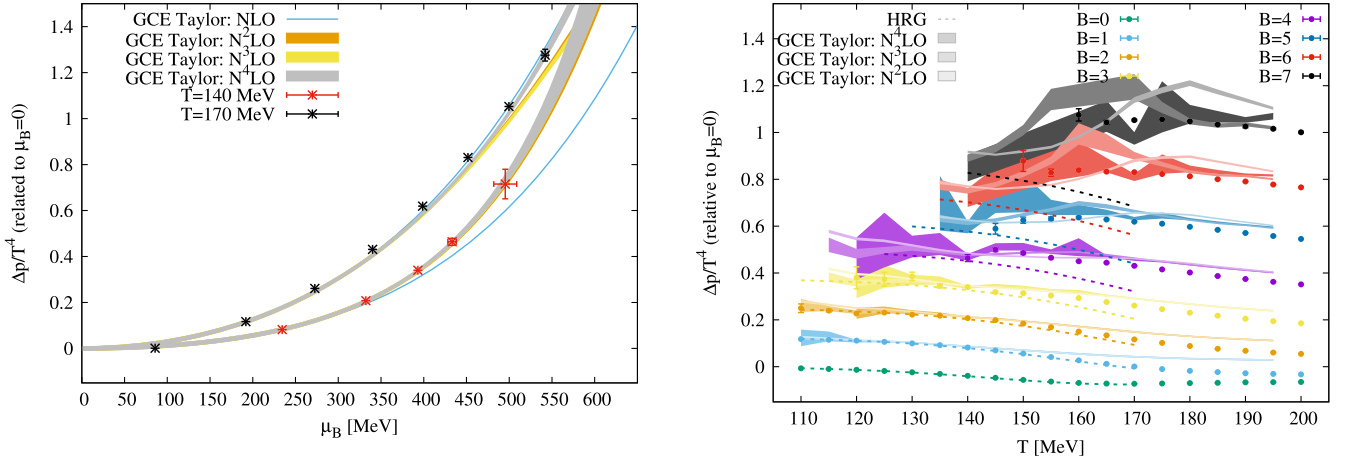


FIG. 5. Left: The relative pressure at two temperatures in the canonical ensemble. We show the Taylor expanded grand canonical results (based on the same ensemble) as color bands. Right: The relative pressure as a function of the temperature at fixed baryon number. We also show the grand canonical extrapolation as bands and the prediction of the HRG model as dotted lines.

distribution, which we show as a red curve in Fig. 4. The parameter of the Skellam distribution [see $\hat{p}_B$ in Eq. (A2)] is the leading term in the fugacity expansion that we extracted from the grand canonical data, not by fitting the points in Fig. 4.

The agreement with data is good, though the statistical error (orange line) decreases with N more slowly than the signal, eventually resulting in 100% errors for $N \geq 6$ in this case. The apparent slope of noise-dominated data reflects the error's scaling with N , and the algorithm does not protect us from unphysical, negative values ($N = 8$). In our analysis we will discard the marginally significant data points based on the error on Z_N .

From $Z_C(T, V, N)$ the computation of μ_B is straightforward, using the backward discrete derivative of Eq. (17), while the canonical pressure requires a separate Fourier transformation [see Eq. (23)]. The relative pressure that can be readily extracted from our data employs a hybrid definition: it subtracts the grand canonical pressure at $\mu_B = 0$ from the canonical pressure with particle number N , with this difference possibly negative, especially for $N = 0$. We show the relative pressure according to this definition in Fig. 5. In the left panel we plot the result of Eq. (23) against Eq. (17) together with the Taylor extrapolation to four consecutive orders in μ_B^2 .

Throughout this work we will use the GCE label to refer to the Taylor extrapolation using the very same lattice ensembles. Leading order means that the expansion is truncated at the order of $\chi_2^B(T)$, and the $N^4\text{LO}$ order includes up to $\chi_{10}^B(T)$, where $\chi_n^B(T)$ are the Taylor coefficients of the pressure:

$$\chi_n^B(T) = \left(\frac{\partial^n (p/T^4)}{\partial (\mu_B/T)^n} \right)_{\mu_B=0} \quad (48)$$

With these one expands the grand canonical density at finite μ_B as

$$\frac{n_B}{T^3} = \sum_{n=1}^{\infty} \frac{1}{(2n-1)!} \chi_{2n}^B(T) \left(\frac{\mu_B}{T} \right)^{2n-1} \quad (49)$$

The $\chi_{2n}^B(T)$ coefficients for the ensembles in this work have already been published in Ref. [31].

In order to determine the chemical potential, the Taylor expanded result for $n_B(\mu_B)$ was computed to the chosen order, then inverted to translate the density N/V to μ_B . This was not always successful, since high order fluctuations are notoriously noisy and the error on Taylor expanded results is often higher than on canonical results, even though both approaches use the very same set of configurations. One possible reason is a potential cancellation between the noise in higher orders of the Taylor expansion in a resummed setting, like the canonical ensemble. Further, the algorithmic improvement of Sec. III B has not yet been applied to the Taylor coefficients. How many orders in the Taylor expansion are needed for a given accuracy may only be known empirically, and even that is subject to statistical error. Adding one further order might perhaps only increase the error, but it can just as well shift the value enough to be incompatible with the previous order.

In the right panel of Fig. 5 we show a comparison of our canonical results with the three highest orders in the GCE. Especially for higher densities, subsequent orders are not in agreement. Our canonical data, which are compatible with the highest order except at high temperature, have consistently smaller errors. For example, at $T = 160$ MeV the simulation volume is $\sim 15 \text{ fm}^3$, thus, $B = 6$ corresponds to $n_B \sim 0.40 \text{ fm}^{-3}$. We see that the Taylor bands at $N^3\text{LO}$ and $N^4\text{LO}$ orders do not overlap, even if they are quite wide. The canonical data point is on top of the highest grand canonical order and with a much smaller error than the width of the $N^4\text{LO}$ band. We note that, especially at high T , the volume is small and the canonical and grand canonical observables are expected to agree in the thermodynamical

limit only. We also show a canonical prediction from the hadron resonance gas (HRG) model in the same figure, computed by Fourier transforming the exponentiated grand canonical potential within HRG using the simulation volume $8/T^3$ employed in this work. We could crosscheck the canonical HRG thanks to the `Thermal-FIST` package [62]. HRG is expected to describe data in the hadronic phase. As the density is increased, the range of agreement shifts to smaller temperatures, consistent with a density-dependent transition temperature. We find that at fixed density HRG underestimates the pressure difference, which is expected for a repulsive two-baryon interaction. Note that the same interactions in turn cause HRG to overestimate $\Delta p/T^4$ if μ_B is kept fixed, instead. The negative relative pressure at $N = 0$ is also apparent in the right panel of Fig. 5. Here, the fully canonical relative pressure would be the difference between the $N > 0$ and the $N = 0$ results.

In Fig. 6 we plot the chemical potential determined as the discrete (backward) derivative of the Helmholtz free energy for a set of net baryon numbers. We use the standard axes as in the QCD phase diagram, and show the QCD crossover lines from Refs. [10,13,54]. We note that the chiral crossover line of [10] is continuum extrapolated and belongs to the strangeness neutral case, whereas our canonical data come from a finite lattice spacing and a small volume ($16^3 \times 8$), and the strangeness chemical potential is set to zero for simplicity $\mu_S = 0$. In Ref. [54] we estimated the transition line from the static quark entropy (related to the Polyakov loop) in the $\mu_S = 0$ scheme [54], employing the very same ensembles as we used here with updated statistics. From this plot we see that we can chart the phase diagram until $\mu_B \approx 500$ MeV before the sign problem becomes severe. The resolution in density is low, and specific to our simulation volume. For a dense coverage in density we will generalize

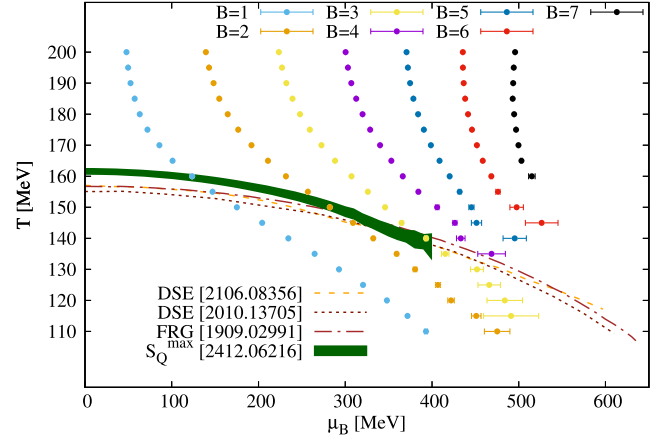


FIG. 6. Contours of constant baryon number in the simulation volume $V = 8/T^3$ on the QCD phase diagram.

this result in the next section using the saddle point technique described in Sec. V and arrive at the results in Fig. 1.

V. GENERALIZED CANONICAL RESULTS AND THE GRAND CANONICAL LIMIT

The goal of this section is to compute predictions at real chemical potentials in the grand canonical context, starting from our canonical setup. In fact, Eq. (1) shows this connection, and the same equation has already been used in this context [52]. Unfortunately, we do not know $Z_C(T, V, N)$ for high N , hence the use of Eq. (1) is not practical if we are interested in a truncation-free result. Instead, we do not start from $Z_C(T, V, N)$, but from one step before: the ratio $Z_{GCR}(T, V, \varphi)$, which we can access directly on the lattice.

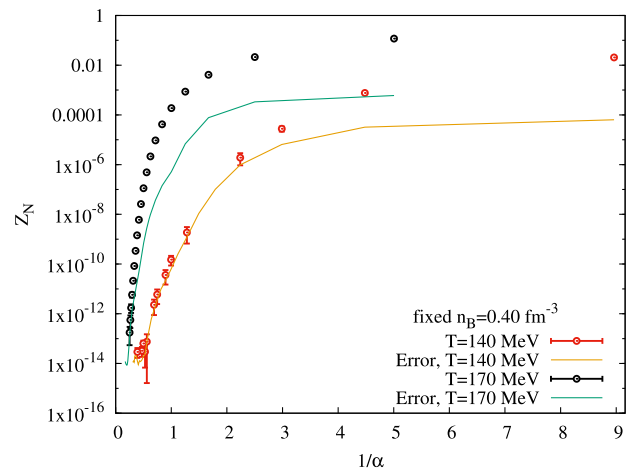
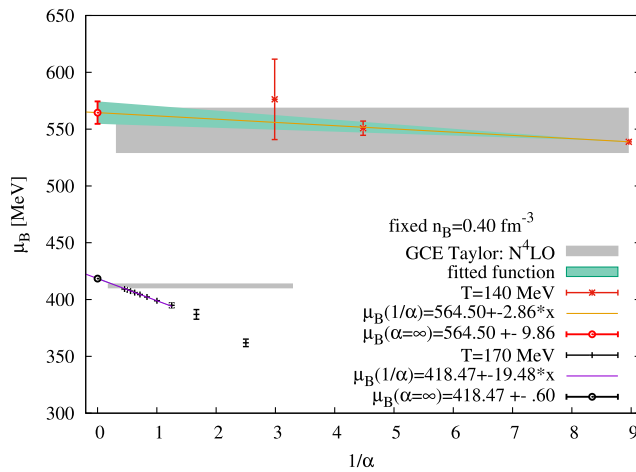


FIG. 7. Left: the baryo-chemical potential as a function of $1/\alpha$ and the $\alpha^{-1} \rightarrow 0$ limit based on simulation data. We show two temperatures at fixed baryon density. The gray band shows the Taylor-extrapolated grand canonical result using coefficients up to χ_{10}^B [31]. Right: the underlying Z_N is shown on a logarithmic scale at fixed density. The solid lines indicate the 1σ error level. For large N (small $1/\alpha$) the signal is lost, limiting the range of $1/\alpha$ usable for the extrapolation.

In Sec. IV we defined all observables starting from the free energy

$$F(T, V, N) = -T \log \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i\varphi N + \log Z_{GCR}(T, V, \varphi)}. \quad (50)$$

In Eq. (8) we introduced the replica parameter (α) that has allowed us to write a rescaled version of the canonical free energy

$$F_\alpha(T, V, N_\alpha/\alpha) = -\frac{T}{\alpha} \log \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i\varphi N_\alpha + \alpha \log Z_{GCR}(T, V, \varphi)} \quad (51)$$

In Sec. II the $\alpha \rightarrow \infty$ limit that connects F_α of Eq. (51) with the Legendre transform F_{LT} was performed at fixed T , V and $\langle N \rangle$. Equivalently, one can fix T , V and the baryon density n with

$$N_\alpha = \alpha n V. \quad (52)$$

The parameter N_α must be an integer, because of the manifest periodicity of the integrand. On the other hand, the density n is not limited to integer multiples of $1/V$. Any non-negative n can be realized by fixing N and α such that N_α is integer valued according to Eq. (52). The definition of Eq. (51) can be easily related to the asymptotic formula in Eq. (15) by

$$F_\alpha(T, V, \langle N \rangle = nV) = F_{LT}(T, V, \langle N \rangle = nV) - \frac{T}{2} \alpha^{-1} \log \alpha^{-1} + \mathcal{O}(\alpha^{-1}) \quad (53)$$

where the asymptotic form is valid for fixed density n . We can conveniently use our direct lattice result on

$Z_{GCR}(T, V, \varphi)$ to evaluate Eq. (51) for an arbitrary positive α parameter.

We propose to use Eq. (53) to take the $\alpha^{-1} \rightarrow 0$ limit numerically on the simulation data with fixed density and obtain

$$\begin{aligned} \Omega(T, V, \mu_B) + nV\mu_B &= F_{LT}(T, V, nV) \\ &= \lim_{\alpha \rightarrow \infty} F_\alpha(T, V, nV), \end{aligned} \quad (54)$$

as a result of the grand canonical limit. This translates on the level of observables to

$$\begin{aligned} \mu_B(T, V, nV) &= F_\alpha(T, V, nV) - F_\alpha(T, V, nV - \alpha^{-1}) \\ &\quad + \mathcal{O}(\alpha^{-1}), \end{aligned} \quad (55)$$

$$\begin{aligned} \Delta p_C(T, V, nV) &= \frac{T}{V} \frac{\int_0^{2\pi} \frac{d\varphi}{2\pi} [Z_{GCR}(\varphi)]^\alpha \log Z_{GCR}(\varphi) e^{-i\varphi N_\alpha}}{\int_0^{2\pi} \frac{d\varphi}{2\pi} [Z_{GCR}(\varphi)]^\alpha e^{-i\varphi N_\alpha}} \\ &\quad + \mathcal{O}(\alpha^{-1}). \end{aligned} \quad (56)$$

$$\begin{aligned} \frac{1}{\chi_2(T, V, nV)} &= VT^2 (F_\alpha(T, V, nV + \alpha^{-1}) \\ &\quad - 2F_\alpha(T, V, nV) + F_\alpha(T, V, nV - \alpha^{-1})) \\ &\quad + \mathcal{O}(\alpha^{-1}). \end{aligned} \quad (57)$$

The particle number argument nV of F_α in Eq. (55) means that the Fourier integral (51) is evaluated with baryon number $N_\alpha = \alpha nV$. The argument $nV \pm \alpha^{-1}$, in turn, means that we evaluate the Fourier integral at particle numbers $N_\alpha \pm 1$. Thus, Eqs. (57) and (55) actually implement Eqs. (17) and (25), respectively.

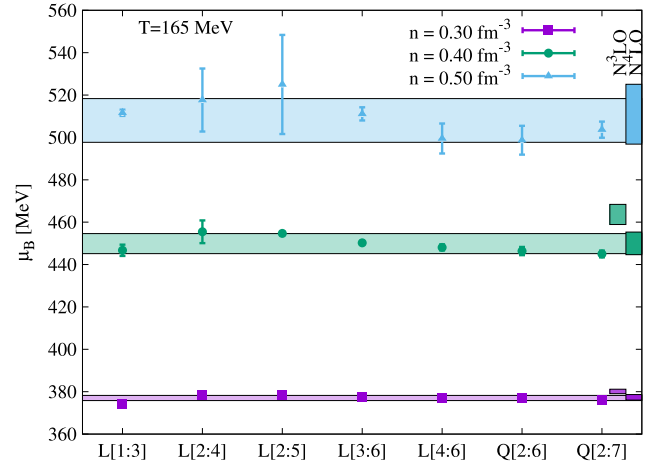
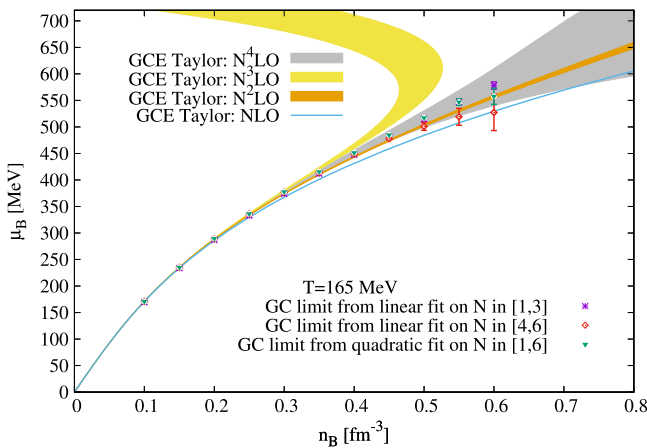


FIG. 8. We illustrate the systematic effects of the extrapolation in $1/\alpha$. In this example ($T = 165$ MeV) we show the baryo-chemical potential as a function of the net-baryon density and compare the results of the $1/\alpha$ extrapolation to various orders (error bars) of the Taylor expansion. In the left panel we show this as a function of temperature. The right panel shows the results of various linear (L) or quadratic (Q) fits in $1/N$ in the given ranges. The horizontal band shows the combined error from this procedure, while the bars in the right edge indicate two consecutive orders of the Taylor expansion.

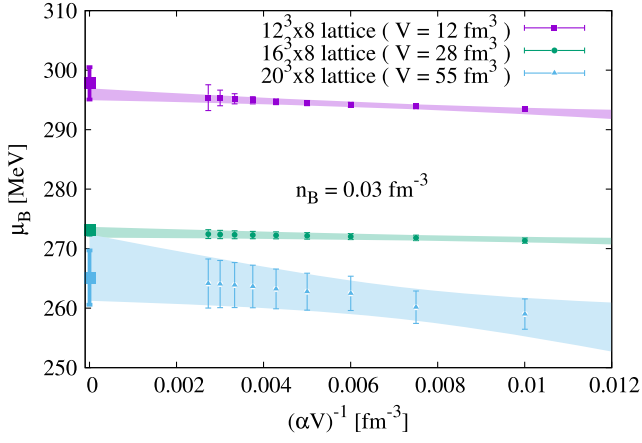


FIG. 9. The lattice data and the corresponding $1/\alpha \rightarrow 0$ limit at fixed density for three different simulation volumes. The different limits reveal the residual volume dependence of the original grand canonical setup. The error bars on the μ_B axis show the N^4 LO Taylor expanded grand canonical result ($T = 130$ MeV).

These quantities can be computed at a fixed value of the density n with several integer choices of N_α . The $\alpha \rightarrow \infty$ limit is implemented by repeating this computation for a list of N_α values, corresponding to a respective value of $\alpha = N_\alpha/(nV)$. This way a limit procedure in $1/\alpha \sim 1/N_\alpha$ can be defined. The range in N_α is limited by the sign problem (especially at low temperature) and numerical precision. Choosing a small N_α will make the higher order corrections (e.g. $\sim 1/N_\alpha^2$) relevant. We see this happen at higher temperatures where the higher precision makes these appreciable. We illustrate the limit procedure of Eqs. (55) and (56) on our simulation data at two temperatures in Fig. 7.

The range of $1/\alpha$ (or $1/N_\alpha$) that can be used in Eqs. (55) and (56) to perform the grand canonical limit ($\alpha^{-1} \rightarrow 0$) depends on data quality and the size of higher order terms. This is very similar to a continuum limit

$\alpha^2 \rightarrow 0$, which can be reached only in the form of an extrapolation. Figure 8 presents various versions of this grand canonical limit, depending on the fitting range and the order (linear or quadratic) of the fit in $1/N_\alpha$. The results mostly agree within 1σ . Below $T < 165$ MeV we do not have the luxury to vary the fitting range, e.g. at the lower temperature in Fig. 7 only three points are available for this extrapolation.

On the other hand, we are able to compare the results of this procedure on three different simulation volumes, namely $12^3 \times 8$, $16^3 \times 8$ and $20^3 \times 8$, as we show in Fig. 9. As expected, we observe the same linear approach to the GCE, and also see that the two larger volumes agree within error.

For our final results in Figs. 1 and 10, we use this range $N = [1, 3]$ below $T < 165$ MeV, and the range $N = [4, 6]$ for $T \geq 165$ MeV. Since this result is not continuum extrapolated, we do not elaborate on the precise magnitude of the systematic errors.

In Fig. 10 we show the baryo-chemical potential (left) and the relative pressure (right) at a set of fixed baryon densities ($n_B = 0.05, 0.10\text{--}0.60$ fm $^{-3}$ in steps of 0.05 fm $^{-3}$), and compare our results with the Taylor expansion. Note that here also the data points represent grand canonical results, since the $\alpha \rightarrow \infty$ limit has already been taken. It is natural that, for large densities, the data points are less controlled due to the combined effect of the sign and overlap problems. The Taylor expansion seems to have a more severe problem near $T = 150$ MeV, although both the Taylor expanded grand canonical and the α -extrapolated canonical data are based on the same set of configurations.

Let us finally turn to the baryon susceptibility $\chi_2(T)$. Equation (57) can, in principle, be used to perform an extrapolation, similar to those for μ_B and Δp_C . However, the range of N for a given density where a linear fit in $1/N$ would be practical is often fewer than three data points.

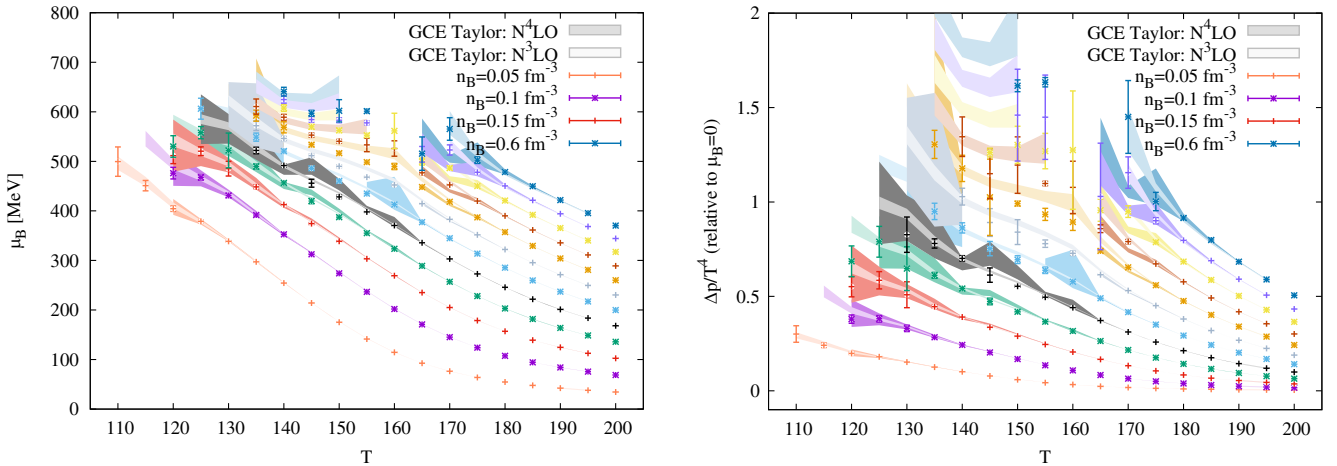


FIG. 10. Infinite α limit of $\mu_B(T, V, n)$ and $\Delta p_C(T, V, n)$ [using Eqs. (55) and (56), respectively]. For μ_B and Δp_C each color represents a density n_B , with the same coloring scheme as in Fig. 1.

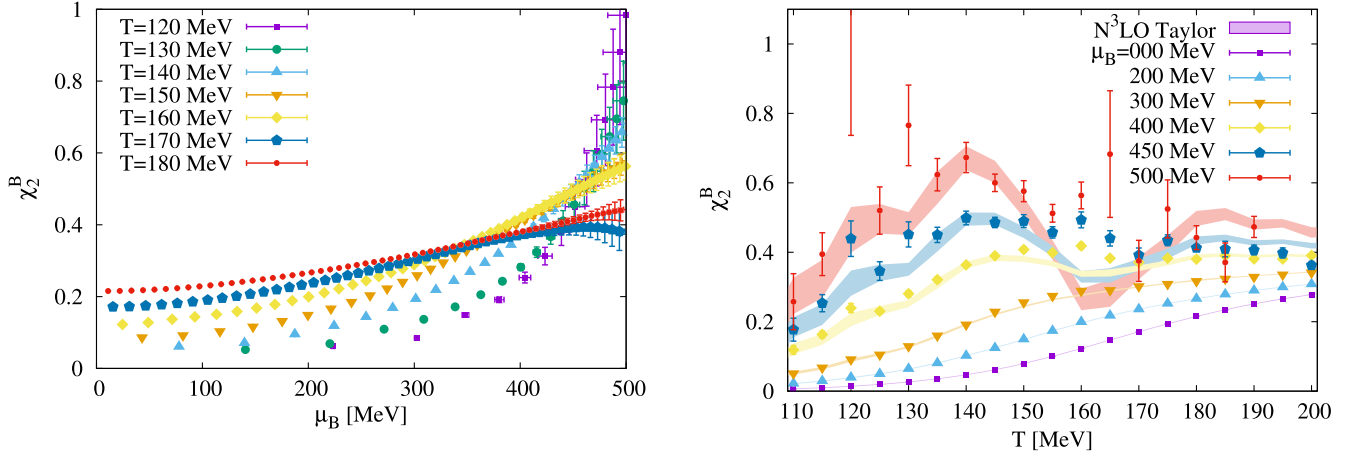


FIG. 11. The net-baryon susceptibility as a function of chemical potential (left), or temperature (right). χ_2 was obtained as the inverse derivative of the $\mu_B(n_B)$ function. The Taylor extrapolation in the right panel uses χ_8^B as its highest order, while using χ_{10}^B would result in much higher errors. Notice, that $\chi_2^B(T)$ starts out as a sigmoid for small μ_B but develops as μ_B is increased.

A much simpler strategy can be used, instead: the function $\mu_B(n_B)$ of Eq. (55) can be derived to yield $\chi_2^{-1} = T^2 d\mu_B/dn_B$. For this, we fix the range in N and compute $\mu_B(n_B)$ up to the point where μ_B reaches the maximal value of interest (here 500 MeV). This function can then be derived with respect to the density (n_B) numerically without any problem.

In Fig. 11 we show the resulting baryon susceptibility. The left panel shows the μ_B dependence of this inverse derivative for a selection of temperatures. In the right panel we interpolate every jackknife sample to a given fixed μ_B so that the error bars are on n_B or χ_2 , not on μ_B . Through this interpolation we finally return to a completely grand canonical picture. In the right panel we also show the Taylor extrapolated prediction, using the coefficients at $\mu_B = 0$ up to χ_8^B . Both the Taylor extrapolation and the data points, i.e., the grand canonical result we obtained through the canonical detour, are from the same set of input configurations, and different temperatures are statistically independent. In the figure we observe that (a) the Taylor extrapolation introduces a nonphysical nonmonotonic temperature dependence, which has already been discussed in the context of the T' expansion [63]; (b) the data points reveal that for small μ_B one recovers the known sigmoid form of $\chi_2(T)$. As μ_B is increased, the inflection point moves to smaller temperatures, as expected. For even larger chemical potential a new maximum develops.

The signal quickly deteriorates as the chemical potential is increased. Moreover, some data points (e.g. those at $T = 120$ and 130 MeV) give higher fluctuations than the neighboring temperatures. Such outliers can be hints for the presence of an overlap problem. Indeed, in this work we have not addressed the overlap nor the sign problem of reweighting. What we did is to use the canonical formalism and derive a new method to extract finite density physics

from $\mu_B = 0$ ensembles, that eliminates some of the shortcomings of reweighting or the Taylor expansion.

VI. CONCLUSIONS AND OUTLOOK

In this work, we used lattice QCD simulations at $\mu_B = 0$ to extract physical observables (baryon density, pressure, fluctuations) at real $\mu_B > 0$. Similar results have already been published with various extrapolation schemes for more than a decade. Specifically, the Taylor expansion has been used extensively to compute the very same observables we presented here. The computation of the Taylor coefficients is not hindered by the complex action problem, but it still suffers from a remnant sign problem [31], making the simulation of higher order coefficients extremely costly, unless the volume is small. Even in a small volume, it is difficult to know how well a fixed order approximates the true result. Adding one more order can be impossible due to its cost, or because simulations deliver results for the highest order with insufficient precision due to the limited statistics. It is also known that the use of imaginary-valued μ_B can boost the range of such extrapolations. In general, the numerical cost of Taylor coefficients is driven by the severity of the cancellation problem, which in turn is proportional to a power of the volume (the exponent depends on the order). Thus, it is generally more cost effective to model the imaginary- μ_B dependence of lower-order susceptibilities than to address directly high order fluctuation observables [29,64]. Yet, the extrapolation itself is ill posed, and is subject to hard-to-control systematic errors. The T' expansion [63] introduced a more physical ground for the μ_B extrapolation where the lowest orders dominate at moderate μ_B .

On the other hand, this work *extracts*, instead of extrapolating, finite density information. In this sense

our method is similar to reweighting with one important technical difference: the simple reweighting cannot be applied to rooted actions, like staggered lattice QCD. While other formulations, e.g. Wilson, twisted mass or minimally doubled fermions might in principle be reweighted from zero to real μ_B , with these actions one struggles to simulate with physical quark masses even at $\mu_B = 0$. As of today, the only lattice formulation where the extreme statistics needed to fight off the sign problem is not prohibitively expensive, is the staggered quark.

Our method can be summarized with three steps: (1) We first reweighted the $\mu_B = 0$ ensembles to imaginary chemical potential, then (2) moved to the canonical ensemble by means of a Fourier transform, and finally (3) performed a limit procedure to return to the grand canonical ensemble at finite μ_B .

Already step (1) required a new algorithmic ingredient, in order to ensure a proper sampling of the center sectors in the center-breaking setup at $\mu_B = 0$. This improvement might also turn out to be beneficial for the computation of the Taylor coefficients, as it effectively eliminates ill-sampled parts of the configuration space. These eliminated parts are not left out of the path integral, but computed precisely through an exact transformation of a well-sampled sector. In this work we did not use simulations at imaginary valued μ_B , but an extension of the method can be easily derived. Quite importantly, the various imaginary- μ_B ensembles should not be constructed based on the range of simulated imaginary chemical potentials, but rather the configuration space should be partitioned. We leave this extension to future work.

Step (2) has been preformed by several authors before us, although never with physical quark masses. We did not address stability and precision, because in most cases the sign problem, stronger in our system than in other literature, was more significant. In the volume of our choice ($LT = 2$) the sign problem is already out of control in the presence of a handful baryons, corresponding to a large density. We demonstrated the magnitude of the sign problem in three simulation volumes.

Leaving the result in the canonical formulation would severely limit its usability. We computed the pressure and the chemical potential for just a handful of densities where N is an integer. The volume matters, too, since canonical effects are very different in our simulation volume and in the entire volume of the quark gluon plasma in a heavy ion collision event.

Thus, we introduced step (3) to recover the grand canonical description. Instead of naively adding up the canonical partition function with weights $e^{N\mu/T}$ we employed a limit procedure with a known asymptotic form. In this step we are relying on certain analytic features of the finite volume grand canonical partition function, and may be limited by the radius of convergence of the Taylor series. We determined the leading coefficient of this

asymptotic form for a noninteracting hadron gas (HRG in the Boltzmann approximation). This limit procedure introduces systematic errors that we studied on a few examples, but did not further elaborate. Moreover, we worked at finite lattice spacing and, most importantly, in a volume where the sign problem can be kept under control up to $\mu_B \leq 500$ MeV.

After step (3) we arrive at grand canonical results where the average particle number is not necessarily an integer. We stress that this is not an interpolation of canonical results at integer valued N . Our procedure is an analytic method that computes the grand potential (and its derivatives) at real μ_B from the grand potential at imaginary μ_B . Our final result after taking the $\alpha \rightarrow \infty$ limit is strictly grand canonical. Both Taylor expansion and our procedure in systematically improvable: adding higher orders in the case of Taylor, and increasing α here. But unlike the Taylor expansion, here we know the asymptotic behavior, namely $\sim 1/\alpha$. Also in our procedure the systematic improvement is performed at fixed density, while Taylor works at fixed zero chemical potential. At a given α we compute the Helmholtz free energy of a fictitious system in the canonical ensemble. For integer α , this canonical system is defined as the union of α pieces of independent replicas of the original system, the replicas are not required to be the same state. The interpolation happens in α . This is possible, since the fictitious system can be easily defined (not imagined) for any positive α . Our numerical work demonstrates that the grand canonical results are correctly reproduced with a limit procedure even if the range in α is rather modest. We could make such a comparison within this dataset, since for the same ensembles the Taylor coefficients have been computed to very high order. In our numerical tests we varied either temperature or simulation volume. In the latter case we found that the grand canonical result is reproduced for the respective simulation volume if the $\alpha \rightarrow \infty$ limit is performed at fixed temperature, volume and density.

We focused on bulk QCD thermodynamics, charting the QCD phase diagram and computing the pressure and its μ_B derivatives, from which the full equation of state can be determined. The results presented here can be extended to account for more than one conserved charge without technical difficulties. The results we presented were defined at $\mu_S = 0$, but an extension to strangeness neutrality can be a natural continuation of this work. It should also be investigated whether the canonical method and reweighting agree when a real isospin chemical potential is introduced. In the latter case it is known that the Taylor extrapolation is limited by the finite radius of convergence of m_π due to the transition to a pion-condensed phase [65].

In this work we employed a finite lattice spacing ($N_t = 8$). Fortunately, the severity of the sign problem does not diverge toward the continuum limit. However, a technical difficulty is the extraction of the eigenvalues from the simulated configurations. This step scales as $\sim N_t^9$, and

its numerical stability is uncertain at $N_t = 12$. We suspect that in such a case a stochastic algorithm would probably be better suited. The final costs on a finer lattice are, thus, hard to estimate, which can be seen as a drawback of the method.

The greater challenge is to increase the simulation volume, which would be a welcome extension. This is mainly because a larger volume would give us access to chiral observables, which are distorted in the volume we employ here. For example, at a chemical potential $\mu_B \approx 500$ MeV we have ca. 5 net-baryons in the $16^3 \times 8$ lattice volume. A lattice size of $20^3 \times 8$ corresponds to doubling the physical volume and having 10 net-baryons. The corresponding partition function (the signal) is then $Z_{16^3 \times 8}(N=5) \sim 10^{-7}$ and $Z_{20^3 \times 8}(N=10) \sim 10^{-14}$, respectively. The signal is, thus, suppressed by a factor of 160 on the smaller lattice, and by a factor of 3.6×10^5 on the larger one. If one does not increase the statistics while doubling the volume, the reachable range in density is approximately halved.

The biggest challenge is to extend this approach to higher baryo-chemical potential. While at high temperature a brute force increase of statistics may work, for the exploration of the cross-over, and eventually a true transition an other problem needs to be addressed. Our low temperature simulation run entirely in the hadronic phase, thus, reading out information on a different phase at high density is problematic and manifests an overlap problem. The relatively small simulation volume in this study allowed fluctuations to at least partially sample configurations relevant for the crossover. If the goal is to study criticality, we must be prepared for a finite size scaling, with bigger volumes where such fluctuations are no longer present, and this approach will be insufficient by its own. One way to enrich the sampled configuration space with data from the high density phase, is to introduce global constraints favoring these. This can be in principle be done with density-of-states type algorithms, which have already found applications in the context of QCD thermodynamics [35,66–68].

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX: EXAMPLE: NONINTERACTING HADRON GAS

In the low temperature phase QCD can be described with very good approximation as a noninteracting hadron gas. Lattice studies have confirmed the concept, that the fugacity series

$$\chi_1(T, V, \mu) = \sum_{k=1}^{\infty} b_k(T) \sinh\left(k \frac{\mu}{T}\right) \quad (\text{A1})$$

converges fast, and already the second coefficient $b_2(T)$ can hardly be distinguished from zero below $T < T_c$ [56,70,71]. Thus, the simple “cosh model”

$$\hat{p}_{GC} \equiv \frac{1}{VT^3} \log Z_{GC} = \hat{p}_M(T) + \hat{p}_B(T) \cosh\left(\frac{\mu}{T}\right) \quad (\text{A2})$$

makes a reasonable choice to illustrate the canonical formalism. Here $\hat{p}_M$ and $\hat{p}_B \equiv b_1$ stand for the mesonic and baryonic contributions, respectively, assuming the validity of the Boltzmann approximation in the hadron resonance gas picture. We will use the “hat” notation to indicate a normalization to temperature:

$$\hat{p} = \frac{p}{T^4}, \quad \hat{\mu} = \frac{\mu}{T} \quad (\text{A3})$$

It is well known, that the canonical partition function of the cosh model (A2) is given by the Skellam distribution.

$$\begin{aligned} Z_C(T, V, N) &= \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-i\varphi N + VT^3 \hat{p}_M + VT^3 \hat{p}_B \cos(\varphi)} \\ &= e^{VT^3 \hat{p}_M} I_N(VT^3 \hat{p}_B) \end{aligned} \quad (\text{A4})$$

where $I_N(z)$ is the modified Bessel function of first kind. The temperature dependence of Z_C enters through the coefficients $\hat{p}^M(T)$ and $\hat{p}^B(T)$. This matches the general form of the Skellam distribution

$$e^{-(\lambda_1+\lambda_2)} \left(\frac{\lambda_1}{\lambda_2}\right)^{N/2} I_N\left(2\sqrt{\lambda_1\lambda_2}\right) \quad (\text{A5})$$

with $\lambda_1 = \lambda_2 = \frac{1}{2}(LT)^3 \hat{p}_B$. Mesons play no role.

The grand canonical relations, which are fully inherited by F_{LT} , such as

$$N = VT^3 \hat{p}_B \sinh \hat{\mu} \quad (\text{A6})$$

are not exactly satisfied if we replace μ with μ^f or μ^b . Having an exact form for $Z_C(T, V, N)$ we are in the position to quantify these canonical volume effects.

Let us start with the backward definition of the chemical potential

$$\begin{aligned} \hat{\mu}^b(T) &= F(T, V, N) - F(T, V, N-1) \\ &= -\log \left(\frac{I_N(VT^3 \hat{p}_B)}{I_{N-1}(VT^3 \hat{p}_B)} \right) \end{aligned} \quad (\text{A7})$$

We will keep the density $\hat{n} = N/(VT^3)$ fixed, which is set by the chemical potential $\hat{\mu}_B$,

$$\hat{n} = \hat{p}_B \sinh(\hat{\mu}_B) = \frac{\hat{p}_B}{c}, \quad c = \frac{1}{\sinh(\hat{\mu}_B)}. \quad (\text{A8})$$

Through the shorthand c we can simply write

$$\hat{\mu}^b = \log \left(\frac{I_{N-1}(Nc)}{I_N(Nc)} \right) \quad (\text{A9})$$

where we can now take the $N \rightarrow \infty$ thermodynamic limit. The asymptotic formula for the Bessel functions with simultaneously growing index and argument reads [(9.7.7) of Ref. [72]]

$$\begin{aligned} I_N(z) &= \frac{1}{\sqrt{2\pi z}(1 + \frac{N^2}{z^2})^{1/4}} \exp \left(-N \operatorname{arsinh} \left(\frac{N}{z} \right) \right. \\ &\quad \left. + z \sqrt{1 + \frac{N^2}{z^2}} \right) \left(1 + \mathcal{O} \left(\frac{1}{z \sqrt{1 + \frac{N^2}{z^2}}} \right) \right) \end{aligned} \quad (\text{A10})$$

Inserting $z = Nc$ we have

$$\begin{aligned} I_N(Nc) &= \frac{1}{\sqrt{2\pi N}(1 + c^2)^{1/4}} \exp \left(-N\mu_B/T \right. \\ &\quad \left. + N\sqrt{1 + c^2} \right) (1 + \mathcal{O}(N^{-1})). \end{aligned} \quad (\text{A11})$$

The same asymptotic form was used in [73] to derive baryon/antibaryon cumulant in canonical HRG. With this asymptotic form we can calculate F near the thermodynamic limit:

$$\begin{aligned} \frac{F(T, V = N \frac{c}{\hat{p}_B T^3}, N)}{VT^4} &= -\hat{p}_M(T) - \frac{1}{VT^3} \log I_N(Nc) \\ &= -\hat{p}_M(T) + \frac{\hat{p}_B}{Nc} \log \sqrt{2\pi N}(1 + c^2)^{1/4} + \hat{p}_B \frac{\hat{\mu}_B - \sqrt{1 + c^2}}{c} + \frac{\hat{p}_B}{Nc} \mathcal{O}(N^{-1}) \\ &= \frac{1}{VT^4} (\Omega + \mu N) - \frac{\hat{p}_B}{2Nc} \log \frac{1}{2\pi N} - \frac{\hat{p}_B}{2N} \sinh(\hat{\mu}_B) \log \tanh \hat{\mu}_B + \mathcal{O}(N^{-2}) \end{aligned} \quad (\text{A12})$$

The corresponding generic formula was given in Eq. (15). The $N \rightarrow \infty$ limit has to be understood here at constant density, that is $c = 1/\sinh \hat{\mu}_B$ fixed.

Let us now show that the observables follow the $1/N$ asymptotics, as announced. Applying the asymptotic form to $I_{N\pm 1}(Nc)$ as well, simple algebra yields

$$\begin{aligned} \hat{\mu}^f(N) &= \hat{\mu} + \frac{1}{2N} \frac{1}{\sqrt{1 + c(\hat{\mu})^2}} + \frac{1}{2N(1 + c(\hat{\mu})^2)} + \mathcal{O}\left(\frac{1}{N^2}\right) \\ \hat{\mu}^b(N) &= \hat{\mu} - \frac{1}{2N} \frac{1}{\sqrt{1 + c(\hat{\mu})^2}} + \frac{1}{2N(1 + c(\hat{\mu})^2)} + \mathcal{O}\left(\frac{1}{N^2}\right) \end{aligned} \quad (\text{A13})$$

For small c (i.e. $\mu \gtrsim 1$) there is an approximate cancellation between the two leading correction terms of $\hat{\mu}^b$. In contrast the contributions amplify for $\hat{\mu}^f$. If we reexpand in c , this behavior is exposed as

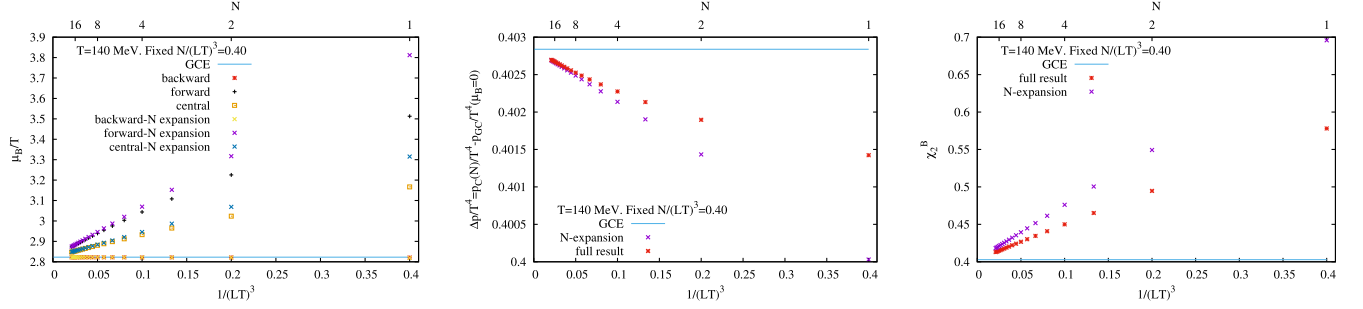


FIG. 12. Left: The forward (μ^f) and backward (μ^b) chemical potentials in a finite volume in a concrete example. $\hat{p}_B$ is taken from lattice at $T = 140$ MeV. The volume independent grand canonical value $\hat{\mu} = \text{arsinh}(\hat{n}/\hat{p}_B)$ is shown as a line “GCE.” We also show the central chemical potential ($(\mu^f + \mu^b)/2$) and evaluate the leading asymptotic formulas text to the exact results in Eqs. (16) and (17). Center: the analogous result for the pressure at finite volume. Right: the corresponding χ_2 coefficient.

$$\hat{\mu}^f(N) = \hat{\mu} + \frac{1}{N} - \frac{3c^2}{4N} + \mathcal{O}(N^{-2}) + \mathcal{O}(c^4) \quad (\text{A14})$$

$$\hat{\mu}^b(N) = \hat{\mu} - \frac{c^2}{4N} + \mathcal{O}(N^{-2}) + \mathcal{O}(c^4) \quad (\text{A15})$$

We plot the formulas with realistic parameters in Fig. 12.

The pressure [see Eq. (21)] is computed with the same principle

$$\frac{p_C(T, V, N)}{T^4} = \frac{p_{GC}(T, V, \mu)}{T^4} - \hat{p}_B e^{\hat{\mu}} (\hat{\mu} - \hat{\mu}^b) + \mathcal{O}(N^{-2}), \quad (\text{A16})$$

here the leading $\sim 1/N$ terms are encoded in $\hat{\mu}^b$.

We can also extract $\chi_2 = \hat{p}_B$ as

$$\frac{1}{\chi_2^{\text{discrete}}(N)} \equiv (VT^3)(\hat{\mu}^f(N) - \hat{\mu}^b(N)) \quad (\text{A17})$$

For the leading asymptotics in $1/\chi_2$ we will need one more order in the $1/N$ expression of $\hat{\mu}^b$ and $\hat{\mu}^f$. A tedious computation then gives

$$\frac{1}{\chi_2^{\text{discrete}}(N)} = \frac{1}{\hat{p}_B \cosh(\hat{\mu}) \left(1 - \frac{1}{2N\sqrt{1+c^2}} + \frac{5}{4} \frac{1}{(1+c^2)^{3/2}} \frac{1}{N}\right)} + \mathcal{O}(N^{-2}) \quad (\text{A18})$$

recovering the grand canonical result in the $N \rightarrow \infty$ limit with an $\mathcal{O}(1/N)$ correction. The actual numerical result on the finite N observables, and their approach to the grand canonical limit we show in Fig. 12.

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