Lattice QCD Equation of State for Nonvanishing Chemical Potential by Resumming Taylor Expansions

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Taylor expansion in powers of baryon chemical potential (μ_B) is an oft-used method in lattice QCD to compute QCD thermodynamics for $\mu_B > 0$. Based only upon the few known lowest order Taylor coefficients, it is difficult to discern the range of μ_B where such an expansion around $\mu_B = 0$ can be trusted. We introduce a resummation scheme for the Taylor expansion of the QCD equation of state in μ_B that is based on the n-point correlation functions of the conserved current (D_n). The method resums the contributions of the first N correlation function $D_1, \ldots, D_N$ to the Taylor expansion of the QCD partition function to all orders in μ_B. We show that the resummed partition function is an approximation to the reweighted partition function at $\mu_B \neq 0$. We apply the proposed approach to high-statistics lattice QCD calculations using $2+1$ flavors of Highly Improved Staggered Quarks with physical quark masses on $32^3 \times 8$ lattices and for temperatures $T \approx 145$–176 MeV. We demonstrate that, as opposed to the Taylor expansion, the resummed version not only leads to improved convergence but also reflects the zeros of the resummed partition function and severity of the sign problem, leading to its eventual breakdown. We also provide a generalization of scheme to include resummation of powers of temperature and quark masses in addition to μ_B, and show that the alternative expansion scheme of [S. Borsányi *et al.*, Phys. Rev. Lett. **126**, 232001 (2021).] is a special case of this generalized resummation.

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Introduction.—Lattice quantum chromodynamics (QCD) results for the QCD equation of state (EOS) plays a critical role in the dynamical modeling of heavy-ion collisions [1–4] and, thereby, in the experimental explorations of the QCD phase diagram in the T-μ_B plane. Because of the fermion sign problem it is difficult to carry out lattice QCD computations directly at $\mu_B \neq 0$. Despite some recent progress [5–10], direct lattice computations of the QCD EOS $\mu_B \neq 0$ with physical quark masses, fine lattice spacings, and large lattice volumes have remained elusive. Instead, the present state-of-the-art lattice QCD EOS at $\mu_B > 0$ has been obtained using the Taylor expansion [11,12] and the analytic continuation [13,14] methods. In the Taylor expansion method one expands the pressure in powers of μ_B around $\mu_B = 0$ and directly computes the Taylor coefficients at $\mu_B = 0$. For the analytic continuation, one avoids the fermion sign problem using simulations at purely imaginary values μ_B, fits these results with a power series in μ_B to determine the Taylor coefficients at $\mu_B = 0$ and then provides the EOS at real $\mu_B > 0$ based on these Taylor coefficients. On the other hand, it is well known that the applicability of the Taylor expansion as well as the analytic continuation should be limited by the zeros, nearest to $\mu_B = 0$, of the partition function in the entire complex-μ_B plane [15–17]. In principle, it is possible to estimate the zeros of the partition function by re-expressing the power series in real or imaginary μ_B in terms of Padé approximants [12] or in a power series of the fugacity [18–20]. Armed, in reality, with only the few lowest order Taylor coefficients, this becomes a very difficult task and, in practice, one just restricts the EOS to $\{T, \mu_B\}$ that avoids any pathological nonmonotonicity in the truncated Taylor series [11,14]. Furthermore, these methods provide very little guidance on the severity of the fermion problem, i.e., how rapidly the phase of the partition function fluctuates as μ_B is increased. It is possible to determine the zeros of the partition function as well as its average phase by reweighting the fermion determinant to $\mu_B \neq 0$ [21–25]. However, due to the computational cost associated with exact evaluation of the fermion determinant, at present this method is restrained within coarse lattice spacings and small lattice volumes.

In this work, we introduce a method for the calculation of the lattice QCD EOS that genuinely resums the truncated Taylor series to all orders in μ_B and whose breakdown encodes the severity of the sign problem and zeros of the resummed partition function.

The resummation method.—The Taylor expansion to $\mathcal{O}(\mu_B^N)$ of the excess pressure, $\Delta P(T,\mu_B) \equiv P(T,\mu_B) - P(T,0)$, is given by

$$\frac{\Delta P_N^E}{T^4} = \sum_{n=1}^{N} \frac{\chi_n^B}{n!}\left(\frac{\mu_B}{T}\right)^n, \tag{1}$$

where the Taylor coefficients are defined as

$$\chi_n^B(T) = \frac{1}{VT^3}\frac{\partial^n \ln Z(T,\mu_B)}{\partial(\mu_B/T)^n}\bigg|_{\mu_B=0}. \tag{2}$$

Here, the QCD partition function is denoted as $Z = \int e^{-S}\det[M]\mathcal{D}U$, V is the spatial volume, U is the SU(3) gauge fields, S is the pure gauge action, and M is the fermion matrix. Each χ_n^B consists of a sum of terms like $\langle D_i^a D_j^b \cdots D_k^c\rangle$ with $i\cdot a + j\cdot b + \cdots + k\cdot c = n$ [26,27], where

$$D_n(T) = \bar{D}_n \cdot n! = \frac{\partial^n \ln\det[M(T,\mu_B)]}{\partial(\mu_B/T)^n}\bigg|_{\mu_B=0}, \tag{3}$$

and the $\langle\cdot\rangle$ denotes the average over gauge field ensembles at $\mu_B = 0$, i.e., $\langle O\rangle = \int O e^{-S}\det[M(T,0)]\mathcal{D}U/Z$. The physical interpretation of D_n is simple for the continuum theory: $D_n = \int d\mathbf{x_1}\cdots d\mathbf{x_n} J_0(\mathbf{x_1})\cdots J_0(\mathbf{x_n})$ is the integrated n-point correlation function of the 0th component of the conserved (baryon) current $J_0(\mathbf{x})$ at a space-time point $\mathbf{x}$. Note that, due to CP symmetry of QCD all D_n for $n =$ odd(even) are purely imaginary(real) and only the $n =$ even terms contribute to Eq. (1). In practice, lattice QCD computations of the χ_N^B involve computations of all D_n for $n \le N$ as intermediate steps, and χ_N^B are obtained from combinations of D_n and their powers.

Contributions of various combinations of D_n to the few lowest order Taylor coefficients are sketched in Fig. 1.

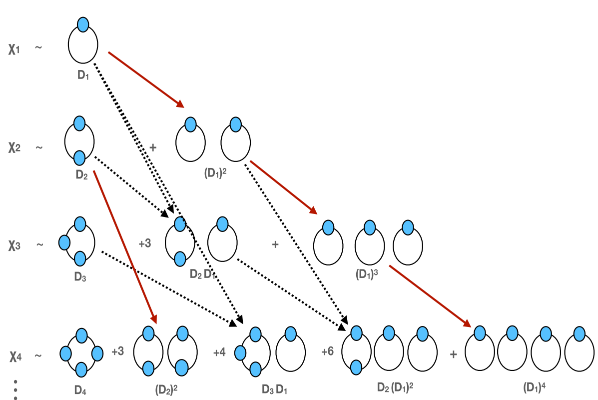

FIG. 1. Contributions of different D_n to the χ_n^B. Each blob represents insertion of the 0th component of the conserved current. Solid red and dotted black lines represent directly exponentiated and cross terms, respectively.

If one considers the factorials and the powers of μ_B/T associated with each D_n in the sum of Eq. (1), it is not difficult to realize that all contributions of each D_n to ΔP^E can be resummed into exponential forms. For example, contributions of D_1^n from all χ_n^B in Eq. (1) can be resummed as $\exp[\bar{D}_1(\mu_B/T)]$. Similarly, contributions of all D_2^n can be resummed as $\exp[\bar{D}_2(\mu_B/T)^2]$, and so on. Also it is easy to see that the contributions of the mixed terms like $D_1^n D_2^m$ arise from $\exp[\bar{D}_1(\mu_B/T)] \times \exp[\bar{D}_2(\mu_B/T)^2]$. Thus, it is possible to write down a resummed version of Eq. (1), viz.

$$\frac{\Delta P_N^R}{T^4} = \frac{1}{T^3 V}\ln\left\langle \exp\left[\sum_{n=1}^{N}\bar{D}_n\left(\frac{\mu_B}{T}\right)^n\right]\right\rangle, \tag{4}$$

providing the EOS up to infinite orders in μ_B. The ΔP_N^R can be considered as a μ_B-dependent effective action obtained by resumming up to N-point correlation functions of the conserved current. Expansion of ΔP_N^R in powers of μ_B/T yields an infinite series in μ_B/T, in addition to the truncated Taylor series: $\Delta P_N^E + \sum_{n>N}^{\infty}\langle \bar{D}_1^i \cdots \bar{D}_N^j\rangle(\mu_B/T)^n$, where $i,j = 0,\ldots,N$ satisfying $1\cdot i + \cdots + Nj = n$. The Taylor expanded ($\mathcal{N}_N^E$) and the resummed ($\mathcal{N}_N^R$) net baryon-number densities can be straightforwardly obtained as a single μ_B derivative of ΔP^E and ΔP^R in Eqs. (1) and (4), respectively.

The resummed version in Eq. (4) also highlights the connection between the Taylor expansion and the reweighting method. In the reweighting method $Z(T,\mu_B)/Z(T,0) = \langle\det[M(T,\mu_B)]/\det[M(T,0)]\rangle$ can be calculated, if computationally feasible, by exactly evaluating the ratio of the fermion matrix determinants on the gauge fields generated at $\mu_B = 0$. In more realistic lattice calculations with large volumes, exact evaluations of the determinant ratios might not be computationally feasible and one may consider evaluating $\det[M(T,\mu_B)]$ within some approximation scheme to obtain approximate partition function $Z_N^R(T,\mu_B) \approx Z(T,\mu_B)$. Following the spirit of the Taylor expansion, one such approximation scheme can be expansion of $\det[M(T,\mu_B)]$ in powers of μ_B/T. Keeping in mind $\det[M] = \exp[\mathrm{Tr}\ln M]$ and Eq. (3), one can immediately recognize

$$\frac{Z_N^R(T,\mu_B)}{Z(T,0)} = \left\langle \exp\left[\sum_{n=1}^{N}\bar{D}_n\left(\frac{\mu_B}{T}\right)^n\right]\right\rangle. \tag{5}$$

Since CP symmetry dictates that the even(odd) D_n are purely real(imaginary) and the partition function must be real, a measure of the severity of the sign problem is given by the average phase factor for Z_N^R (with μ_B real),

$$\langle\cos\Theta_N^R\rangle = \left\langle \cos\left(\sum_{n=1}^{N/2}\mathrm{Im}[\bar{D}_{2n-1}]\left(\frac{\mu_B}{T}\right)^{2n-1}\right)\right\rangle. \tag{6}$$

An expansion of $\langle\cos\Theta_N^R\rangle$ in μ_B/T leads to the Taylor expanded measure of the average phase of the partition function [23,26], which we will denote by Θ_N^E. As the sign problem becomes more severe the average phase $\langle\cos\Theta_N^R\rangle\approx 0$ and resummed results will also show signs of breakdown. Furthermore, although ΔP_N^E can be evaluated for any complex value of μ_B, ΔP_N^R becomes undefined when $\mathrm{Re}[Z_N^R]\le 0$ for a given N and statistics, leading to a natural breakdown of the resummed results. The location of the zeros of Z_N^R in the complex-μ_B plane will indicate the μ_B region where such resummation can be applicable. Obviously, for any given N the region of applicability of ΔP_N^E cannot exceed the same for ΔP_N^R.

Lattice QCD computations.—For this work, we used the data for χ_n^B and D_n generated by the HotQCD Collaboration for calculations of the QCD EOS [11] and the chiral crossover temperature [28] at $\mu_B>0$ using the Taylor expansion method. The HotQCD ensembles were generated with $2+1$ flavors of Highly Improved Staggered Quarks and the tree-level improved Symanzik gauge action [29–31]. Bare quark masses were chosen to reproduce, within a few percent, the physical value of the kaon mass and a pseudo-Goldstone pion mass of 138 MeV in the continuum limit at $T=\mu_B=0$ and the lattice spacing were calibrated against the physical value of the kaon decay constant [32]. We present lattice QCD results from a single lattice size $32^3\times 8$ and for 6 temperatures $T=145$, 151, 157, 166, 171, 176 MeV. About 475, 520, 716, 522, 232, and 152 K gauge field configurations were used to measure D_n at these temperatures, respectively. The gauge field configurations were separated by 10 Rational Hybrid Monte Carlo trajectories of unit length. The D_n were calculated within the formalism adopted in Refs. [11,28], i.e., using the exponential-μ formalism [33] for $n\le 4$ and the linear-μ formalism [34,35] for $n>4$. The expressions for D_n in terms of the traces involving the inverse of the staggered fermion matrix and its μ_B derivatives are well known [26,36]. Each trace was calculated stochastically for each configuration by employing 2000 random Gaussian volume sources for the trace D_1 and 500 random sources for the rest [36].

Results.—To demonstrate the superiority of the resummation method over the Taylor expansion, we chose the temperature where we had the largest statistics, i.e., $T=157$ MeV, which is also closest to the QCD crossover temperature [28]. In Fig. 2, we compare ΔP_N^E with ΔP_N^R (top) and $\mathcal{N}_N^E$ with $\mathcal{N}_N^R$ for different orders N. Comparisons are shown both for real as well as imaginary values of μ_B, corresponding to positive and negative values of $(\mu_B/T)^2$, respectively. The ΔP_N^R and $\mathcal{N}_N^R$ show very good convergence between different orders $N=2$, 4, 6, 8. The Taylor-expanded results seem to approach their respective resummed results as contributions from higher orders in μ_B are included; however, the convergence of the Taylor-expanded

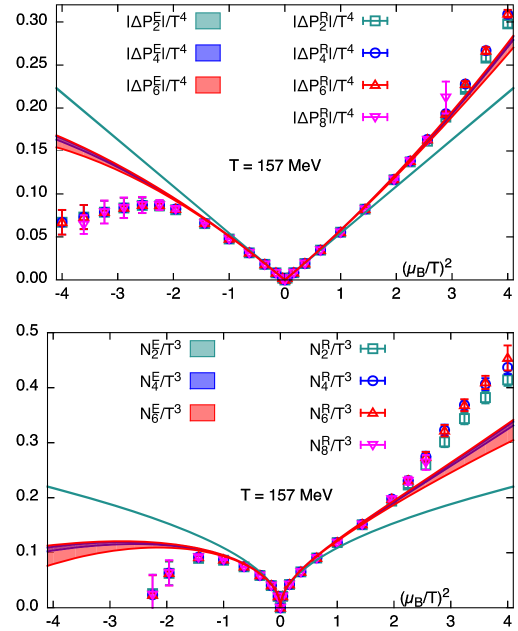

FIG. 2. Comparisons between the Taylor expanded and resummed results for different orders for the excess pressure (top) and net baryon-number density (bottom) at $T=157$ MeV. Results for real and imaginary μ_B/T are plotted on the positive and negative x axis, respectively.

results is slow due to the alternating signs of the higher order χ_n^B near the QCD crossover [11–13]. The resummation method overcomes this problem by including contributions from all orders in μ_B and shows markedly improved convergence.

We checked that such a breakdown is not a mere statistical issue by repeating the calculations using only parts of the gauge configurations available at this temperature. Similar breakdown for $\mu_B/T\gtrsim 1.5$ was also observed in Refs. [12,37,38] when the EOS was reconstructed from the Padé approximants of the Taylor series in μ_B. While Padé-based continuations of the QCD crossover temperature from imaginary values μ_B did not encounter such breakdowns [39,40], the same in the case of the EOS seemed to break down due to singularities in the complex-μ_B plane [41].

To investigate the origin of this breakdown, we computed the average phase as a function of real μ_B, cf. Eq. (6). The results are shown in Fig. 3 (top). Also, $\langle\cos\Theta_N^R\rangle\approx 0$ for $\mu_B/T\gtrsim 1.5$, which shows that the sign problem is uncontrollably severe where the EOS calculations broke down. The resummation method thus faithfully captures the severity of the sign problem, as opposed to the Taylor expansion. The phase factor cannot be calculated exactly within the Taylor series approach. Its Taylor series expansion too converges very slowly, as the bands plotted in Fig. 3 (top) show. Further, we searched for the zeros of resummed partition function, cf. Eq. (5), in the complex μ_B plane. We solved for $Z_N^R=0$ using the Newton-Raphson

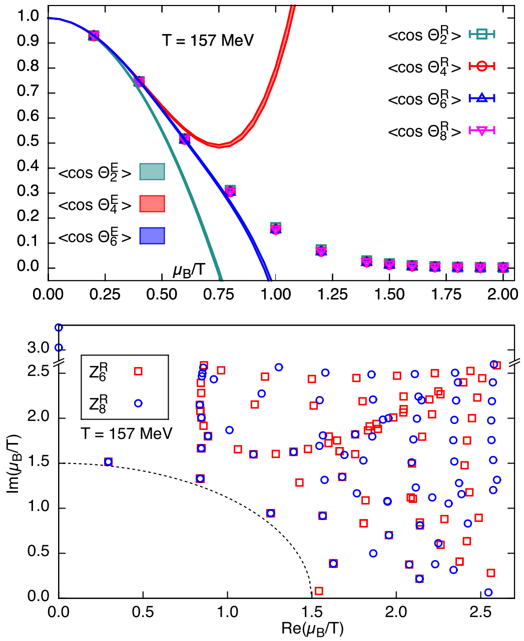

FIG. 3. (Top) The average phase factor $\langle \cos \Theta_N^R \rangle$ as a function of μ_B/T. The bands are the Taylor series expansions of the phase factor to different orders. (Bottom) Zeros of Z_N^R in the complex-μ_B plane. Only roots in the first quadrant are shown since the distribution is symmetric in the four quadrants. Both top and bottom plots are for $T = 157$ MeV.

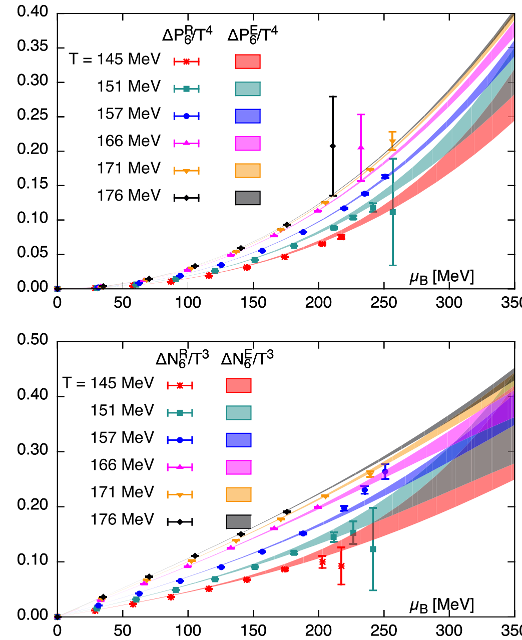

FIG. 4. Comparisons between the excess pressure (top) and the net baryon-number density (bottom) obtained the sixth order resummation (ΔP_6^R and $\mathcal{N}_6^R$) and Taylor expansion (ΔP_6^E and $\mathcal{N}_6^E$) methods for all six temperatures that were considered in this work.

algorithm with initial guesses chosen from a uniform distribution over a grid $0 \leq \{\mathrm{Re}(\mu_B/T), \mathrm{Im}(\mu_B/T)\} \leq 2.5$. The results are shown in Fig. 3 (bottom). The zeros of Z_6^R and Z_8^R are more or less consistent with each other and appears only for $|\mu_B/T| \gtrsim 1.5$. The exact nature of the singularity responsible for breakdown of the resummation method is certainly of great interest, i.e., whether it is associated with the Yang-Lee edge singularity of the QCD chiral transition [15,17] or the QCD critical point and approaches the real axis [12,21,22,37,38], etc. This will need detailed quantitative studies involving careful finite-volume scaling analyses using more sophisticated techniques [18,20,42] and is beyond the scope of the present work. But our results demonstrate that the breakdown of the resummation method reflects the associated singularities of the partition function, at least qualitatively.

Finally, in Fig. 4 we summarize results for all $T =$ 145–176 MeV by showing comparisons between ΔP_6^R and $\mathcal{N}_6^R$ with the corresponding ΔP_6^E and $\mathcal{N}_6^E$. As in the case of $T = 157$ MeV, ΔP^R and $\mathcal{N}^R$ show improved convergence over ΔP^E and $\mathcal{N}^E$ at all temperatures. Again, in contrast to the Taylor expansion the resummation method shows signs of breakdown for $\mu_B \gtrsim$ 200–250 MeV, depending on the temperature. As before, we checked that in all cases, these breakdowns reflect the severity of the sign problem and the singularities of the partition function in the complex-μ_B plane.

Generalization to multiparameter and joint expansion in T, μ_B.—Since our resummation scheme is equivalent to an approximate reweighting method, for large values of μ_B the results obtained using this method are subjected to the so-called overlap problem. The distribution of the gauge configurations at $\mu_B = 0$ might be drastically different from that at large μ_B, leading to smaller overlap between the two gauge field distributions and inaccurate results with increasing μ_B. A hint of such an overlap problem may be seen in Fig. 2, where the resummed results for $\mathrm{Im}(\mu_B)$ not only deviate from the corresponding Taylor expansion results but also from the direct lattice QCD computations at $\mathrm{Im}(\mu_B)$ [14]. To mitigate such overlap problems, we propose a generalized resummation scheme that is akin to multiparameter reweighting [21–24] in the bare gauge coupling, $\Delta\beta = \beta - \beta_0$, and quark mass, $\Delta m = m - m_0$. Our resummation scheme also can be extended to obtain $Z_N^R(T, \mu_B)$ starting from a different temperature $T_0(\beta_0)$ and bare quark mass m_0,

$$\frac{Z_N^R(T, \mu_B)}{Z(T_0, 0)} = \langle e^{-S_G \Delta\beta + \sum_{i+j=1}^{N} \bar{\mathcal{G}}_{ij} (\frac{\mu_B}{T})^i (\frac{\Delta m}{T})^j} \rangle, \tag{7}$$

where the expectation value is taken over gauge fields associated with $\{\beta_0, m_0, 0\}$. Here, S_G is the pure gauge action and

$$\bar{\mathcal{G}}_{ij}(\beta_0, m_0) = \frac{\partial^i \partial^j \ln \det[M(m, \mu_B)]}{i!j!\partial(\mu_B/T)^i \partial(m/T)^j}\Bigg|_{(m_0,0)}. \quad (8)$$

Note, $\bar{\mathcal{G}}_{i0} = \bar{D}_i$ [Eq. (3)], $\bar{\mathcal{G}}_{0j}$ are the chiral condensate and higher order chiral susceptibilities, and general $\bar{\mathcal{G}}_{ij}$ are μ_B derivatives of various chiral observables [26,36,43,44]. This generalization can possibly mitigate the overlap problem that one might encounter while resumming only in μ_B. Further, a systematic expansion of the logarithm of Eq. (7) in powers of $\Delta\beta$, Δm, and μ_B yields the expansion of the pressure difference, $P(T, \mu_B)/T^4 - P(T_0, \mu_B)/T_0^4$, in powers of $\Delta T = T - T_0$ and μ_B; particular choice of $T_0(\mu_B)$ defined by a line of constant physics in the T-μ_B plane reproduces the expansion scheme used in Ref. [45] (see Supplemental Material [46]). Thus, our method also generalizes the alternative expansion scheme of Ref. [45] by resumming up to N-point baryon-current correlations to all orders in μ_B and ΔT.

Conclusions.—We have introduced a new method to compute lattice QCD EOS by resumming contributions of up to N-point baryon-current correlations to all orders in μ_B. When expanded in powers of μ_B this resummed partition function exactly reproduces the Taylor expansion up to $\mathcal{O}(\mu_B^N)$, plus an infinite series in μ_B capturing all possible contributions involving only the $n \leq N$-point baryon-current correlations. This resummation method also amounts to an approximate reweighting method, thereby bridging two traditional lattice QCD techniques for $\mu_B \neq 0$. With illustrative high-statistics lattice QCD computations we have demonstrated that the resummation method shows improved convergence over the Taylor expansion method. The method also faithfully captures the severity of the sign problem as well as reflects the singularities in the complex-μ_B plane that are responsible for its eventual breakdown. Thus the resummation method not only provides a more convergent lattice QCD EOS but also a more reliable one by enabling us to judge its validity with increasing μ_B. Although the resummation method is more general and powerful than the Taylor expansion, computationally it is somewhat simpler. The resummation method relies on the computations of D_n which come as an intermediate step in the computations of the Taylor coefficients. Comparison with the resummed results and the direct lattice QCD simulations for purely imaginary μ_B will help us to decide up to what values $\mathrm{Im}(\mu_B)$ an analytic continuation using only the power series of μ_B is justified and whether Padé-type analytic continuations [39–41] are necessary to avoid singularities in the complex-μ_B plane. We have also introduced a generalized multiparameter version of the resummation, Eq. (7), and shown that the method of Ref. [45] is a special case of this—Taylor expansion of Eq. (7) in T and μ_B along a specific line in the T-μ_B plane. While the success of the method of Ref. [45] indicates that our generalized multiparameter resummation will mitigate the overlap problem to a large extent, the QCD equation of state presented in this work was not obtained using the generalized method and might suffer from the overlap problem.

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[46] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.128.022001 for a generalization of the method presented here to resummation in both μ_B and T. The generalized method resums the alternative expansion scheme presented in S. Borsányi *et al.* [45] to all orders in μ_B and T and is equivalent to multi-parameter reweighting in μ_B and T.