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A new method for computation of QCD thermodynamics: EOS, specific heat and speed of sound

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We propose a new variant of the operator method for the computation of the equation of state of QCD, which yields positive pressure for all temperatures and all values of temporal lattice spacings. Using this new method, we calculate the continuum limit of pressure, P, energy density, ϵ, entropy density, s, specific heat, c_V, and the speed of sound, c_s, in quenched QCD, for $0.9 \leq T/T_c \leq 3$.

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1. Introduction

The equation of state (EOS) of quantum chromodynamics (QCD) has been perused for a long time, not only because it is theoretically interesting but also for its growing importance in the relativistic heavy-ion collision experiments. Almost two decades back, an operator method formalism was devised [1] to study the EOS of QCD numerically by using lattice gauge theory. Later it was found that computations on coarse lattices, using this method, gave negative pressure near the phase transition region. It was argued then, that this problem arises due the use of perturbative formulae for the various derivatives of the coupling. To cure this problem a new elegant method, the integral method, was proposed in [2]. This method assumes the system to be homogeneous, bypassing the use of those derivatives. It uses another non-perturbatively determined derivative of the coupling, namely the QCD β-function. Unfortunately, the assumption of homogeneity does not hold at a first order phase transition. Moreover, the method also has other limitations like the pressure being ill-defined below an arbitrarily chosen cut-off temperature and the fluctuation measures being obtained only by taking numerical derivatives, resulting in large errors.

In view of this situation we propose [3] a new variant of the operator method which gives non-negative, well-defined pressure for the entire temperature range. This method can also be extended to the calculation of fluctuation measures [4], starting from the first principle. We choose the temporal lattice spacing to set the scale of the theory, in contrast to the choice of the spatial lattice spacing in the approach of [1]. Thus, our method [3] could be called the t-favoured operator method and the method of [1] may be called the s-favoured operator method.

2. Formalism

As in most finite temperature lattice gauge theory formulation, our t-favoured formalism is defined on a $3+1$ dimensional hypercubic, asymmetric lattice having different lattice spacings a_τ and a_s in the temporal and spatial directions respectively. The temperature(T) and the spatial volume(V) are defined as $T=(a_\tau N_\tau)^{-1}$ and $V=(a_s N_s)^3$, N_τ and N_s being the number of lattice sites in the temporal and spatial directions. In our t-favoured scheme we introduce the anisotropy parameter ξ and the scale a by the relations—

$$\xi = \frac{a_s}{a_\tau}, \qquad \text{and} \qquad a = a_\tau. \tag{2.1}$$

The partial derivatives with respect to temperature and volume can easily be written in terms of these variables—

$$T\,\frac{\partial}{\partial T}\bigg|_V = \xi\,\frac{\partial}{\partial \xi}\bigg|_a - a\,\frac{\partial}{\partial a}\bigg|_\xi, \qquad \text{and} \qquad V\,\frac{\partial}{\partial V}\bigg|_T = \frac{\xi}{3}\,\frac{\partial}{\partial \xi}\bigg|_a. \tag{2.2}$$

In finite temperature lattice gauge theory simulations the scale is set by the temperature $T = 1/a_\tau N_\tau$. In that sense our choice of scale $a = a_\tau$ corresponds to the situations in actual simulations, giving rise to the most natural procedure for the scale setting. On the other hand, in the case of the s-favoured scheme [1], for any $\xi \neq 1$, the scale is set by $a = a_s$ and only in the $\xi \to 1$ limit this natural choice of the scale emerges.

For a pure gauge $SU(N_c)$ theory on an asymmetric lattice, the Wilson action and the corresponding partition function are defined as—

$$S[U] = K_s P_s + K_\tau P_\tau, \qquad \text{and} \qquad \mathscr{Z}(V,T) = \int \mathscr{D}U e^{-S[U]}, \tag{2.3}$$

where periodic boundary conditions are assumed. P_s denotes the sum of spatial plaquettes over all lattice sites, and P_τ is the corresponding sum of mixed space-time plaquettes. The couplings in the temporal and spatial directions are given by $K_s = 2N_c/\xi g_s^2$, and $K_\tau = 2N_c\xi/g_\tau^2$ respectively.

In the weak coupling limit, g_i^{-2} 's ($i = s,\tau$) can be expanded [5] around their symmetric lattice value $g^{-2}(a)$,

$$g_i^{-2}(a,\xi) = g^{-2}(a) + c_i(\xi) + O[g^2(a)], \tag{2.4}$$

with the condition $c_i(\xi = 1) = 0$. The value of $g^2(a)$ depends on the identification of the scale a.

We are now in a position to calculate different thermodynamic quantities. Let us first look at the energy density (ε) and the pressure (P). Starting from the standard definitions of ε and P in terms of $\ln\mathscr{Z}$, operating the lattice derivatives of eq. (2.2) on the partition function given in eq. (2.3) and making use of the relation mentioned in eq. (2.4) one can derive the expressions for ε and P. In the $\xi \to 1$ limit these expressions reduces to—

$$\begin{aligned}
\frac{\varepsilon}{T^4} &= 6N_cN_\tau^4\left[\frac{D_s - D_\tau}{g^2} - (c_s' D_s + c_\tau' D_\tau)\right] + 6N_cN_\tau^4\frac{B(\alpha_s)}{2\pi\alpha_s^2}\left[D_s + D_\tau\right] \qquad \text{and} \\
\frac{P}{T^4} &= 2N_cN_\tau^4\left[\frac{D_s - D_\tau}{g^2} - (c_s' D_s + c_\tau' D_\tau)\right].
\end{aligned} \tag{2.5}$$

Here the primes denote derivatives with respect to ξ, $B(\alpha_s)$ is the QCD β-function, with the usual definition of $\alpha_s = g^2(a)/4\pi$. An ultraviolet divergence in the values of the plaquettes is removed by a subtraction of the corresponding vacuum ($T = 0$) values to yield $D_i = \langle P_i\rangle - \langle P_0\rangle$ above. In [6], c_i' 's have been calculated for a weakly coupled $SU(N_c)$ gauge theory upto one-loop order. Since these Karsch coefficients are known only upto one-loop order, we also use one-loop order $B(\alpha_s)$ for logical consistency. We use the one-loop order renormalized coupling $g^2(a)$ as has been suggested in [7].

Our expressions for energy density and pressure, eq. (2.5), can be compared to the expression of ε and P in the s-favoured operator method of [1]. It is clear that the P in the t-favoured method is exactly $\varepsilon/3$ of the s-favoured method. The positivity of the ε in the s-favoured scheme guarantees the positivity of P in the t-favoured scheme. The interaction measure—

$$\frac{\Delta}{T^4} = \frac{(\varepsilon - 3P)}{T^4} = 6N_cN_\tau^4\frac{B(\alpha_s)}{2\pi\alpha_s^2}\left[D_s + D_\tau\right], \tag{2.6}$$

is same for both the t and s-favoured methods. Since Δ is always positive our expression for ε is also bound to give positive values for the energy density.

Let us now turn our attention to specific heat at constant volume (c_V) and the isentropic speed of sound (c_s). These quantities are defined as—

$$c_V = \left.\frac{\partial\varepsilon}{\partial T}\right|_V, \qquad \text{and} \qquad c_s^2 \equiv \left.\frac{\partial P}{\partial\varepsilon}\right|_s = \left.\frac{\partial P}{\partial T}\right|_V\left(\left.\frac{\partial\varepsilon}{\partial T}\right|_V\right)^{-1} = \frac{s/T^3}{c_V/T^3}. \tag{2.7}$$

Here we have used the definition of entropy density, $s = (\partial S/\partial V)_T = (\varepsilon + P)/T$, and the thermodynamic identity $(\partial P/\partial T)_V = (\partial S/\partial V)_T$, S being the total entropy. In [4] it has been argued that the specific heat can most easily be obtained by working in terms of the dimensionless variable $\mathscr{C}$, the so-called conformal measure, —

$$\mathscr{C} = \frac{\Delta}{\varepsilon}, \qquad \text{and} \qquad \Gamma = T\,\frac{\partial \mathscr{C}}{\partial T}\bigg|_V . \tag{2.8}$$

By doing some straight forward algebraic manipulations it is very easy to see that—

$$\frac{c_V}{T^3} = \left(\frac{\varepsilon/T^4}{P/T^4}\right)\left[\frac{s}{T^3} + \frac{\Gamma}{3}\frac{\varepsilon}{T^4}\right], \qquad \text{and} \qquad c_s^2 = \left(\frac{P/T^4}{\varepsilon/T^4}\right)\left[1 + \frac{\Gamma\varepsilon/T^4}{3s/T^3}\right]^{-1}. \tag{2.9}$$

In [3], an expression for Γ has been calculated in terms of the plaquettes and the co-variances of the plaquettes. It has also been shown in [4] that c_V/T^3 and c_s^2 reaches their respective ideal gas values in the $g \to 0$ limit. The expression for Γ contains the second derivatives of the Karsch coefficients c_i'''s. Numerical values of these second derivatives have already been evaluated in [4] for an $SU(3)$ gauge theory. Using all these we can determine the specific heat and the speed of sound directly from numerical simulations.

3. Results

We have performed simulations in the temperature range $0.9 \leq T/T_c \leq 3$, with temporal lattice sizes $N_\tau = 8,\ 10,\ 12$. Spatial lattice sizes were chosen to be $2N_\tau + 2$ for $T \leq 2T_c$, and $3N_\tau + 2$ for $3T_c$. For the zero temperature simulations, a minimum lattice size of 22^4 were chosen and then lattice sizes were scaled up with changes in lattice spacings. Typical number of sweeps used for the measurements of the plaquettes were around few hundred thousand in finite temperature runs, and around one hundred thousand in zero temperature simulations. The details of our simulations can be found in [3].

From the computations for the above mentioned three temporal lattices we performed continuum extrapolations by linear fits in $a^2 \propto 1/N_\tau^2$ at all temperatures. In Figure (1a) and Figure (1b) we compare the continuum limits of pressure and energy density for the t-favoured method [3], s-favoured method [1] and the integral method [2]. The most important thing to be noted is that, unlike the old s-favoured operator method, the new t-favoured operator method gives positive pressure for all the temperatures, and also for all lattice spacings. The t-favoured method pressure agrees well with the integral method pressure in the high temperature ($T \geq 2T_c$) region and both differ from the ideal gas value by about 20%. In contrast, even in the continuum limit, and on N_τ as large as $8-12$, the s-favoured method does not yield positive pressure near T_c. On the other hand in the phase transition region the t-favoured method pressure shows a steeper rise than that of the integral method pressure. Compared to the integral method the energy density in the t-favoured method is harder near T_c and agrees with that of the integral method for $T \geq 2T_c$. This indicates a difference in the latent heat determined by the two methods.

Part of the disagreement between the t-favoured and the integral method results can be traced back to the fact the integral method pressure is simply set to zero at T_c and below this cut-off temperature the integral method pressure is ill-defined. Also the assumption of a homogeneous

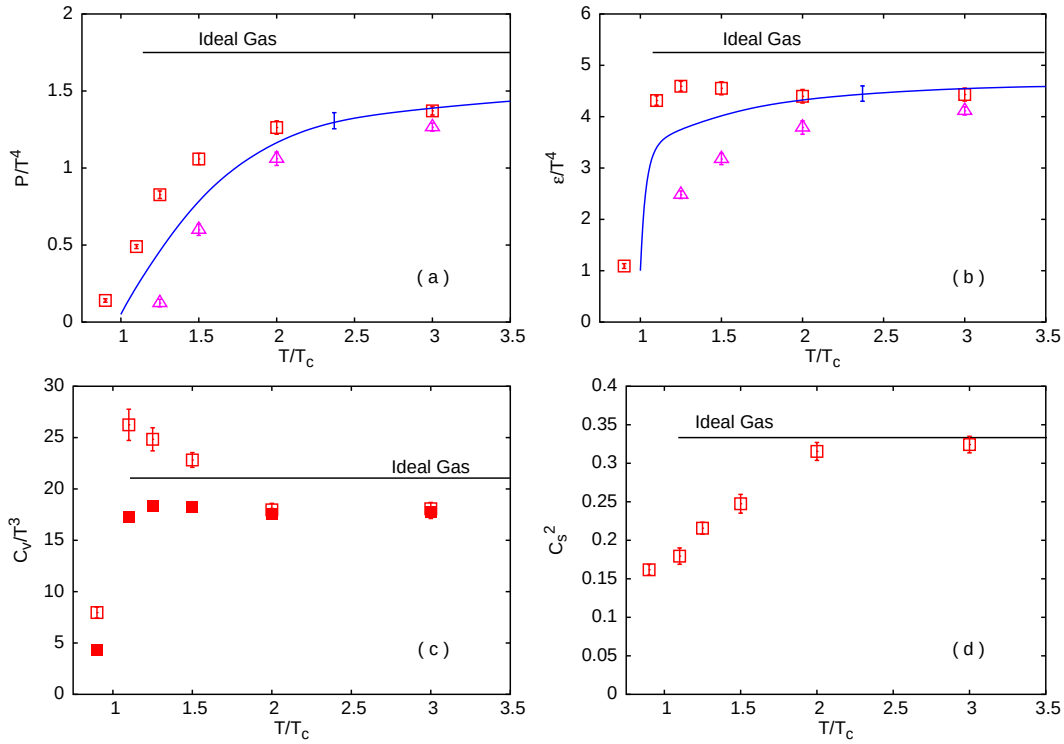

Figure 1: We show comparisons between the continuum results of different thermodynamic quantities for our new method (boxes), the old operator method (triangles) and the integral method (line). In panel (c) we show a comparison between our continuum results for c_V/T^3 (open boxes) and continuum $4\varepsilon/T^4$ (filled boxes). The data for the integral method has been taken form Ref. [2].

system breaks down at a first order phase transition that takes place for a pure $SU(3)$ gauge theory. Along with these, the integral method results of [2] shown here are for coarser lattices, uses non-perturbative β-function and different scheme to determine the renormalized coupling. We plan to investigate these issues in future, in view of all the differences in these two computations.

We present the continuum results for the specific heat and the speed of sound in Figure (1c) and Figure (1d) respectively. For $T \geq 2T_c$, c_V/T^3 is far from its ideal gas value, but is quite consistent with the prediction in conformal theories that $c_V/T^3 = 4\varepsilon/T^4$. In the neighbourhood of T_c, c_V shows a peak-like structure. Whereas c_s is consistent with its ideal gas value (in accordance with the prediction for a conformal theory) for $T \geq 2T_c$, it decreases dramatically near T_c.

We find that the pressure in the t-favoured method agrees with that obtained from a dimensionally reduced theory, matched with the 4-d theory perturbatively upto order $g^6 \ln(1/g)$ [8], almost all the way down to T_c. This has been shown in Figure (2a).

In Figure (2b) we compare our result for the entropy density s with that of the strongly coupled $\mathcal{N} = 4$ Super Yang-Mills (SYM) theory obtained by using the AdS/CFT correspondence [9]. We find that the deviation of s/s_0, s_0 being the entropy density for an ideal gluon gas, from $3/4$ is in good agreement with the predicted results for a strongly coupled $\mathcal{N} = 4$ SYM from $T > 1.5T_c$. This, along with our results for c_V/T^3 and c_s^2, gives a hint that QCD behaves like a quasi-conformal

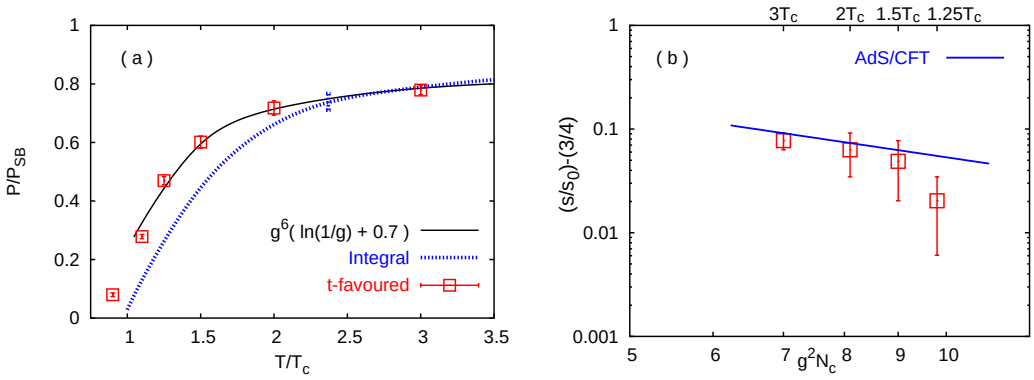

Figure 2: In panel (a) we compare the pressure obtained by t-favoured method (boxes), integral method (dotted line) and the $g^6 \ln(1/g)$ order perturbative expansion (solid line). The data for the integral method and the perturbative expansion are taken from Ref. [2] and Ref. [8] respectively. The values of the $T/\Lambda_{\overline{MS}}$ in Ref. [8] has been converted to T/T_c using the $T_c/\Lambda_{\overline{MS}}$ quoted in [7]. In panel (b) we show the deviation of s/s_0 from $3/4$ (boxes) as a function of the t'Hooft coupling. The line shows the same quantity as predicted by the AdS/CFT correspondence [9].

theory for t' Hooft couplings $g^2N_c < 9$.

4. Summary

We presented a new variant of the operator method, namely the t-favoured scheme, for the calculation of the EOS of QCD. This methods gives positive pressure for all temperatures and all lattice spacings, even when the old operator method gives negative pressure. Using this new method we have computed the continuum limit of the energy density and pressure. We have also extended this method to determine the continuum limit of specific heat at constant volume and speed of sound, both above and below the transition temperature. To the best of our knowledge this is the first continuum results for these two quantities. We have also compared our results with the predictions of perturbation theory and also with the results for strongly coupled $\mathcal{N} = 4$ SYM. We find good agreement with both in certain ranges of temperature.

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