Results from Lattice QCD

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Abstract. I present our recent results on the critical end point in the $\mu_B-T$ phase diagram of QCD with two flavours of light dynamical quarks and compare them with similar results from other groups. Implications for a possible energy scan at the RHIC are discussed. I also comment briefly on the new results of great relevance to heavy ion collisions from finite temperature lattice QCD simulations on speed of sound, specific heat and on the fate of $J/\psi$.

Submitted to: J. Phys. G: Nucl. Phys.
1. Introduction

Lattice Quantum Chromo Dynamics (QCD), defined on a space-time lattice, has been our best and most reliable tool to extract non-perturbative physics of the strongly interacting theory for over a decade now. In many cases, such as the hadron spectra or the weak decay constants, the focus of lattice QCD has now shifted to obtaining more precise results. In the fields of strong interest to this conference, namely Relativistic Heavy Ion Collisions and the possible transition to the new Quark-Gluon Plasma (QGP) phase, also there are similar examples: the quark-hadron transition temperature $T_c$, the Wróblewski Parameter $\lambda_s$, and the the equation of state $[1]$. Already a lot of reliable theoretical information on these physical observables of interest has been predicted by lattice QCD and again the focus is now for better precision. Due to the strong influence of dynamical fermions on thermodynamics and the nature of the phase transition, one still has some way to go before precise prediction for realistic world of two light ($u$ and $d$) and one heavy ($s$) flavour become available. Nevertheless, the continuing progress in lattice QCD makes it perhaps a reachable goal. I shall be unable to review all the important recent lattice results in the time available. I have therefore chosen to focus on those with thrust on something new, either conceptually or quantitatively. In particular, I shall cover the new results on the $T-\mu_B$ phase diagram and the physically interesting question of $J/\psi$-dissolution/persistence. An interesting theoretical issue these days has been the comparison of predictions of conformally invariant theories with lattice QCD results. I shall show one such comparison along with new results for speed of sound.

2. QCD Phase Diagram

The first principles exploration of the QCD phase diagram has the lattice QCD partition function as its focal point. Assuming three flavours of quarks, $u$, $d$, and $s$ and denoting by $\mu_f$ the corresponding chemical potentials, it is defined by:

$$Z = \int DU \exp(-S_G) \prod_{f=u,d,s} \text{Det} M(m_f, \mu_f).$$

Note that the quark mass $m_f$ and the corresponding chemical potential $\mu_f$ enter only through the Dirac matrix $M$ for each flavour. The baryon and isospin chemical potentials are related to those for quarks by $\mu_B = \mu_u + \mu_d + \mu_s$ and $\mu_3 = \mu_u - \mu_d$.

Progress in unravelling the phase diagram using lattice QCD has been slow due to so-called “fermion problem”: for nonzero $\mu$, the determinant in eq. (1) is complex. This renders both analytical and numerical investigations very difficult. Recently, progress was made by a key observation. Following the phase transition from the $\mu_B = 0$ axis into the $\mu_B$-$T$ plane is relatively easier. Various methods have been employed to achieve this. In addition to the original re-weighting method [3] in two couplings, imaginary chemical potential [4] and Taylor series expansion [5] have been used to find and locate the critical end point, expected for a world with two light flavours on the basis of a variety of
model considerations [6]. I shall describe below our results obtained by using the Taylor series method. One of its primary advantages is the ease of taking the continuum and thermodynamic limit which is mandatory for all such lattice computations. This is especially difficult for the re-weighting method [3] due to the $\exp(-\Delta S)$ factor it has which becomes exponentially small for bigger lattices. Furthermore, the discretization errors propagate in an unknown manner in a re-weighting computation, making reliable estimates in continuum limit very difficult. A much better control of the systematic errors is, on the other hand, achieved in the method we employ. We study volume dependence of the Taylor coefficients at several temperature $T$ to i) bracket the critical region and then to ii) track its change as a function of volume. As shown in Figure 1, one expects to pin down the critical region much more precisely this way in going from a smaller volume $V_1$ to a bigger one $V_2$.

Various quark, baryon and isospin densities and the corresponding susceptibilities can be obtained from eq. (1) as:

$$n_i = \frac{T}{V} \frac{\partial \ln Z}{\partial \mu_i}, \quad \chi_{ij} = \frac{T}{V} \frac{\partial^2 \ln Z}{\partial \mu_i \partial \mu_j}.$$  

Higher order susceptibilities, $\chi_{n_u,n_d}$, can be similarly defined as $n_u(n_d)$ partial derivatives of $\ln Z$ with respect to $\mu_u(\mu_d)$. Using them, the pressure $P$ has the following expansion in $\mu$:

$$\frac{\Delta P}{T^4} = \frac{P(\mu, T)}{T^4} - \frac{P(0, T)}{T^4} = \sum_{n_u,n_d} \chi_{n_u,n_d} \frac{1}{n_u!} \left( \frac{\mu_u}{T} \right)^{n_u} \frac{1}{n_d!} \left( \frac{\mu_d}{T} \right)^{n_d}$$  

(3)

Quark number susceptibilities in (2) are crucial for many quark-gluon plasma signatures which are based on fluctuations in globally conserved quantities such as baryon number or electric charge. Theoretically, they serve as an important independent check on the methods and/or models which aim to explain the large deviations of the
lattice results for pressure $P(\mu=0)$ from the corresponding perturbative expansion. This has been discussed elsewhere in details. Here we will be concerned with using them with the higher order terms to learn about the critical end point. Indeed, a series for baryonic susceptibility $\chi_B$ can be constructed using them, whose radius of convergence gives the nearest critical point [7]. Limited by the finite (and even small) number of terms available, one uses standard tests for series convergence on them to do the best one can. Successive estimates for the radius of convergence can be obtained from these using $r_{n+2} = \sqrt{\chi_B^{n+2}/\chi_B^n}$. We use terms up to 8th order in $\mu$, i.e., the estimates from 2/4, 4/6 and 6/8 terms in eq. (3). It may be noted here that a similar construction of a series goes through for the off-diagonal susceptibility, $\chi_{11}$ as well. The ratio $\chi_{11}/\chi_{20}$ can be shown to yield the ratio of widths of the measure in the imaginary and real directions at $\mu = 0$, i.e., a measure of the difficulty of the ‘fermion sign’ problem mentioned above. With some care, this argument can be generalized to nonzero $\mu$.

2.1. Our Results

Our results [7] were obtained by simulating full QCD with two flavours of dynamical staggered quarks of mass $m/T_c = 0.1$, where $T_c$ is the transition temperature for zero chemical potential, on lattices of size $4 \times N_s^3$, with $N_s = 8, 10, 12, 16$ and 24. R-algorithm [8] with a trajectory length of one unit of molecular dynamics time on $N_s = 8$ was used for simulations of full QCD. The trajectory length was scaled with $N_s$ on larger spatial lattices. Earlier investigations have pinned down the physical parameters for our simulations at zero chemical potential [9]: $m_\rho/T_c = 5.4 \pm 0.2$ and $m_\pi/m_\rho = 0.31 \pm 0.01$. We used the canonical methods to fix the lattice spacing $a$ in physical units for which we made runs on symmetric $16^4$ lattices. Their details as well as other details about evaluation of the higher order susceptibilities can be found in [7]. Here I shall be brief and state only that our simulations were made at $T/T_c = 0.75(2), 0.80(2), 0.85(1)$,
0.90(1), 0.95(1), 0.975(10), 1.00(1), 1.05(1), 1.25(1), 1.65(6) and 2.15 (10) with a typical statistics of 50-100 in the units of (maximum) autocorrelation length.

Using terms of up to 8th order in $\mu$ in the expansion in eq. (3), we obtained estimates for the radius of convergence shown in Figure 2. The left panel shows $r_6$ as a function of $N_s$ at three temperatures whereas the right panel exhibits $r_6$ and $r_8$ at $T/T_c = 0.95$. The latter also shows on top the spatial lattice size in units of inverse pion length. As seen from the left panel of the figure, our estimate of the radius of convergence for the smaller lattices with $N_s \sim 10$ is consistent with the critical end point estimate of the re-weighting method [3] with appropriate size, i.e, $N_s m_\pi = 3-4$. Note that $m_\pi/m_\rho = 0.31$ in that case as well. Figure 2 shows, however, large finite size effects for these small lattices and a strong change in the estimate around $N_s m_\pi \sim 6$. Such finite size effects are expected theoretically [10] and have been seen in other cases such as chiral condensates [11] and lattice QCD evaluations of structure functions [12].

A key consequence of our use of larger volumes than before is that we find a shift in the critical end point to $\mu_B/T \sim 1 - 2$, as is evident from Figure 2. Recently, similar computations but up to 6th order have been reported on a large lattice with $N_s m_\pi \sim 15$, and were also discussed in this conference [13]. These use, however, large quark masses, and consequently a a large $m_\pi/m_\rho \sim 0.7$. It will be interesting to see if lowering their quark mass leads to results similar to ours.

### 2.2. Measure of Sign Problem

![Figure 3](attachment:image.png)

**Figure 3.** The ratio of quark number susceptibilities $\chi_2$ and $\chi_{11}$ on $4 \times 16^3$ (circles) and $4 \times 24^3$ (boxes) lattices.

Figure 3 displays the ratio of the two susceptibilities $\chi_{11}$ and $\chi_{20}$ as a function of temperature on two different lattice sizes. This ratio, which is a measure of the seriousness of sign problem, shows how the increase in both its value and fluctuations make the simulations progressively more difficult as one lowers the temperature to $T_c$ and below. The success of the current round of finite density lattice simulations can also be traced from this figure to the fact that all current efforts, regardless of the details of their methods, attempt to explore the phase diagram starting from $T_c$, the transition point at zero chemical potential. An important check one can make in the
Taylor series expansion technique is that each coefficient in the Taylor expansion must be volume independent. Since the actual evaluation of these terms entails cancellation of divergences, this is indeed a nontrivial check which has been made successfully [7]. In fact, care is needed in extracting any equation of state at finite chemical potential from these coefficients: a systematic study on different volumes (spatial lattices) with a subsequent extrapolation to infinite volume is necessary to ensure that some peak-like behaviour in, e.g., $\chi_{40}$, is real and does not give spurious results for thermodynamic quantities.

3. Speed of Sound

![Figure 4](image_url)

**Figure 4.** Specific heat $C_v$ and $4\epsilon$ (left) and the speed of sound $c_s$ as a function of temperature for quenched QCD. See text for more details.

An important physical property of the strongly interacting matter at finite temperature, which has been computed [14] since long using lattice techniques, is the speed of sound. Its relevance to many aspects of heavy ion physics, such as the elliptic flow or the hydrodynamical studies can hardly be overemphasized. A related quantity of interest is the specific heat which has been related to event-by-event fluctuations of the transverse momentum ($p_T$). There are various measures of these fluctuations currently in use in the literature. It may actually be better to relate them to the specific heat in order to make them both more physical as well as uniform in convention.

A recent development in this direction on the lattice is a new way to obtain these by relating them to the temperature derivative of an anomaly measure $\Delta/\epsilon \equiv (\epsilon - 3P)/\epsilon$ [15]. Using lattices with 8, 10, and 12 temporal sites ($38^3 \times 12$ and $38^4$ lattices) and with statistics of 0.5-1 million iterations, $\epsilon, P, s, C_s^2$ and $C_v$ were obtained in continuum using this differential method at $2T_c$ and $3T_c$ for quenched QCD. Sizable deviations from the corresponding ideal gas results were found although $C_v$ was consistent with $4\epsilon$, as expected in a weak coupling scenario. On the other hand the result for entropy density at $3T_c$ also seemed to agree with a strong coupling (super Yang-Mills) prediction [16]:

$$s/s_0 = f(g^2N_c),$$

where $f(x) = \frac{3}{4} + \frac{45}{32}\zeta(3)(2x^{-3/2}) + \cdots$ and $s_0 = \frac{2}{3}\pi^2 N_c^2 T^3$. However, curiously it too failed at $2T_c$. 


New results for the specific heat and the speed of sound, obtained by using a new method, called the $t$-method, were presented at this conference in a poster \cite{17}. While the differential method \cite{18} for obtaining thermodynamic quantities has lesser systematic errors and is convenient to use, it was abandoned in favour of the integral method \cite{19} due to the former’s problem of yielding negative Pressure. It was shown that this problem of negative pressure can be completely avoided even in the differential method by writing the derivatives with respect to temperature and volume using a parameter $t$: the old (Bielefeld) method \cite{18} corresponds to $t = 1$ and leads to negative pressure but $t = 0$ results in positive pressure always. Figure 4 shows these new results of \cite{17} for the specific heat (the left panel) and the speed of sound (right panel). While the corresponding pressure is not shown here, it is positive even around $T_c$, an input which went in getting the speed of sound (squares), shown in Figure 4. Note that these continuum results have been obtained by simulating lattices with many lattice spacings and then extrapolating to zero unlike the results for the integral method (dotted line) in Figure 4 which are for $N_t = 8$. The interesting and noteworthy features are: i) the specific heat does tend to peak near $T_c$ and is widely different there from the weak coupling expectation of $4\epsilon$, ii) for $T \geq 2T_c$, this weak coupling expectation is fulfilled but the resulting value is very different from that for an ideal gas, iii) speed of sound is about 10% smaller than the ideal gas for higher temperatures but drops close to $T_c$, and iv) the results are in good agreement with the integral method but could differ significantly in the neighbourhood of $T_c$. Further investigations are needed to see if $c_s^2$ dips close to zero near $T_c$.

4. Persistence of $J/\psi$

![Figure 5. Spectral functions \cite{20} of the vector $J/\psi$ and scalar $\chi$ mesons as a function of energy at various temperatures. See text for more details.](image)

An intriguing result on the $J/\psi$ and similar heavy quarkonia has recently emerged \cite{20, 21} from the lattice QCD investigations. As is well known, Matsui and Satz \cite{22} proposed $J/\psi$ suppression as a signal of quark-gluon plasma. Quarkonium potential model calculations with an ansatz for temperature dependence of the heavy quark-antiquark potential lead to the result that $J/\psi$ and $\chi_c$ states dissolve in QGP by
1.1\( T_c \). The impressive results from the CERN NA50 did suggest an anomalous suppression of \( J/\psi \) in Pb-Pb collisions, bringing forth detailed theoretical questions on this suppression mechanism and the above mentioned ansatz. In particular, one approach taken by the lattice experts has been to study the spectral function of these states in QGP to look for their dissolution from first principles. The recognition of the maximum entropy method (MEM) as a reliable tool to extract the spectral functions from temporal lattice correlators at zero temperature lead to its application at finite temperature. Caution is, however, called for in doing so since nonzero and high temperatures are obtained by making the temporal lattice smaller whereas MEM works better for longer temporal lattices.

Figure 4 shows the results of the Bielefeld group, obtained by simulating lattices from \( 48^3 \times 12 \) to \( 64^3 \times 24 \) in sizes in the quenched approximation of no dynamical quarks. The vertical bars are drawn to indicate the size of the error on the integrated spectral function in the area shown by the horizontal bars. One observes that the \( \chi_c \) does seem to indeed dissolve by 1.1\( T_c \), as expected from naive potential model considerations. However, the \( J/\psi \) and \( \eta_c \) persist up to 2.25 \( T_c \) and are gone only at 3\( T_c \). Similar results have been obtained by other groups as well, although there seems to be some disagreement on the precise value of the temperature at which the \( J/\psi \) peak vanishes.

While these results have to be still confirmed in a full QCD simulation with light dynamical quarks, they already can have strong consequences for the \( J/\psi \) signal. Recall that only about 30-40 % of the \( J/\psi \) come through \( \chi \) decays (with a substantial fraction from \( \chi_2 \) which has not yet been investigated), thus the predicted suppression will be rather small until temperatures close to 3\( T_c \) are reached (or energy densities 81 times that of critical energy density is reached), which seems to be a tall order for the current round of CERN and BNL experiments. An interesting observable consequence could, however, be a change of the suppression pattern as a function of \( \sqrt{s} \) or the energy density reached.

5. Summary

The QCD phase diagram in \( T - \mu_B \) plane has begun to emerge. Since all results so far have been obtained on \( N_t = 4 \), i.e, very coarse, lattices, several quantitative issues related to continuum limit still have to wait. It may be noted that the existence of equally legitimate different prescriptions of introduction of the chemical potential on the lattice can, and do, lead to even larger lattice artifacts on such coarse lattices. Nevertheless, it is very heartening to find that different methods lead to a similar qualitative picture.

Our results, using Taylor expansion, permit us to take the thermodynamic limit, unlike other methods. Our investigation of volume dependence suggests \( N_s m_\pi > 6 \) approximates the thermodynamic volume limit reasonably. The \( \mu_B/T \) of the critical end point, identified from the radius of convergence using up to, and including the 8th order terms, drops strongly around that volume. We find that \( \mu_B/T \sim 1 - 2 \) is
indicated for the critical point with a corresponding temperature of \( \simeq 0.95 T_c \), where \( T_c \) is the transition temperature for the baryon-free case.

![Figure 6. The QCD phase diagram with a freeze-out curve superimposed. The filled circle denotes the estimate of the critical point which has been obtained in [7]. The open circle is an earlier estimate from [3] using smaller lattices and nearly the same quark mass.](image)

Figure 6 shows our results, together with the earlier determination [3] on small volumes but similar quark mass, i.e., the pion mass. A freeze-out curve [25], obtained by treating a resonance gas as ideal, has been superimposed on the Figure. From the marked values of the CM energy, \( \sqrt{s} \), per nucleon needed to reach that point on the curve, one notes that the critical end-point may be in the reach of future RHIC energy scans.

I also presented new continuum results on the speed of sound and the specific heat for quenched QCD. A new method, which revives the earlier differential method but without its drawback of negative Pressure was used to obtain these results. Interesting quantitative agreement was found with strong coupling predictions from super Yang-Mills theory at \( 3T_c \) but not at \( 2T_c \).

Finally, the intriguing persistence of \( J/\psi \) in QGP was discussed. The MEM technique has been used to obtain the spectral function at finite temperature. While it showed the peak in the \( \chi \) spectral function to go away by \( 1.1T_c \), the peak in the vector spectral function persists up to \( 2.25-3T_c \). Extension of these simulations to incorporate dynamical quarks would be crucial to be sure of the phenomenological consequences of these results.

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