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Lattice Simulations of the Thermodynamics of Strongly Interacting Elementary Particles and the Exploration of New Phases of Matter in Relativistic Heavy Ion Collisions

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Abstract. At high temperatures or densities matter formed by strongly interacting elementary particles (hadronic matter) is expected to undergo a transition to a new form of matter - the quark gluon plasma - in which elementary particles (quarks and gluons) are no longer confined inside hadrons but are free to propagate in a thermal medium much larger in extent than the typical size of a hadron. The transition to this new form of matter as well as properties of the plasma phase are studied in large scale numerical calculations based on the theory of strong interactions - Quantum Chromo Dynamics (QCD). Experimentally properties of hot and dense elementary particle matter are studied in relativistic heavy ion collisions such as those currently performed at the relativistic heavy ion collider (RHIC) at BNL.

We review here recent results from studies of thermodynamic properties of strongly interacting elementary particle matter performed on Teraflops-Computer. We present results on the QCD equation of state and discuss the status of studies of the phase diagram at non-vanishing baryon number density.

1. Introduction

During recent years our faith in numerical calculations of properties of strongly interacting matter at high temperature and non-vanishing baryon number density greatly increased. The steady improvement of discretization schemes for the fermion sector of QCD and the development of new simulation algorithms [1] now allow to perform calculations with greatly reduced systematic errors. Moreover, the widespread availability of a new generation of Teraflops-Computer for lattice gauge theory calculations now allows to perform studies of thermal properties of matter formed by strongly interacting elementary particles with an almost realistic quark mass spectrum [2, 3, 4].

Numerical calculations with small systematic errors also form the basis for further quantitative studies of the QCD phase diagram at non-zero quark chemical potential ($\mu_q$) [5, 6, 7, 8, 9] or, equivalently, non-zero baryon number [10, 11]. The different approaches developed for this purpose are still limited to the regime of temperatures close to and above the transition temperature, $T_0$, as well as small values of the chemical potential, $T \cong 0.9T_0$, $\mu_q/T \leq 1$. As such they do not yet allow to explore the interesting low temperature and high density part of the QCD phase diagram, where various color superconducting phases
are expected to show up [12, 13]. They, however, allow to study the phase diagram and thermodynamic properties of matter in a regime accessible to heavy ion experiments and cover a regime that will be studied in future experiments planned at RHIC and the GSI in Germany to explore matter at high baryon number density. The generic form of the QCD phase diagram is shown in Fig. 1(left). Various model calculations suggest that at low temperature the low and high density regions in the QCD phase diagram are separated by a line of first order phase transitions. On the other hand, lattice calculations suggest that at small values of $\mu_q/T$ the transition from low to high temperature is not a phase transition; thermodynamic quantities like the energy density or the chiral condensate change smoothly, although quite rapidly, in a narrow temperature interval. It thus has been speculated [14] that a 2nd order phase transition point exists somewhere in the interior of the QCD phase diagram. Lattice calculations have provided first indications for the existence of such a critical point [5, 15, 16]. Its exploration and the detailed quantitative analysis of transition parameters characterizing the separation line between the low and high density regime are currently being performed in large scale numerical simulation of QCD.

Experimentally properties of hot and dense matter are studied in relativistic heavy ion collisions performed at CERN and BNL. In particular, recent results from RHIC experiments on on jet modifications and flow properties of matter created in Au-Au collisions suggest that in the collision of two heavy nuclei a dense medium is generated which equilibrates quickly after the collision at temperatures well above the transition temperature estimated in lattice calculations. A hot and dense system thus seems to be generated in the plasma phase of QCD; once equilibrated it expands isentropically and cools down again. Its constituents, quarks and gluons, then 'freeze-out', i.e. recombine to ordinary hadrons that become experimentally detectable. The relative abundances of various hadron species at freeze-out seem to be well described by a hadron resonance gas which allows to relate the observed particle yields to temperature and baryon chemical potential ($\mu_B = 3\mu_q$) at freeze-out. The freeze-out parameters extracted from heavy ion experiments performed with different collision energies [17] are shown in Fig. 1(right). At least for small values of $\mu_q$ the freeze-out temperature seems to be close to the transition temperature determined in lattice calculations [18, 19]. To quantify this agreement and the relation between freeze-out conditions and phase transitions also at larger values of $\mu_q$. 

Figure 1. Sketch of the QCD phase diagram (left) as well as the freeze-out curve determined in heavy ion collisions at various center of mass energies (right) [17]. The freeze-out curve is parametrized by $T = 0.17 - 0.13\mu_B^2 - 0.06\mu_B^4$. 
2. The QCD equation of state at vanishing baryon number density

Most information on the structure of the high temperature phase of QCD and the nature of the transition itself has been obtained through lattice calculations performed in the limit of vanishing baryon number density or, equivalently, vanishing quark chemical potential ($\mu_q = 0$). This limit is most relevant for our understanding of the evolution of the early universe. It also corresponds to the regime which currently is studied experimentally in heavy ion collisions at RHIC (BNL) and soon will be explored also at the LHC (CERN). The experimental accessibility of this regime of dense matter also asks for a thorough quantitative study of the QCD phase transition and of basic parameters that characterize the thermodynamics of dense matter at high temperature, e.g. the transition temperature $T_0$ and the energy density $\epsilon_c$ at this temperature. Good quantitative control over the temperature dependence of basic quantities that characterize bulk properties of a thermal medium also is needed to extract the equation of state, $p(\epsilon)$, which controls the evolution of dense matter created in heavy ion collisions. We will in the following present some of the recent results on the QCD transition and the equation of state obtained in large scale numerical simulations of lattice regularized QCD.

2.1. Deconfinement and chiral symmetry restoration

The transition to the high temperature phase of QCD is closely related to two fundamental properties of QCD - chiral symmetry breaking and confinement. In QCD at low temperature chiral symmetry is spontaneously broken; the chiral condensate, obtained as the derivative of the logarithm of the QCD partition function, $Z(T, V, m_q)$ with respect to the quark mass,

$$\langle \bar{\psi} \psi \rangle = \frac{T}{V} \frac{\partial \ln Z}{\partial m_q},$$  \hspace{1cm} (1)
remains non-zero even in the limit of vanishing quark mass $m_q$. In this limit the chiral condensate is an order parameter for the phase transition to the high temperature phase; it is non-zero at low temperature and vanishes for temperatures larger than the transition temperature. Lattice calculations give evidence for chiral symmetry restoration as is apparent from Fig. 2(left) which shows a recent analysis of $\langle \bar{\psi} \psi \rangle$ performed for QCD with two light and a heavier strange quark mass as well as for QCD with three degenerate quark masses [20]. Although the transition is not a true phase transition but a smooth crossover, it clearly is signaled by a rapid change in the chiral condensate.

The chiral transition also is deconfining, i.e. at the transition temperature a large number of new degrees of freedom gets liberated. These degrees of freedom can be identified as quarks and gluons. At (very) high temperatures bulk thermodynamic observables resemble the behavior of an ideal quark-gluon gas, i.e. the pressure and energy density approach the corresponding Stefan-Boltzmann values,

$$\frac{P_{SB}}{T^4} = \frac{1}{3} \frac{\epsilon_{SB}}{T^4} = \frac{\pi^2}{45} \left( 8 + \frac{21}{4} n_f \right).$$

This becomes apparent when one compares, for instance, results for the temperature dependence of the pressure calculated in QCD with different number of quark species ($n_f$ flavors). As can be seen in Fig. 2(right) the pressure rises rapidly at the transition temperature and at higher temperatures approaches (slowly) the Stefan-Boltzmann limit for an ideal gas with the relevant number of quark and gluon degrees of freedom.

2.2. The QCD transition temperature

Determining the transition temperature accurately is one of the basic goals of numerical studies of QCD thermodynamics. This involves several independent steps. First of all one has to determine the bare coupling, $g^2$, at which the transition takes place, on a four dimensional lattice with fixed extent, $N_T$, in the fourth direction. This determines the transition temperature in units of the lattice spacing $T = 1/N_T a(g^2)$. In a second step one has to determine the lattice spacing, $a(g^2)$, that corresponds to this value of the gauge coupling. This can be done by calculating another physical observable in lattice units that is known experimentally, e.g. a hadron mass, $m_H a(g^2)$, or a phenomenologically known observable like the heavy quark potential. Finally one has to increase the lattice extent $N_T$ and reduce the quark masses to perform a controlled extrapolation to the continuum limit with physical values of the quark masses. In Fig. 3 we show results from an ongoing analysis [23] that follows this program. Shown there is the transition temperature expressed in terms of the square root of the string tension, $\sqrt{\sigma}$, which characterizes the long distance behavior of the heavy quark potential,

$$V_{q\bar{q}}(r) = -\frac{\alpha}{r} + \sigma r.$$  

Similar studies with almost physical light quark masses and a heavier strange quark mass have been performed recently by the MILC collaboration [20]. These analyses have been performed with significantly smaller quark masses and a smaller lattice spacing than earlier studies. They indicate that the transition temperature expressed in units of the string tension, $T_0/\sqrt{\sigma} \simeq 0.39 - 0.4$, is in fact somewhat smaller than earlier estimates. Nonetheless, recent studies of heavy quarkonium spectra, suggest a value for the string tension, $\sqrt{\sigma} \simeq 460$ MeV, which is about 10% larger than values used previously to convert the QCD transition temperature to physical units. This leads to somewhat larger estimates for $T_0$ than the value $T_0 \simeq 175$ MeV used in the past. Current estimates suggest a transition temperature of about $190$ MeV for QCD with almost physical light quark masses and a heavier strange quark mass.
Figure 3. The transition temperature in QCD expressed in units of the square root of the string tension. Shown are results obtained from a simulation of QCD with two light quark masses and a heavier strange quark mass [23]. They are plotted versus the lightest pseudo-scalar meson mass expressed in terms of the commonly used scale parameter $r_0$ which is determined from the slope of the heavy quark potential at short distances (for more details on the scale $r_0$ see for instance [20]).

2.3. The QCD equation of state at $\mu_q = 0$

As has been discussed in Section 2.1 we learn from the temperature dependence of the equation of state about the relevant degrees of freedom in the high temperature phase of QCD. Reaching accurate quantitative results on the temperature dependence of pressure and energy density also is needed for the comparison of experimental results obtained in heavy ion collisions with theoretical calculations performed in equilibrium QCD. The dense system created in a heavy ion collision rapidly expands and cools down after its generation and equilibration. This expansion process may be described using hydrodynamic models. In these models the equation of state is a basic input.

While earlier studies of the equation of state of QCD have been performed with rather heavy quark masses and large lattice spacings, recent studies significantly improved over this situation and allow to get better control over systematic effects arising from the use of unphysically large quark mass values as well as from the use of too coarse lattices. Although the calculations with light quarks have still been performed in rather small physical volumes, $TV^{1/3} \approx 2$, they do support earlier findings on the temperature dependence of the pressure and energy density in the transition region and also confirm that quark mass effects are small at high temperature. In particular, they show that the contribution of strange quarks, which have a mass of the order of the transition temperature, $T_0$, has little influence on the thermodynamics in the vicinity of $T_0$. In Fig. 4(left) we compare the recent calculation of the pressure in (2+1)-flavor QCD [2] and earlier results for 2-flavor QCD [24, 25] which both have been performed with unimproved staggered fermions. The good agreement in the vicinity of $T_0$ suggests that the strange quark contribution to the pressure is small. Only for $T \gtrsim 1.5T_0$ differences show up; the positive strange quark contribution to the pressure in $(2 + 1)$-flavor QCD becomes sizeable.

In Fig. 4(right) we compare results for the energy density calculated in QCD with two light quark masses and a heavier strange quark mass [3] with results obtained in 3-flavor QCD with a quark mass that rises with temperature but stays small on the scale given by the temperature, $m/T < 1$ [21]. The good agreement between these calculations is quite reassuring. These calculations confirm that thermodynamics in the high temperature phase is rather insensitive
Figure 4. Cut-off dependence of the pressure calculated with the standard staggered fermion action on lattices with temporal extent \( N_T = 4 \) and 6 in 2-flavor QCD [24, 25] and (2+1)-flavor QCD [2] (left). The right hand figure shows the energy density calculated with improved staggered fermion actions. Shown are results for 3-flavor QCD obtained with the so-called p4-action on lattices with temporal extent \( N_T = 4 \) [21] and for (2+1)-flavor QCD obtained with the asqtad-action for \( N_T = 6 \) [3].

to changes of the quark mass; a reduction of the light quark masses by almost an order of magnitude does not lead to drastic changes in the energy density at the transition point and in the high temperature phase. These recent calculations also show that the transition itself is not strongly influenced by discretization errors, which in the staggered fermion formulation show up prominently in the distortion of the light hadron spectrum; reducing \( m_q \) and thus the masses of light hadrons as well as reducing flavor symmetry breaking effects drastically [2] does not significantly change the energy density at the transition temperature. The estimate, \( \epsilon_c/T_0^4 = 6 \pm 2 \) [21], is consistent with the recent calculations in (2+1)-flavor QCD performed with lighter quark masses. The weak dependence of transition parameters on the quark mass can be understood in phenomenological models of the low temperature phase of QCD; it seems to reflect the importance of numerous heavy resonances that are necessary to build up the particle and energy density needed for the transition to occur [26].

Like earlier calculations with improved staggered fermions also the recent studies of the equation of state performed at vanishing quark chemical potential suggest that for physical values of the quark masses the transition to the high temperature phase of QCD only is a rapid crossover rather than a phase transition which on finite lattices would be signaled by metastabilities and a strong volume dependence of bulk thermodynamic observables or the chiral condensate. None of the calculations performed so far for QCD with two light quarks with or without the inclusion of a heavier strange quark gave direct evidence for a first order phase transition.

3. Thermodynamics at non-zero baryon number density

3.1. Isentropic equation of state and freeze-out in heavy ion collisions

Studies of the QCD equation of state have recently been extended to the case of non-zero quark chemical potential (\( \mu_q \)). Calculations of bulk thermodynamic quantities for \( \mu_q > 0 \) based on the reweighting approach [27], using the Taylor expansion of the partition function [28, 29, 30], as well as analytic continuation of calculations performed with imaginary values of the chemical potential [31] show that the \( \mu_q \)-dependent contributions to energy density and pressure are dominated by the leading order \( (\mu_q/T)^2 \) correction. For RHIC energies, \( \mu_q/T \approx 0.1 \), even this
Figure 5. Temperature dependence of the Taylor expansion coefficients for $p/T^4$ in 2-flavor QCD and for quark masses corresponding at $T_0$ to a pseudo-scalar (pion) mass of about 770 MeV.

We will focus in the following on a discussion of Taylor expansions of the partition function of 2-flavor QCD around $\mu_q = 0$. At fixed temperature and small values of the chemical potential the pressure may be expanded in a Taylor series around $\mu_q = 0$,

$$
\frac{p}{T^d} = \frac{1}{VT^3} \ln Z = \sum_{n=0}^{\infty} c_n(T, m_q) \left( \frac{\mu_q}{T} \right)^n,
$$

where the expansion coefficients are given in terms of derivatives of $\ln Z(T, \mu_q)$, i.e. $c_n(T, m_q) = \frac{1}{n!VT^3} \frac{\partial^n \ln Z}{\partial (\mu_q/T)^n}$. The series is even in $\mu_q/T$ which reflects the invariance of $Z(T, \mu_q)$ under exchange of particles and anti-particles. The Taylor series for the energy density can then be obtained using the thermodynamic relation, $(\epsilon - 3p)/T^4 = Td(p/T^4)/dT$,

$$
\frac{\epsilon}{T^4} = \sum_{n=0}^{\infty} \left( 3c_n(T, m_q) + c'_n(T, m_q) \right) \left( \frac{\mu_q}{T} \right)^n,
$$

with $c'_n(T, m_q) = Tdc_n(T, m_q)/dT$. A similar relation holds for the entropy density [30]. The coefficients $c_n(T, m_q)$ calculated for a fixed value of the bare quark mass up to $n = 6$ are shown in Fig. 5.

Knowing the dependence of the energy density and the pressure on the quark chemical potential one can eliminate $\mu_q$ in favor of a variable that characterizes the thermodynamic boundary conditions for the system under consideration [30]. In the case of dense matter created in heavy ion collisions this is a combination of entropy and baryon number. Both quantities stay constant during the expansion of the system. In Fig. 6 we show the resulting isentropic equation of state as function of temperature as well as energy density obtained from a 6th order Taylor expansion of pressure and energy density [30]. The three different entropy and baryon number ratios, $S/N_B = 30$, 45 and 100, correspond roughly to isentropic expansions of matter formed at the AGS, SPS and RHIC, respectively. It is quite remarkable that $p(\epsilon)$ is to a good approximation independent of $S/N_B$; for temperatures $T > T_0$, or equivalently $\epsilon \gtrsim 0.8$ GeV/fm$^3$, the equation of state is well described by

$$
\frac{p}{\epsilon} = \frac{1}{3} \left( 1 - \frac{1.2}{1 + 0.5 \epsilon \text{ fm}^3/\text{GeV}} \right).
$$
Figure 6. Equation of state of 2-flavor QCD on lines of constant entropy per baryon number. The left hand figure shows three lines of constant $S/N_B$ in the QCD phase diagram relevant for the freeze-out parameters determined in various heavy ion experiments. The right hand figure shows the equation of state on these trajectories using $T_0 = 175$ MeV to set the scale. The solid curve in the right hand figure is the parametrization of the high temperature part of the equation of state given in Eq. 6.

Figure 7. The velocity of sound in QCD vs. temperature expressed in units of the transition temperature $T_0$. Shown are results from calculations with Wilson [32] and staggered fermions [2] as well as for a pure SU(3) gauge theory [22]. Also shown is $v_s^2$ deduced from the isentropic equation of state, Eq. 6 [30].

For large energies this agrees well with a bag equation of state, $3p = e - 4B + O(e^{-1})$, with $B^{1/4} \approx 260$ MeV. Deviation from the simple bag EoS, however, become large close to $T_0$; corrections in an expansion in terms of $e^{-1}$ exceed the leading bag term contribution in magnitude for for $e \lesssim 5$ GeV/fm$^3$ or equivalently $T \lesssim 1.5T_0$.

The insensitivity of the isentropic equation of state on $S/N_B$ also implies that the velocity of sound, $v_s = \sqrt{\frac{dp}{de}}$, is similar along different isentropic expansion trajectories. In fact, the parametrization given in Eq. 6 suggests that the velocity of sound approaches rather rapidly the ideal gas value, $v_s^2 = 1/3$. In Fig. 7 we summarize results for $v_s^2$ obtained in lattice calculations for a $SU(3)$ gauge theory [22], for 2-flavor QCD with Wilson fermions [32], (2 + 1)-flavor QCD with staggered fermions [2] as well as from the isentropic equation of state for 2-flavor QCD [30].

3.2. The chiral critical point

Various model calculations [14] suggest that a second order phase transition point (chiral critical point) exists in the QCD phase diagram which separates a region of first order phase transitions at high baryon number density and low temperatures from a cross-over region at low baryon number density and high temperature. Evidence for the existence of such a critical point may come from lattice calculations at non-zero quark chemical potential by either determining the
location of Lee-Yang zeroes [5] or by determining the convergence radius of the Taylor series for the logarithm of the partition function which directly yields the pressure, \( p/T = V^{-1} \ln Z \) [28].

If there exists a 2\(^{nd}\) order phase transition point in the QCD phase diagram, this could be determined from an analysis of the volume dependence of Lee-Yang zeroes of the QCD partition function. In any finite volume zeroes of \( Z(V, T, \mu_q) \) only exist in the complex \( \mu_q \) plane with \( \text{Im} \mu_q \neq 0 \). Only for \( V \to \infty \) some of these zeroes may converge to the real axis and will then give rise to singularities in thermodynamic quantities. The relation between phase transitions and zeroes of the partition function has been exploited using a reweighting technique to extend lattice calculations performed at \( \mu_q = 0 \) to \( \mu_q > 0 \) [5]. Recent results based on this approach [15] suggest that a critical point indeed exists and occurs at \( \mu_B = 3\mu_q \simeq 360 \text{ MeV} \). This estimate is about a factor two smaller than earlier estimates [5] which have been obtained on smaller lattices and with larger quark masses. This suggests that a detailed analysis of the quark mass and volume dependence [33] still is needed to gain confidence in the analysis of Lee-Yang zeroes.

The radius of convergence of the Taylor series is controlled by a singularity in the complex \( \mu_q \) plane closest to the origin. It is related to the location of the critical point only if this singularity lies on the real axis. A sufficient condition for this is that all expansion coefficients in the Taylor series are positive. For temperatures below the transition temperature at \( \mu_q = 0 \) this indeed seems to be the case for all expansion coefficients calculated so far. The first coefficient, \( c_0 \), gives the pressure at \( \mu_q = 0 \) shown in Fig. 2(right) and thus is positive for all temperatures. This also is the case for \( c_2 \), which is proportional to the quark number susceptibility at \( \mu_q = 0 \) [34],

\[
\frac{X_2}{T^2} = \left. \frac{\partial^2 p}{\partial (\mu_q/T)^2} \right|_{\mu_q=0} = \sum_{n=0}^{\infty} d_n \left( \frac{\mu_q}{T} \right)^n \quad \text{with} \quad d_n = (n+2)(n+1)c_{n+2}. \tag{7}
\]

As can be seen in Fig. 4 also the next-to-leading order coefficient, \( c_4 \), is strictly positive.

A new feature shows up in the expansion coefficients at \( \mathcal{O}(\mu^6) \). The coefficient \( c_6 \) is positive only below \( T_0 \) and changes sign in its vicinity. If this pattern persists for higher order expansion coefficients one may conclude that the irregular signs of the expansion coefficients for \( T > T_0 \) suggest that the radius of convergence of the Taylor series is not related to critical behavior at these temperatures, whereas it determines a critical point for \( T < T_0 \).

Ratios of subsequent expansion coefficients provide an estimate for the radius of convergence of the Taylor expansion,

\[
\rho(T) = \lim_{n \to \infty} \rho_n = \lim_{n \to \infty} \sqrt[2n]{\frac{c_n}{c_{n+2}}}, \quad \rho(T) = \lim_{n \to \infty} \sqrt[2n]{\frac{d_n}{d_{n+2}}}. \tag{8}
\]

The expansion coefficients \( d_n \) for the quark number susceptibility have been analyzed recently for unimproved staggered fermions [16] up to \( n = 6 \). It has been shown that an accurate determination of these expansion coefficients requires large physical volumes. Based on a finite volume analysis the radius of convergence has been estimated from the Taylor series of the quark number susceptibility to be \( \mu_B \simeq 180 \text{ MeV} \) [16]. As the expansion coefficients \( d_n \) are directly related to the expansion coefficients \( c_n \) of the pressure the radius of convergence coincides in the limit \( n \to \infty \). For finite \( n \), i.e. \( n \simeq 6 \), estimates based on the Taylor series for the pressure will be about 30\% higher than those based on the Taylor series for susceptibilities. In any case, current estimates for the location of the critical point in the QCD phase diagram differ quite a bit and these calculations need to be refined in the future.

4. Conclusions

We have presented recent results obtained on the QCD equation of state at vanishing and non-vanishing quark chemical potential. These calculations now can be performed with an almost realistic quark mass spectrum. At vanishing chemical potential one now can start a systematic
analysis of lattice artefacts which allows a controlled extrapolation of lattice results on the equation of state and the transition temperature to the continuum limit. Also studies of the QCD phase diagram at non-zero quark chemical potential made significant progress in recent years. However, in this case much work is still needed to perform high precision calculations that would allow for a controlled continuum extrapolation.

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