Exploring matter under extreme conditions with numerical simulations

Péter Petreczky
Physics Department, Brookhaven National Laboratory, Upton NY 11973, USA
E-mail: petreczk@bnl.gov

Abstract. In this contribution I am going to summarize recent progress in exploring the phase diagram as well as the properties of strongly interacting matter at extreme conditions using lattice QCD. Current status and prospectives of calculating quantities crucial for RHIC program ( quarkonia spectral functions, critical energy density, equation of state ) is discussed in detail. The role of the SciDAC program in reaching the outlined goals is emphasized.

1. Introduction
It is expected that strongly interacting matter shows qualitatively new behavior at temperatures and/or densities which are comparable or larger than the typical hadronic scale. It has been argued that under such extreme conditions deconfinement of quarks and gluons should take place, i.e. thermodynamics of strongly interacting matter could be understood in terms of these elementary degrees of freedom and this new form of matter was called Quark Gluon Plasma [1]. On the lattice the existence of the deconfinement transition at finite temperature was first shown in the strong coupling limit of QCD [2], followed by numerical Monte-Carlo simulations of lattice SU(2) gauge theory which confirmed it [3]. Since these pioneering studies QCD at finite temperature became quite a large subfield of lattice QCD (for recent reviews on the subject see Refs. [4, 5, 6]). One of the obvious reasons for this is that phase transitions can be studied only non-perturbatively. But even at high temperatures the physics is non-perturbative beyond the length scales \(1/(g^2 T)\) (\(g^2 T\) being the gauge coupling) [7]. Therefore lattice QCD remains the only tool for theoretical understanding of the properties of strongly interacting matter under extreme condition which is important for the physics of the early universe as well as heavy ion collisions.

2. Finite temperature transition in full QCD
One of the basic questions, we are interested in, is what is the nature of the transition to the new state of matter and what is the temperature where it happens \(^1\). In the case of QCD without dynamical quarks, i.e. SU(3) gauge theory these questions have been answered. It is well established that the phase transition is 1st order [8]. Using standard and improved actions the corresponding transition temperature was estimated to be \(T_c/\sqrt{\sigma} = 0.632(2)\) [4] (\(\sigma\) is the string tension). The situation for QCD with dynamical quarks is much more difficult. Not

\(^1\) I will talk here about the QCD finite temperature transition irrespective whether it is a true phase transition or a crossover and \(T_c\) will always refer to the corresponding temperature.
only because the inclusion of dynamical quarks increases the computational costs by at least two orders of magnitude but also because the transition is very sensitive to the quark masses. Conventional lattice fermion formulations break global symmetries of continuum QCD (e.g. staggered fermion violate the flavor symmetry) which also introduces additional complications. Current lattice calculations suggest that transition in QCD for physical quark masses is not a true phase transition but a crossover [9, 10, 11, 12, 13]. Recent lattice results for the transition temperature \(T_c\) from Wilson fermions [14, 15], improved [9, 12, 13] and unimproved staggered fermions [11] with 2 and 2+1 flavors of dynamical quarks are summarized in Fig. 1. The errors shown in Fig. 1 are only statistical with the exception of the data point from the MILC collaboration. The MILC collaboration which is largely supported by the SciDAC project performed a detailed study of the transition temperature at several value of the quark masses and three lattice spacings. The simultaneous extrapolation to the continuum limit and to the limit of physical \(u, d\) -quark masses [13] enhanced the error in \(T_c\). In order to reduce the error in \(T_c\) much higher statistics is required. Since the “critical” energy density \(\epsilon_c = \epsilon(T_c)\) (i.e. the energy density at the transition) scales as \(T_c^4\) the error in \(T_c\) is the dominant source of error in \(\epsilon_c\) [6].

3. Equation of state
Lattice calculations of the QCD equation of state are very difficult because equation of state are very senstive to high momentum modes and thus to the effect of finite lattice spacings. This makes the use of improved actions mandatory. In addition because the pressure and the energy density are calculated with respect to the corresponding vacuum values the signal to noise ratio is proportional to \(a^4\), with \(a\) being the lattice spacings. As the consequence the total computational costs grow as \(a^{-11}\) compared to \(a^{-7}\) growth for zero temperature calculations. For this reason current lattice calculations of the equation of state are limited to very course lattices and quite large values of the quark masses, corresponding to pion masses of 700 – 800 MeV. The results of these calculations for pressure and energy density are shown in Fig. 2.

4. Heavy quarks at finite temperature
In this section I am going to summarize some recent progress made in understanding the interaction of heavy quarks at finite temperature. Apart from being an interesting problem from a theoretical perspective understanding the interaction of heavy quarks at finite temperature also
Figure 2. The energy density and pressure versus the temperature calculated using improved staggered fermion action [16].

Figure 3. The singlet free energy in three flavor QCD at different temperatures in MeV (left) and the coupling constant $\alpha_s$ at finite temperature (right).

is very important for phenomenology. It has been suggested that quarkonium suppression due to color screening at high temperatures can serve as signature of Quark Gluon Plasma formation in heavy ion collisions [17]. For static quarks one can calculate the free energy difference for the system with static quark anti-quark pair and the system without static charges. This quantity is often referred to as finite temperature potential, though it should be emphasized that it is a free energy and thus contains an entropy contribution [18]. In Fig. 3 I show the free energy of static $Q\bar{Q}$ in the singlet state calculated in three flavor QCD [19]. As one can see from the Figure the free energy goes to a constant at distances $r > 0.9$ fm at low temperatures. This happens because once enough energy is accumulated the string can break due to creation of a light quark-antiquark pair. As the temperature increases the distance where the free energy levels off becomes temperature dependent and decreases with increasing temperature. This reflects the onset of chromo-electric screening. Similar results have been obtained in two flavor QCD [20, 21].

It should be noticed that at short distances ($r < 0.4$ fm) the free energy of static $Q\bar{Q}$ is temperature independent. As expected at short distance medium effects are not important. This is also confirmed by studies of the coupling constant at finite temperature [22] which I also show in Fig. 3. The running of the coupling constant at finite temperature is controlled by the distance between the static quarks and its value is never larger than at zero temperature [22]. This disfavors the picture of strongly coupled plasma where $\alpha_s$ runs to large value above the transition temperature [23].

Though the study of the free energy of a static quark anti-quark pair gives some useful insight
into the problem of quarkonium binding at high temperatures (for a recent review on this subject see Ref. [24]), it is not sufficient for detailed understanding quarkonium properties in this regime. To gain quantitative information on this problem quarkonium correlators and spectral functions should be studied at finite temperature. Such studies became possible only recently and still are restricted to the so-called quenched approximation, where the effect of dynamical quarks is neglected. [25, 26, 27, 28, 29, 30]. The results of these studies are summarized in Fig. 4. The 1S states ($J/\psi, \eta_c$) seem to survive to temperatures as high as $1.5T_c$ (maybe even higher, cf. the figure) while the 1P states ($\chi_{c0}, \chi_{c1}$) are dissolved at $1.1T_c$ [27]. The survival of the 1S state is also confirmed by two other groups [25, 26]. The temperature dependence of the charmonia correlators also suggests that the properties of 1S charmonia are not affected significantly above $T_c$, at least at zero spatial momentum [27, 29]. In the $J/\psi$ spectral functions only the first state corresponds to physical state, the higher peaks are artifacts of the finite lattice spacing [27].

Very recently with my collaborators I have performed a detailed study of quarkonia spectral functions at several values of the lattice spacing and have shown that the properties of the first peak do not depend on the lattice spacing while the position and the amplitudes of all the other peaks strongly depend on the lattice spacing [31]. In addition to charmonia spectral functions we have also calculated bottomonia spectral functions. These calculations were done on QCDOC supercomputers using the Columbia Physics System. It has been shown that $\Upsilon$ can exist in the plasma up to much higher temperatures [30] but surprisingly enough the $\chi_b$ state is dissociated at temperatures smaller than $1.5T_c$ [30] as shown in Fig. 4.

5. Outlook

Current lattice calculations of the transition temperatures suffer from the lack of the continuum extrapolations or from insufficient statistical accuracy. Furthermore to firmly establish the nature of the transition to the new state of strongly interacting matter simulations at even smaller quark masses are required. Equations of state has been calculated so far only on coarse lattices (with lattice spacing of about 0.25 fm) and quite large values of quark masses. To improve this situations computers resources of several Teraflops are required. In Brookhaven National Laboratory 4 Teraflops on QCDOC supercomputer, developed through the SciDAC project and RIKEN-BNL, are allocated to QCD thermodynamics. This will allow to calculate equation of state for quark masses corresponding to pion masses of about 200 MeV and smaller lattice spacing.

In this paper I only discussed the QCD transition at finite temperature and zero baryon density. Calculations at finite baryon density are extremely difficult because complex action (weights) make importance sampling impossible. Recently several methods have been proposed
to circumvent this problem (for a review see e.g. Ref. [5]). In general, simulations at finite baryon density are at least by an order of magnitude more demanding computationally than at zero baryon density. Thus Teraflop computing facilities are required to make progress in this field.

Lattice calculations of quarkonia spectral functions are in the stage of infancy. All calculations have been performed with Wilson action and in quenched approximation. To reduce lattice artifacts in the quarkonium spectral functions discussed above better fermion actions are required. This will increase the cost of computations significantly. To be relevant for the RHIC experimental the effect of dynamical quarks has to be included in such calculations which will require computer resources beyond 10 Teraflops.

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