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QCD Thermodynamics: The Numerical Study of Strongly Interacting Matter under Extreme Conditions

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The basic building blocks of the matter we get in touch with in our daily life are atoms; its central part, the nucleus, is made up of protons and neutrons. Stable nuclei contain up to a few hundred of them. This is the form of nuclear matter we have to our disposal in a laboratory. Nuclear matter in bulk exists in the universe at much higher densities for instance in the form of neutron stars. We also believe that extremely hot and dense forms of strongly interacting matter existed in the early universe shortly after the Big Bang. Its properties must have been qualitatively different, protons and neutrons as well as all the other hadrons known to us must have dissolved into their constituents - quarks and gluons. It commonly is expected that this change to the quark-gluon plasma state of strongly interacting matter happened through a phase transition. The theoretical framework to describe this phase transition, the dense nuclear matter and its thermodynamic properties is known to us; it is the theory of strong interactions – Quantum Chromo Dynamics. The complexity of this theory, however, prohibits a direct analytic analysis of most of the interesting phenomena related to complex thermodynamic processes, in particular the critical behaviour related to phase transitions. To analyze the thermodynamics of strongly interacting matter we need large scale numerical calculations. We will discuss here some of the results obtained from such calculations.

1 Introduction

The conjecture that the structure of strongly interacting hadronic matter will undergo a qualitative change at high temperature and/or densities has been around for a long time. Two basic properties of hadrons were essential for the development of these ideas. In high energy experiments it had been observed that strongly interacting particles produce a large number of new resonance particles. This mechanism, in fact, is so effective that the number of resonances in a given energy or mass interval rises exponentially (resonance production $\Rightarrow$ Hagedorn's bootstrap model[1]). As the average energy of hadrons increases with temperatures copious production of new particles will take place in a hot hadron gas; a dense equilibrated system results from this as a mixture of different particle species distributed according to the exponentially rising mass spectrum. Moreover hadrons are known to be extended particles with a typical size of about 1 fm$\simeq 10^{-13}$ cm. At high temperature extended hadrons thus would start to "overlap" and loose their identity as independent particles (see Fig. 1). This has been formulated in terms of percolation models[2] and led to the expectation that some form of new physics has to occur under the extreme conditions that are realized at high temperature and/or densities.

With the formulation of Quantumchromodynamics (QCD) as a theoretical framework for the strong interaction force among elementary particles it became clear that this "new physics" indeed meant a phase transition to a new phase of strongly interacting matter –

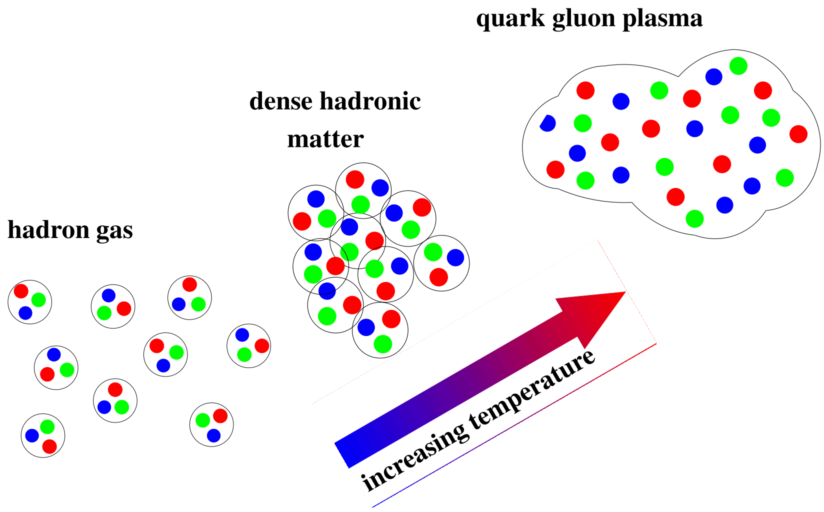


Figure 1. The transition from a gas of extended hadrons to the quark gluon plasma.

the quark-gluon plasma (QGP)[3]. QCD is an asymptotically free theory; the interaction between the elementary constituents, quarks and gluons, is known to vanish logarithmically with increasing temperature. It thus is expected that at least at very high temperatures the dominant degrees of freedom are the constituents of QCD – quarks and gluons – which behave almost like free particles. Bulk thermodynamics of the high temperature phase thus asymptotically should look like that of an ideal (free) gas of quarks and gluons. An interesting question then is to understand how our phenomenological picture of the transition which has been derived from bootstrap and percolation models is realized within the framework of QCD. The basis for answering such questions is given by the lattice discretized version of QCD – lattice QCD. This opens the possibility to study complex non-perturbative processes like phase transitions in dense matter with the help of numerical simulation techniques based on more or less standard Monte Carlo or molecular dynamics algorithms. Results from such calculations will be discussed in the next section.

A further important aspect that makes the study of QCD thermodynamics so attractive is that quantitative numerical studies can also be confronted with results obtained in relativistic heavy ion collision experiments. A great challenge, of course, is to directly verify that basic hadron properties indeed change qualitatively in a thermal environment as suggested by our discussion given above. In-medium modifications of hadron properties can be studied in numerical calculations on the lattice either through the analysis of static screening mechanisms that lead to modifications of the potential (binding) energy between quarks or directly through the study of thermal modifications of hadron masses and the width of resonances. These effects lead to experimentally observable modifications of particle production cross sections for heavy quark bound states and light mesons, respectively. We will discuss lattice calculations of these quantities in Section 3.

2 QCD Thermodynamics

Numerical studies of the thermodynamics of strongly interacting matter are performed on 4-dimensional space-time lattices[4]. These calculations have shown that a transition to the quark gluon plasma does take place, although this is a true phase transition only in limiting cases, *i.e.* in the limit where the masses of the quarks either vanish or are infinite. In nature the masses of two quark species (up and down quarks) are small but finite, whereas a third species (strange quark) has a mass which is of the order of the transition temperature itself. The latter thus is expected to play a marginal role in thermodynamic processes which take place in the vicinity of the transition temperature but should become as important as the lighter up and down quarks at higher temperatures. At low temperature only hadronic bound states can exist. The lightest particles which will dominate the thermodynamics are pions with a mass of 140 MeV. The pion mass vanishes in the limit of vanishing quark masses (*chiral limit*) while all other states remain massive with masses larger than 500 MeV. Their contribution to the thermodynamics is suppressed by the corresponding Boltzmann weight factor $\mathcal{O}(\exp[-m_H/T])$. Approximating the pions by massless particles the expectation thus is that bulk thermodynamic observables like the pressure or energy density will change from values corresponding to those of a free pion gas to that of a free quark-gluon gas. As the number of degrees of freedom is much larger in the latter case this should lead to a drastic change in the normalized energy density ϵ/T^4,

$$\frac{\epsilon}{T^4} = \begin{cases} (n_f^2 - 1)\frac{\pi^2}{30} & , T \to 0 \\ (16 + \frac{21}{2} n_f)\frac{\pi^2}{30} & , T \to \infty \end{cases} \quad , \tag{1}$$

where n_f denotes the number of light quark species (flavours). In fact, the transition between these limiting forms occurs in a rather narrow temperature interval as can be seen in Fig. 2. The numerical calculations performed with different number of light quark species indeed show that the energy density of the QGP rapidly approaches that of an (almost) ideal quark-gluon gas. This strongly suggests that our basic picture about the relevant degrees of freedom in this phase is correct and that hadrons should have dissolved during the transition to the QGP. Moreover, one finds that the transition temperature shifts to smaller values as the number of light degrees of freedom increases. This is particularly drastic, when one compares transition temperatures in the cases $n_f = 0$ and $n_f > 0$. In a purely gluonic world ($n_f = 0$) the transition temperature is found to be about 270 MeV[a] while it drops to 175 MeV for $n_f = 2$ and 155 MeV for $n_f = 3$[6].

Despite the significant change in the transition temperature it, however, turns out that the critical energy density is not at all that different. It changes a lot when expressed in units of T_c^4; however, this is compensated by a corresponding shift of T_c. For the case of two and three light quark flavours shown in Fig. 2 one finds,

$$\epsilon_c/T_c^4 = (6 \pm 2) \quad . \tag{2}$$

This amounts to an energy density $\epsilon_c \simeq (0.3 - 1.3)\text{GeV/fm}^3$ which is at most three times larger than the energy density in an ordinary nucleon. An exciting prediction of these calculations thus is that the transition takes place at an energy density which can be produced in relativistic heavy ion experiments which currently are performed at the SPS at

[a] 100 MeV $\equiv 1.1605\ 10^{12}$ Kelvin

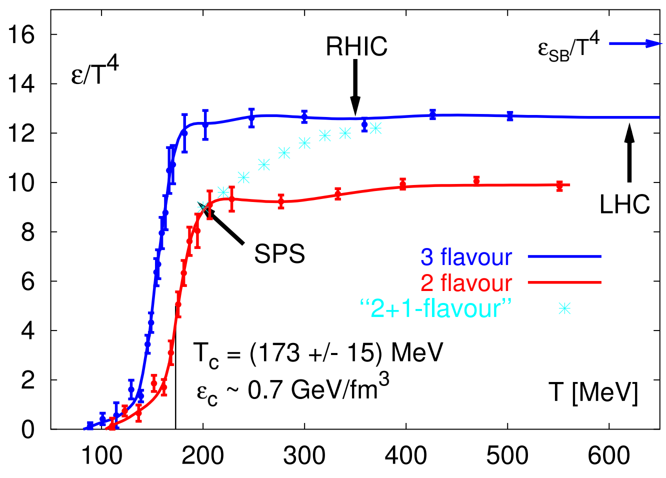


Figure 2. The energy density for QCD with two and three light quark species. The figure is based on data obtained in connection with the analysis of the flavour dependence of the pressure[5]. The crosses give an estimate for the temperature dependence of the energy density for QCD with a realistic quark mass spectrum with nearly massless up and down quarks and a strange quark mass $m_s \simeq T_c$. It shows that the thermodynamics is dominantly that of 2 light quark flavours in the vicinity of T_c and approaches that of 3-flavour QCD at higher temperatures.

CERN (Geneva) and the RHIC at Brookhaven National Laboratory (New York). At RHIC as well as at the future Large Hadron Collider (LHC), which will be build at CERN, it is expected that energy densities corresponding to several times the transition temperature will be produced so that long lived plasma states will be created.

When decreasing the values of light quark masses numerical calculations become increasingly difficult. This generally prohibits to perform numerical calculations directly at the physical values of the light, nearly massless up and down quarks; numerical results are generally extrapolated to the physical values realized in nature. This difficulty, however, can also be turned into a virtue. In a numerical calculation we can analyze the dependence of observables, e.g. the transition temperature, on the quark mass. In particular, we can analyze how the transition temperature depends on the values of the lightest hadron mass, the pseudo-scalar pions m_{PS}. While certain model calculations suggest a strong dependence of T_c on m_{PS} the general arguments on resonance production and the related resonance gas models would suggest that such a dependence is only minor and the crucial mechanism for a phase transition in fact arises from the exponential rise of heavy resonance states. A systematic analysis of the quark mass dependence of T_c is shown in Fig. 3. The line shown in this figure is a representative fit to the 3-flavour data, which gave

$$T_c(m_{PS}) = T_c(0) + 0.04(1)\, m_{PS} \quad . \tag{3}$$

It thus seems that the transition temperature does not react strongly to changes of the lightest hadron masses. Their contribution to the overall energy density, however, rapidly decreases with increasing mass. The light hadrons thus will not be able to induce any form of critical behaviour. The weak dependence of T_c on m_{PS} favours the interpretation that contributions of heavy resonance masses are equally important for the occurrence of the transition. In fact, this also can explain why the transition still sets in at quite low temper-

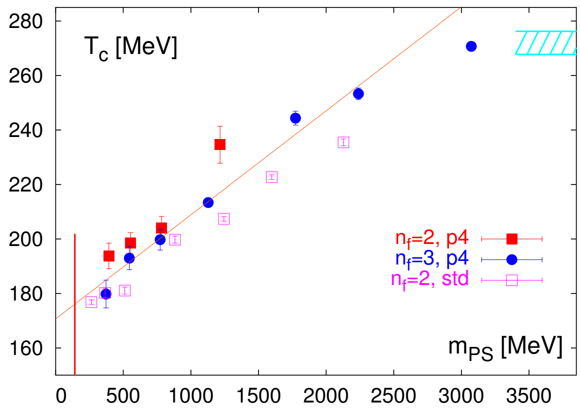


Figure 3. The transition temperature in 2 (filled squares) and 3 (circles) flavour QCD versus m_{PS} using an improved staggered fermion action (p4-action)[6]. Also shown are results for 2-flavour QCD obtained with the standard staggered fermion action (open squares). The difference between the two data sets for 2-flavour QCD gives a feeling for the systematic errors still present in current estimates of the transition temperature. The dashed band indicates the uncertainty on T_c in the pure gauge theory ($n_f = 0$) which corresponds to the limit $m_{PS} \rightarrow \infty$. The straight line is the fit given in Eq. 3.

atures even when all hadron masses, including the pseudo-scalars (pions), attain masses of the order of 1 GeV or more. Also the observation that the critical energy density is only weakly dependent on the quark mass suggests that properties of the light hadron sector in general are not responsible for the transition to the plasma phase. For the quark masses currently used in lattice calculations a resonance gas model combined with a percolation criterion thus provides an appropriate description of the thermodynamics close to T_c. From a theoretical point of view it would, of course, still be interesting to analyze whether the role of the light meson sector becomes more dominant when calculations closer to the massless limit are performed, *i.e.* in a regime where the mass of the lightest hadronic state would be significantly smaller than the relevant temperatures.

3 Thermal Properties of Hadrons from Lattice QCD

Basic properties of the experimentally known zero temperature hadron spectrum are controlled by symmetries of QCD or, more precisely, by the fact that some of them are spontaneously broken in the vacuum. The spontaneous breaking of symmetries leads to non-vanishing condensates and lifts the degeneracy of mass eigenstates which differ only by a quantum number related to this condensate. The condensates, however, will be temperature dependent and eventually they will disappear in the high temperature phase. As the splitting of mass eigenstates is related to the strength of the condensates, it is natural to expect that hadron properties will change with temperature.

Lattice calculations of hadronic screening lengths and hadronic susceptibilities[7], which are based on the analysis of hadronic correlation functions did indeed provide evidence for significant changes of hadron properties in a thermal medium. These observables, however, provide only indirect information on thermal modifications of hadron masses or their widths. If we want to get direct access to thermal changes of these basic hadron properties we have to understand the propagation of hadrons in a thermal medium and their interaction with this medium. In fact, all the information we are interested in is contained in the energy and momentum dependence of the retarded hadron propagator $\tilde{G}_H^R(\omega,\vec{p})$ in momentum space. Its imaginary part defines the spectral function, which in particular provides the information on hadron masses and their width,

$$\begin{aligned}\sigma_H(\omega,\vec{p},T) &= \frac{1}{\pi}\mathrm{Im}\ \tilde{G}_H^R(\omega,\vec{p},T) \\ &= \frac{\mathrm{Im}\Sigma(T,\vec{p})}{(\omega^2-\vec{p}^2-\mathrm{Re}\ \Sigma(T,\vec{p}))^2+(\mathrm{Im}\Sigma(T,\vec{p}))^2} \quad . \end{aligned} \tag{4}$$

Here $\Sigma(T,\vec{p})$ is the self-energy of the hadron. Its imaginary part will receive thermal in-medium contributions from scattering processes, which in general will lead to a broadening of the width of hadronic states (collision broadening).

In a lattice calculation we can analyze the Euclidean time correlation functions $G_H(\tau,\vec{p})$ which through a dispersion relation also depend on the spectral functions σ_H,

$$\begin{aligned}G_H(\tau,\vec{p}) &= T\sum_n \mathrm{e}^{-i\omega_n\tau}\ \tilde{G}_H^R(i\omega_n,\vec{p}) \quad , \quad \omega_n = 2n\pi T \\ &= \int_0^\infty \mathrm{d}\omega\ \sigma_H(\omega,\vec{p},T)\ \frac{\cosh(\omega(\tau-1/2T))}{\sinh(\omega/2T)} \quad . \end{aligned} \tag{5}$$

It is this correlation function which is accessible to numerical lattice calculations. The main problem thus in general is to reconstruct from the correlation functions the spectral functions from which we can get information on hadron masses and their width. However, even before doing so we can learn a lot from the correlation functions themselves. Comparing correlation functions in different quantum number channels, we directly see the drastic changes that occur when going from the low to the high temperature phase of QCD. Moreover, we see that correlation functions which are clearly different at low temperature become degenerate in the high temperature phase[8,9]. This is, for instance, the case for correlation functions in the pseudo-scalar and scalar quantum number channels shown in Fig. 4. Here the splitting of the degeneracy at low temperature is due to the spontaneous breaking of chiral symmetries which get restored in the plasma phase[b].

Similar results as those obtained for the scalar and pseudo-scalar correlation functions can be obtained for vector and pseudo-vector correlation functions. The vector correlation function is of particular interest as it carries the quantum numbers of a photon, which couples to hadrons as well as leptons. The latter are accessible in heavy ion experiments. Once they have been formed they can leave the interaction region without any further strong interaction and thus carry important information about the structure of matter formed in at an early stage in these collisions. For this reason, the analysis of dilepton pair production is expected to give important information on thermal effects in heavy ion collisions. The cross section for dilepton (e.g. electron-positron pair) production is directly related to the vector spectral function. For pairs with vanishing total momentum this is given by,

$$\frac{\mathrm{d}W}{\mathrm{d}\omega\mathrm{d}^3p} = \frac{5\alpha^2}{27\pi^2}\frac{1}{\omega^2(\mathrm{e}^{\omega/T}-1)}\sigma_V(\omega,T) \quad , \tag{6}$$

[b]The scalar correlation function shown in Fig. 4 is the so-called connected part of the correlation function.

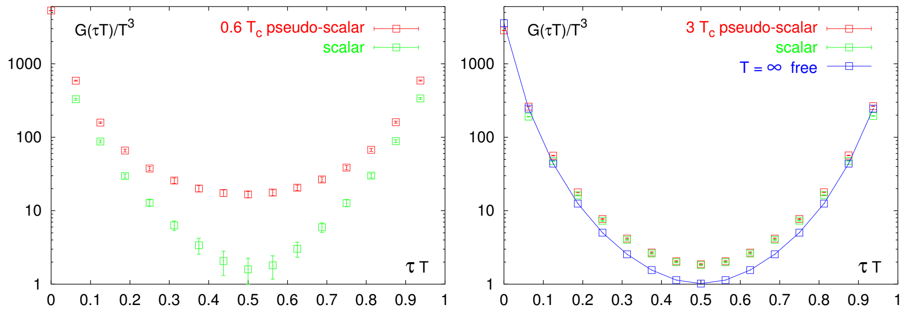


Figure 4. Zero momentum projected temporal correlation functions, $G_H(\tau T) \equiv G_H(\tau T, \vec{p} = 0)$, for scalar and pseudo-scalar mesons at $T = 0.6T_c$ and $3T_c$. The correlation functions have been calculated in the quenched approximation of QCD using Wilson fermions with a non-perturbatively improved Clover term[10] on $32^3 \times 16$ and $64^3 \times 16$ lattices, respectively[9].

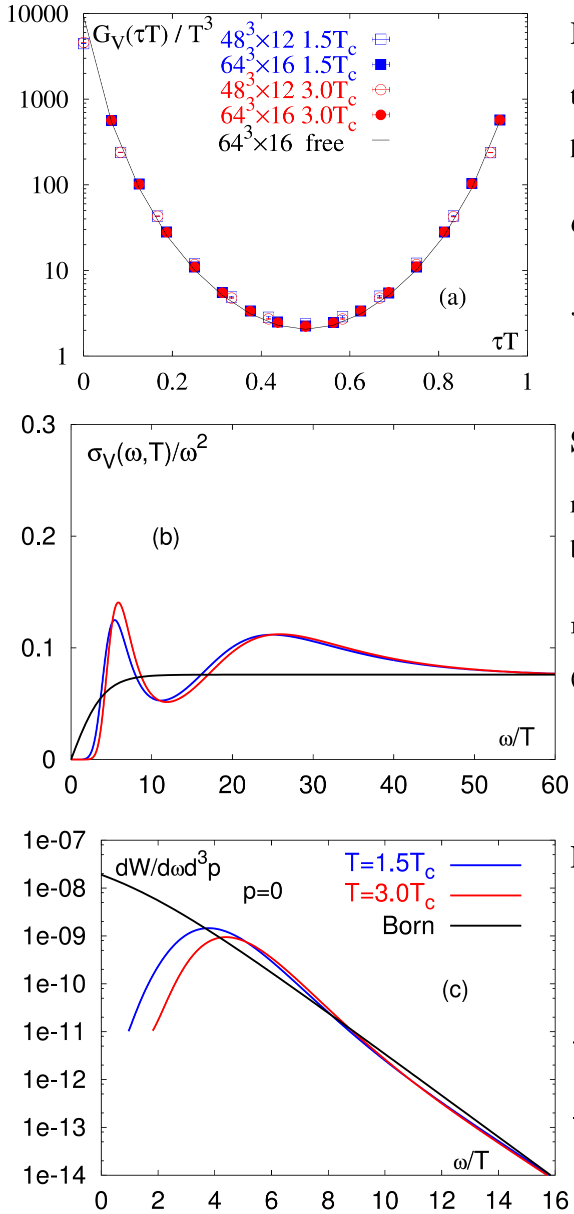
with $\sigma_V(\omega, T) \equiv \sigma_V(\omega, \vec{p} = 0, T)$. The steps needed to get from the numerical calculation of the vector correlation functions to the experimentally accessible cross section is illustrated in Fig. 5. The crucial part is the reconstruction of the spectral function from the correlation function. The latter is known only at a discrete set of Euclidean times, $\tau T = k/N_\tau$, $k = 0,\ 1, ...,\ N_\tau - 1$. The inversion of the integral equation Eq. 5 thus is an ill-posed problem. However, using statistical tools like the maximum entropy method (MEM)[11] it is, nonetheless, possible to determine the most likely form of the spectral function which is consistent with any given prior knowledge on its structure. In the case of QCD this in general means that we have information about the behaviour of $\sigma_H(\omega, T)$ for large ω, *i.e.* we can control the short distance structure of the correlation functions in perturbation theory. This defines an initial guess for the spectral function; the default model $m(\omega, T)$. The spectral function is then determined by maximizing the function $Q \equiv \gamma S - L$ with respect to σ and the additional parameter $\gamma > 0$. Here S is the Shannon-Jaynes entropy

$$S(\sigma) = \int_0^\infty \mathrm{d}\omega \Big[\sigma(\omega, T) - m(\omega, T) - \sigma(\omega, T) \ln(\sigma(\omega, T)/m(\omega, T))\Big] \qquad (7)$$

and L is the χ^2 constructed from the data sample for the correlation function at a discrete set of Euclidean times, $\{D_i(k) \equiv G_H(k/N_\tau) | k = 0,\ 1, ...,\ N_\tau - 1;\ i = 1, .., \#conf.\}$, and the fitting function $G_H^{fit}(k/N_\tau)$ constructed from Eq. 5 with the current trial version for $\sigma(\omega, T)$,

$$L(\sigma) = \frac{1}{2} \sum_{k,l} (G_H^{fit}(k/N_\tau) - D(k)) C_{kl}^{-1} (G_H^{fit}(l/N_\tau) - D(l)) \quad , \qquad (8)$$

with $D(k) = \frac{1}{\#conf} \sum_i D_i(k)$ and C_{kl} denoting the covariance matrix of the data sample. First tests of this approach at zero temperature[12] and in the infinite temperature limit[8] indicated that a MEM analysis of hadron correlation functions is feasible already on lattices with moderate temporal extent.



Lattice Calculation

temporal correlation function of hadronic vector current:

$$G_V(\tau T) = \int_0^\infty \mathrm{d}\omega\ \sigma_V(\omega, T)\ \frac{\mathrm{ch}(\omega(\tau - 1/2T))}{\mathrm{sh}(\omega/2T)}$$

Statistical Analysis

reconstructed spectral function based on Maximum Entropy Method

$$\max_{\gamma,\sigma_V}[\exp(\gamma S - L)]$$

(see Eqs. 7 and 8)

Experimental Observable

predicted thermal contribution to the dilepton cross section:

$$\frac{\mathrm{d}W}{\mathrm{d}\omega \mathrm{d}^3p} = \frac{5\alpha^2}{27\pi^2}\,\frac{1}{\omega^2(\mathrm{e}^{\omega/T}-1)}\sigma_V(\omega, T)$$

Figure 5. The vector correlation function $G_V(\tau T)$ and the corresponding free correlation function for massless quark anti-quark pairs, $G_V^{free}(\tau T)$ versus Euclidean time in units of the temperature (a), reconstructed vector spectral functions σ_V in units of ω^2 at zero momentum (b) and the resulting zero momentum differential dilepton rate (c) at $T/T_c = 1.5$ and 3. Also shown with solid lines is the free spectral function in (b) and the resulting Born rate for thermal dilepton production in (c).

The vector spectral function reconstructed from lattice calculations on large lattices of size $64^3 \times 16$ at two values of the temperature is shown in Fig. 5b and the resulting dilepton rate is given in Fig. 5c[13]. The most exciting aspect of this result is that the rate stays close to the Born rate calculated in leading order perturbation theory and that the rate is cut-off at low energies. In particular, the low energy behaviour is difficult to control in perturbation theory which suffers from infrared singularities. The lattice results, on the other hand, suggest that the low energy part of the spectral function is cut-off, which can be understood in terms of a threshold generated by non-vanishing thermal quark masses. This also is supported by studies of the quark propagators in fixed gauges and its spectral analysis[14].

4 Conclusions

Numerical studies of lattice regularized QCD allow a detailed quantitative analysis of the thermodynamics of strongly interacting matter. The basic techniques and tools used to analyze the QCD equation of state and the transition to the quark gluon plasma have been developed during the last 20 years. However, it is only now that computing facilities with Teraflops computing power are within reach and will allow us to reach the accuracy needed to make definite predictions that can be confronted with experimental data. The critical temperature and critical energy density of the QCD phase transition clearly will be the most fundamental observables which we are asked to provide. At present the critical temperature still is known to us only with a statistical and systematic error of about 10%. This alone leads to a 45% error in the prediction of the critical energy density. There is, however, no doubt that we will soon be able to improve on this.

Lattice calculations also did provide ample evidence for the modification of hadron properties in a thermal medium. However, it is only now that a direct investigation of thermal masses and their widths, which are of direct experimental interest, is within reach. To some extent this also is due to the improved computational resources and the fact that simulations on large thermal lattices at small values of the lattice cut-off now become possible. Equally important, however, it was to realize that statistical tools, which previously have been successfully applied in statistical physics, could also be of use in our studies of correlation functions in quantum field theory[12]. We only have started to explore the possibilities the maximum entropy method offers for the analysis of static correlation functions. In the context of finite temperature field theory it seems to give access to a whole range of open questions that can be addressed in the future.

Acknowledgments

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