Quark-Gluon Plasma: from lattice simulations to experimental results

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Abstract. Theoretical studies of quarkonia can elucidate some of the important properties of the quark–gluon plasma, the state of matter realised when the temperature exceeds $O(150)\text{ MeV}$, currently probed by heavy-ion collisions experiments at BNL and the LHC. We report on our results of lattice studies of bottomonia for temperatures in the range $100\text{ MeV} \lesssim T \lesssim 450\text{ MeV}$, introducing and discussing the methodologies we have applied. Of particular interest is the analysis of the spectral functions, where Bayesian methods borrowed and adapted from nuclear and condensed matter physics have proven very successful.

1. The plasma of quarks and gluons
Heavy ions colliding at ultrarelativistic energies produce a tiny fireball of a plasma of quarks and gluons — the state of matter thought to have existed slightly after the Big Bang. This experimental program started at the SPS in the 1980s, continued at RHIC and it is now running at the LHC, where the
experiments ALICE, ATLAS and CMS are collecting and analyzing data from the collisions of lead nuclei. The most recent runs reached temperatures of about 500 MeV — approximately $5 \times 10^{12}$ K — well above the temperature of the crossover from ordinary matter to the plasma of quarks and gluons, estimated to be at about 155 MeV [1,2].

The analysis of the transition from ordinary matter to the quark-gluon plasma, and the nature of the plasma itself — the spectral properties and the residual interactions — is a very active field of theoretical research [3]. We are concerned with temperatures well above those where the synthesis of the lightest nuclei takes place, so strong interactions alone suffice to describe the system. Hence, the appropriate microscopic description is the relativistic field theory of the strong interactions, Quantum Chromodynamics, QCD. We also know that $\alpha_s$, the QCD coupling at the scale of the temperatures of interest, can be as large as 0.5 and even larger, so that perturbation theory, which will ultimately be valid for very high temperatures, does not work, at least quantitatively, in the region which we wish to explore here. We therefore need a non-perturbative method, and we choose numerical simulations of QCD discretized on a lattice.

This note is devoted to the presentation of lattice results obtained by the FASTSUM collaboration, in particular those appearing in Refs. [4–7]. It updates and expands previous reviews [8, 9].

1.1. Why bottomonium?

Why is bottomonium such an interesting probe of the medium? We will be concerned with phenomena occurring at, or above, the crossover to a chirally symmetric, deconfined phase. In general both chiral symmetry restoration and deconfinement affect the spectrum of the theory: chiral symmetry will be seen in the light sector, by the degeneracy of the chiral partners. The heavier quarks, however, will be blind to chiral symmetry: $m_u, m_d \ll m_s \approx T_c \approx \Lambda_{QCD} \ll m_c, m_b$. For instance only about 15% of the strange mass is due to the breaking of chiral symmetry, and for charm and bottom this contribution is completely negligible — modifications of the spectrum of charmonia and bottomonia come entirely from the gauge dynamics. In very short summary, then, quarkonia are ideal probes of the gluodynamics. Since their size is small, however, the sensitivity to deconfinement is not immediate: the short-range component of the potential, which is responsible for their binding, and hence the fundamental bound states, might well survive in the plasma, while the excited states dissolve. We talk of sequential suppression of quarkonia, and the goal of our studies is to make quantitative these very qualitative considerations.

Charmonia — which are easier to produce experimentally — have been studied since early SPS days. We know by now [10] that the experimental results for charmonia are also sensitive to cold nuclear matter effects which reduce the primordial charmonium number significantly — for instance by about 60% at SPS. There are also competing temporal scales — thermalization of the plasma and formation time of the bound states, as well as the intriguing observation that charmonia production rates at SPS and RHIC are quite similar. The latter effect can be at least in part explained by taking into account a regeneration
mechanism for charmonia (feed-down): the higher dissociation rate at RHIC is compensated by a richer feed-down. All these considerations make the study of charmonium suppression patterns extremely fascinating but also challenging.

Bottomonium production, on the other hand, is much less prone to regeneration effects, and as such is a more promising observable for the spectral analysis of the quark–gluon plasma [10]. Since bottomonium production requires the larger energies available at the LHC, such data have become available only very recently. In the last few years, results showing sequential Upsilon suppression in PbPb collision at LHC energies have appeared [11, 12], and we will comment on those at the end.

2. Lattice QCD, relativistic and non–relativistic

Lattice calculations are performed in a discretized Euclidean space-time, which introduces technical scales: the lattice spacing $a$ and the lattice spatial size, $L$. Each characteristic physical scale $l$ should obviously fulfill the constraint $a \ll l \ll L$. Accommodating quarks with vastly different masses then poses a computational challenge.

Our strategy is to treat as accurately as possible the light quarks: in all our studies gauge configurations with dynamical light Wilson-type quark flavours are produced on highly anisotropic lattices. Details of the lattice action and parameters can be found in Refs. [13,14]. For the $b$ quarks we use non-relativistic QCD (NRQCD). In our work we use a mean-field improved action with tree-level coefficients, which includes terms up to and including $O(v^4)$, where $v$ is the typical velocity of a bottom quark in bottomonium, $v^2_b \simeq 0.1$. There is no (rest) mass term in the NRQCD action so one can dispense with the demanding constraint $a \ll 1/m_b$. In general, NRQCD relies on the separation of scales between the bottom quark and any other physical scale of the theory: in our work we study temperatures up to $2T_c \simeq 400$ MeV, hence $m_b \gg T$ and the application of NRQCD is fully justified.

3. Correlators in the plasma

In our studies we considered the $S$ wave states $\Upsilon$ and $\eta_b$ and the $P$ wave states $\chi^{0}_b$, $\chi^{1}_b$, $\chi^{2}_b$ and $h_b$. We found that the correlators in the different $P$ wave channels behave in a very similar way, hence from now on for the $P$ wave states we present results for the $\chi^{1}_b$ channel only. The gauge configurations are generated with a dynamical first generation of quarks. More recently the strange quark has been added as well [15]: the general features of the results are unchanged, and a systematic, detailed analysis of the effect of a dynamical strange quark is in progress.

There is a further important simplification in NRQCD: to compute propagators we only need to solve an initial value problem, in contrast to the relativistic case where the same computation requires the inversion of a large sparse matrix. In the hadronic phase we expect that the large Euclidean time behaviour of the propagators is dominated by an exponential decay. In the QGP phase, one can use as guidance the behaviour found for free quarks in
Figure 1. Effective exponents $\gamma_{\text{eff}}(\tau)$ for the $\Upsilon$ (left) and $\chi_{b1}$ (center), as a function of Euclidean time for various temperatures. The dotted line indicates the non-interacting result in the continuum, which is approached by the $\chi_{b1}$ results at the higher temperature $T = 2.1T_c$ [4]. Effective mass for the $\chi_{b1}$ (right), as a function of Euclidean time for various temperatures [5].

NRQCD [4,5,16], which yields the spectral functions

$$\rho_{\text{free}}(\omega) \propto (\omega - \omega_0)\alpha \Theta(\omega - \omega_0), \quad \text{where} \quad \alpha = \begin{cases} 1/2, & \text{S wave.} \\ 3/2, & \text{P wave.} \end{cases}$$

Here we supplemented [15] the free results by a threshold, $\omega_0$, to account for the additive shift in the quarkonium energies which describes the residual interactions in the thermal medium. The correlation functions then have the following behaviour

$$G_{\text{free}}(\tau) \propto \int d\omega e^{-\omega \tau} \rho(\omega) \propto e^{-\omega_0 \tau \tau^{\alpha+1}}. \quad (2)$$

To visualize the temperature dependence and at the same time monitor the approach to a quasi-free behaviour we construct effective power plots [4], using the definition

$$\gamma_{\text{eff}}(\tau) = \frac{G'(\tau)}{G(\tau)} = \frac{-\tau G(\tau + a_\tau) - G(\tau - a_\tau)}{2a_\tau G(\tau)}, \quad (3)$$

where the prime denotes the (discretized) derivative. For a pure power law decay this yields a constant, $\gamma_{\text{eff}}(\tau) = \alpha + 1$. Taking into account the threshold $\omega_0$, one finds $\gamma_{\text{eff}}(\tau) = \alpha + 1 + \omega_0 \tau$. The results are shown in Fig. 1. We see that the $\Upsilon$ displays a very mild temperature dependence, while for the $\chi_{b1}$ the asymptotic behaviour of the effective power tends to flatten out with increasing temperature: this indicates that $\omega_0$ — the slope — decreases with temperature. In the same panel also shown are the effective exponents in the continuum non-interacting limit ($\omega_0 = 0$). In the case of the $\chi_{b1}$, we observe that the effective exponent — which can be read off the intercept of the asymptotic straight line
with the $\tau = 0$ axis — seems to approach the non-interacting result. Note that, even for $T \to \infty$ where $\omega_0 = 0$, the effective exponents on the lattice only become a straight line, $\gamma_{\text{eff}}(\tau) \to \alpha + 1$, at large enough $\tau$ due to the presence of lattice discretisation effects at smaller temporal separations.

A complementary description is offered by the effective masses,

$$a_{\tau} m_{\text{eff}}(\tau) = - \log [G(\tau)/G(\tau - a_{\tau})],$$

(4)

which are shown in the rightmost panel of Fig. 1. When the correlator takes the form of a sum of exponentials, the ground state will show up as a plateau at large Euclidean times, provided that it is well separated from the excited states. This is indeed the case at the lowest temperature and leads to the zero-temperature spectrum discussed in Refs. [4, 5]. Above $T_c$, we observe that the effective masses no longer follow the trend given by the correlator below $T_c$, but instead bend away from the low-temperature data. The results shown in Fig. 1 imply that the spectrum of the $\chi_{b1}$ has changed drastically. If isolated bound states persist, the ground state has to be much lighter and excited states cannot be well separated. A more natural explanation is that there is no exponential decay and bound states have melted, immediately above $T_c$. This interpretation is supported by the spectral function analysis presented next.

4. Spectral functions

Spectral functions play an important role in understanding how elementary excitations are modified in a thermal medium, from many-body physics — see the talk by Giuseppina Orlandini at this meeting [17] — to QCD, which is discussed here.

In general, the spectral decomposition of a (relativistic) zero-momentum Euclidean propagator $G(\tau)$ at finite temperature $T$ is given by

$$G(\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, K(\tau, \omega) \rho(\omega),$$

(5)

where $\rho(\omega)$ is the spectral function and the kernel $K$ is given by

$$K(\tau, \omega) = \frac{\cosh [\omega(\tau - 1/2T)]}{\sinh(\omega/2T)}.$$  

(6)

In NRQCD the kinematical temperature dependence is always absent. This can be seen in a number of ways. Following Ref. [16], we write $\omega = 2M + \omega'$ and drop terms that are exponentially suppressed when $M \gg T$. The spectral relation [5] then reduces to its zero-temperature limit,

$$G(\tau) = \int_{-2M}^{\infty} \frac{d\omega'}{2\pi} \exp(-\omega'\tau) \rho(\omega'),$$

(7)

even at nonzero temperature. Since the interesting physics takes place around the two-quark threshold, $\omega \sim 2M$, the region of interest is around $\omega' \sim 0$ and the lower limit becomes irrelevant. In summary, in the heavy-quark limit the
Figure 2. Spectral functions $\rho(\omega)$, normalised with the heavy quark mass, in the vector (Υ) channel (upper panel) and in the pseudoscalar ($\eta_b$) channel (lower panel) for all temperature available. The subpanels are ordered from cold (top left) to hot (bottom right). Every subpanel contains two adjacent temperatures to facilitate the comparison [5].

spectral relation simplifies considerably, and temperature effects seen in the correlators are thus only due to changes in the light-quark–gluon system.

Despite these simplifications, the calculation of the NRQCD spectral functions using Euclidean propagators as an input remains a difficult, ill-defined problem. We will tackle it by using the Maximum Entropy Method (MEM) [18], which has proven successful in a variety of applications. We have carefully studied the systematics, including the dependence on the set
of lattice data points in time, and on the default model $m(\omega)$ which enters in the parametrisation of the spectral function,

$$\rho(\omega) = m(\omega) \exp \sum_k c_k u_k(\omega),$$

where $u_k(\omega)$ are basis functions fixed by the kernel $K(\tau, \omega)$ and the number of time slices, while the coefficients $c_k$ are to be determined by the MEM analysis [18]. We find that the results are insensitive to the choice of default model, provided that it is a smooth function of $\omega$. It remains of interest, and it is an open avenue of research, to experiment with alternative prescriptions [19,20], also on ensembles generated with different lattice actions [21].

The results for the spectral functions for the $S$ wave states, $\Upsilon$ and $\eta_b$ [5] can be seen in Fig. 2, which shows that as the temperature is increased the ground state peaks of both states remain visible. One caveat applies also here: the apparent width at zero temperature is most likely due to a lattice/MEM artefact, and this calls for an analysis of the discretization effects on the spectral function, which is one of our ongoing projects [22]. The peaks associated with the excited states become suppressed at higher temperature and are no longer discernible quickly above $T_c$.

Turning now to the $P$ wave states, the result at the lowest temperature is given in Fig. 3 (left). The dotted vertical line indicates the mass of the lowest-energy state obtained with an exponential fit. We see from this that the narrow peak in the spectral function corresponds to the ground state. The second, wider structure is presumably a combination of excited states and lattice artefacts, see below. We note that we have not been able to extract the mass of the first excited state with an exponential fitting procedure. The spectral functions for all temperatures are shown in Fig. 3 (center). We find no evidence of a ground state peak for any of the temperatures above $T_c$. This is consistent

Figure 3. Spectral function in the $\chi_{b1}$ channel at the lowest temperature (left) and at all temperatures (center). The dotted line on the left indicates the position of the ground state obtained with a standard exponential fit. Comparison with the free lattice spectral function above $T_c$ (right) [7].
with the interpretation of the correlator study presented above and supports the conclusion that the $P$ wave bound states melt in the QGP.

In order to interpret the remaining structure, we compare it with the spectral function computed on the lattice, in the absence of interactions [5]. In Fig. 3 rightmost panel, we show the free lattice spectral functions, together with the spectral functions above $T_c$. In that plot we have adjusted the threshold to match our lattice results, and once this is done the lattice spectral function and the free one almost coincide. This lends further support to the conclusion drawn in Ref. [4] from an analysis of the correlators: the system in the $P$ wave channels is approaching a system of noninteracting quarks, and the residual interactions can be described by a shift in the quarkonium energies, which does not affect the shape of spectral functions.

5. Comparison with analytic studies and momentum dependence

In this section we restrict our analysis to the $S$ waves. From the computed spectral functions we can determine the mass (from the peak position) and (an upper bound on) the width of the ground state at each temperature.

In Fig. 4 we show the temperature dependence of the mass shift $\Delta E$, normalised by the heavy quark mass and the temperature dependence of the width, normalised by the temperature.

We now contrast our results with analytic predictions derived assuming a weakly coupled plasma [20,23,28]. According to Ref. [26], the thermal contribution to the width is given, at leading order in the weak coupling and large mass expansion, by

$$\Gamma = \frac{1156}{81} \alpha_s^3 \approx 14.27 \alpha_s^3,$$

i.e. the width increases linearly with the temperature. If we take as an estimate from our results that $\Gamma/T \sim 1$, we find that this corresponds to $\alpha_s \sim 0.4$, which
Table 1. Nonzero momenta [6]. Also indicated are the corresponding velocities \( v = |p|/M_S \) of the ground states in the vector (\( \Upsilon \)) and pseudoscalar (\( \eta_b \)) channels, using the ground state masses determined previously [4]. \( M_\Upsilon = 9.460 \) GeV and \( M_{\eta_b} = 9.438 \) GeV.

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
n & (1,0,0) & (1,1,0) & (1,1,1) & (2,0,0) & (2,1,0) & (2,1,1) & (2,2,0) \\
|p| (GeV) & 0.634 & 0.900 & 1.10 & 1.23 & 1.38 & 1.52 & 1.73 \\
v [\Upsilon(^3S_1)] & 0.0670 & 0.0951 & 0.116 & 0.130 & 0.146 & 0.161 & 0.183 \\
v [\eta_b(^1S_0)] & 0.0672 & 0.0954 & 0.117 & 0.130 & 0.146 & 0.161 & 0.183 \\
\hline
\end{array}
\]

is a reasonable result. (It would be of interest to compute \( \alpha_s \) directly on our configurations.) In the same spirit the thermal mass shift is given in Ref. [26] by

\[
\delta E_{\text{thermal}} = \frac{17\pi}{9} \frac{T^2}{M_S} \approx 5.93 \alpha_s \frac{T^2}{M},
\]

(10)

In these simulations we have \( T_c \approx 220 \) MeV, \( M \approx 5 \) GeV. Taking these values together with \( \alpha_s \sim 0.4 \) as determined above, Eq. (10) becomes

\[
\frac{\delta E_{\text{thermal}}}{M} = 5.93 \alpha_s \left( \frac{T}{T_c} \right)^2 \left( \frac{T}{T_c} \right)^2 \sim 0.0046 \left( \frac{T}{T_c} \right)^2.
\]

(11)

In order to contrast our results with this analytical prediction, we have compared the temperature dependence of the peak positions to the simple expression

\[
\frac{\Delta E}{M} = c + 0.0046 \left( \frac{T}{T_c} \right)^2,
\]

(12)

where \( c \) is a free parameter. This is shown by the dashed line in Fig. 4 (left panel). The numerical results and the analytic ones are not inconsistent, within the large errors.

The analysis from effective theories predicts significant momentum effects at large momenta. Moreover current CMS results have been obtained at large momenta. There is therefore both phenomenological and experimental motivation to extend these studies to non-zero momenta [6]. The momenta and velocities that are accessible on the lattice are constrained by the discretization and the spatial lattice spacing. The lattice dispersion relation reads

\[
a_s^2 p^2 = 4 \sum_{i=1}^{3} \sin^2 \frac{p_i}{2}, \quad p_i = \frac{2\pi n_i}{N_s}, \quad -\frac{N_s}{2} < n_i \leq \frac{N_s}{2}.
\]

(13)

To avoid lattice artefacts, only momenta with \( n_i < N_s/4 \) are used: we consider the combinations (and permutations thereof) given in Table 1. The largest momentum, using \( n = (2,2,0) \), is \( |p| \approx 1.73 \) GeV, corresponding to \( v = |p|/M_S \approx 0.2 \). Therefore, the range of velocities we consider is non-relativistic.
As in the zero-momentum case, we extract masses and widths from our correlators using MEM, and we display them in Fig. 5. We observe that the peak position increases linearly with $v^2$, as expected. Assuming the lowest-order, non-relativistic expression $M(p) = M(0) + p^2/2M(0)$, one finds

$$\frac{M(p)}{M(0)} = 1 + \frac{p^2}{2M^2(0)} = 1 + \frac{1}{2}v^2,$$

which is indicated with the dotted lines in the left figures.

The dependence on the velocity can be compared with EFT predictions. In Ref. [28] a study of the velocity dependence was carried out in the context of QED, working in the rest frame of the bound state (i.e. the heat bath is moving). In order to compare with our setup, we consider the case in which the temperature is low enough for bound states to be present and where the velocities are non-relativistic. In that case, one finds [28], in the rest frame of the bound state and at leading order in the EFT expansion,

$$\frac{\Gamma_v}{\Gamma_0} = \sqrt{1 - \frac{v^2}{2v}} \log \left( \frac{1 + v}{1 - v} \right),$$

where $\Gamma_0$ is the width at rest. Interpreting the width as an inverse lifetime, one can express this result in the rest frame of the heat bath by dividing with the Lorentz factor $\gamma = 1/\sqrt{1 - v^2}$. An expansion for non-relativistic velocities then yields

$$\frac{\Gamma_v}{\Gamma_0} = 1 - \frac{2v^2}{3} + \mathcal{O}(v^4).$$

If we apply this result to our study of bottomonium, we find that the effect of the nonzero velocity shows up as a correction at the percent level (recall that $v^2 \lesssim 0.04$), which is beyond our level of precision but consistent with the observed $v$ independence within errors. Similarly, additional thermal effects in
the dispersion relation are currently beyond our level of precision. In summary, the observations in our low-momentum range are consistent with Ref. \[28\], and in order to observe the predicted non-trivial momentum dependence we need to explore larger momenta.

6. From lattice to experiments
We have presented our results for bottomonium in the quark-gluon plasma, for temperatures up to $2.1T_c$, at the threshold of the region currently explored by LHC heavy-ion experiments. Our analysis uses full relativistic dynamics for the light quarks, and a non-relativistic approach for the bottom quarks. The results are amenable to a successful comparison with effective models which we hope to further pursue in the future.

Our results demonstrate a pattern of suppression of bottomonia which apparently compares well with recent CMS results \[11,12\], once we take into account that the temperatures reached in the collisions studied by CMS are similar to the ones of our lattices. However the systems under investigation are vastly different: Quantum Chromodynamics in thermal equilibrium in one case, and an expanding fireball, with an extremely complex experimental setup, in the other. For instance, our studies include processes between a $b$ quark and thermal light quarks (and gluons), but do not include the thermal scattering of $b$ quarks. Unravelling the details and the limitations of this comparison is a subject of active research, certainly beyond the scope of this note.

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