Flavoured aspects of the QCD thermodynamics

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Abstract. We discuss recent progress in lattice QCD studies on various aspects involving strange and heavy quarks. Appropriate combinations of conserved net strange and net charm fluctuations and their correlations with other conserved charges provide evidence that in the hadronic phase so far unobserved hadrons contribute to the thermodynamics and need to be included in hadron resonance gas models. In the strange sector this leads to significant reductions of the chemical freeze-out temperature of strange hadrons. We have found that a description of the thermodynamics of open strange and open charm degrees of freedom in terms of an uncorrelated hadron gas is valid only up to temperatures close to the chiral crossover temperature. This suggests that in addition to light and strange hadrons also open charm hadrons start to dissolve already close to the chiral crossover. Further indications that open charm mesons start to melt in the vicinity of \( T_c \) is obtained from an analysis of screening masses, while in the charmonium sector these screening masses show a behavior compatible with a sequential melting pattern. In the last section we discuss recent progress in extracting a transport coefficient, the heavy quark momentum diffusion coefficient, based on continuum extrapolated color-electric field correlation functions and estimate the time scale associated with the kinetic equilibration of heavy quarks. Close to \( T_c \) this suggests that charm quark kinetic equilibration appears almost as fast as that of light partons in agreement with qualitative discoveries at RHIC and LHC that charm quarks appear to flow about as effectively as light quarks.

1. Additional strange hadrons and strangeness freeze-out in Heavy Ion Collisions
Fluctuations and correlations of conserved quantum numbers like baryon number \( B \), electric charge \( Q \), strangeness \( S \) and charm \( C \) are important quantities that can be used to analyze different contributions to thermodynamic quantities. Especially in the strange and charm sector they can serve as probes for the liberation of degrees of freedom and the appearance of fractional charge quantum numbers, e.g. by comparing to the limiting cases, i.e. Hadron Resonance Gas (HRG) in the hadronic phase and the non-interaction Stefan Boltzmann limit at high temperatures. Furthermore, by comparing to hadron resonance gas models information on the abundance of open strange and open charm hadrons can be gained.

The mesonic (M) and baryonic (B) pressure contributions of open strange hadrons in the hadron resonance gas model, using the classical Boltzmann approximation, can be evaluated separately by summing over all open strange mesons and baryons respectively,

\[
P_{M/B}^{S,X}(T, \vec{\mu}) = \frac{T^4}{2\pi^2} \sum_{i \in X} g_i \left( \frac{m_i}{T} \right)^2 K_2 \left( \frac{m_i}{T} \right) \cosh \left( B_i \hat{\mu}_B + Q_i \hat{\mu}_Q + S_i \hat{\mu}_S \right),
\]  
(1)
and both sum up to the total partial pressure of open strange hadrons,

\[ P_{\text{tot}}^{S,X} = P_M^{S,X} + P_B^{S,X}. \]  

(2)

Here the chemical potentials related to the conserved quantum numbers are denoted by \( \hat{\mu}_q \equiv \frac{\mu_q}{T} \) with \( q = B, Q, S \) and \( g_i \) is the degeneracy factor for the hadrons of mass \( m_i \). The quark model (X=QM) predicts a larger number of open strange mesons [2] and open strange baryons [3] compared to the ones listed in the particle data tables (X=PDG). While the effect of the additional mesonic contribution on the partial pressure in the QM-HRG compared to the PDG-HRG is small, reflecting a smaller number of experimentally still-unobserved open strange mesons, the partial baryonic pressure is largely enhanced as can be seen in Fig. 1.

Suitable observables to analyze different contributions to the pressure \( P \), that are related to the underlying effective degrees of freedom in the system, are generalized susceptibilities defined by derivatives with respect to the corresponding chemical potentials,

\[ \chi_{BQS}^{klm} = \left. \frac{\partial^{(k+l+m)}P(T, \hat{\mu}_B, \hat{\mu}_Q, \hat{\mu}_S)/T^4}{\partial \hat{\mu}_B^k \partial \hat{\mu}_Q^l \partial \hat{\mu}_S^m} \right|_{\vec{\mu} = 0} \]  

(3)

In Fig. 2(top) the ratio of two such suitable, strangeness sensitive, cumulatants are shown, the correlation of net strangeness with net baryon number fluctuations, \( \chi_{\text{BS}}^{11} \), normalized by the second cumulant of net strangeness fluctuations, \( \chi_S^2 \). While in the validity range of HRG models, the former only contains partial pressure contributions of strange baryons, the latter is dominated by strange mesons. Therefore this ratio is especially sensitive to the enhancement of partial baryonic pressure of strange baryons in the QM-HRG compared to the PDG-HRG. The results for two different lattice sizes together with an estimate for the continuum result shown in Fig. 2 are obtained in (2+1)-flavor QCD using the highly improved staggered quark (HISQ) action with a physical strange quark mass and light quark masses, \( m_l = m_s/20 \), corresponding to a pion mass of around 160 MeV [1].
From the comparison of lattice QCD data with the two HRG models we find a better description of the QCD thermodynamics in the hadronic phase using the QM-HRG model. This shows the importance of the contributions of additional strange baryons to the thermodynamics below the QCD crossover and provides evidence for the existence of additional strange baryons. This is further corroborated when comparing other combinations of second- and fourth-order cumulants of strangeness and net baryon number fluctuations [1], which are identical for a gas of uncorrelated hadrons, shown in Fig. 2(bottom). All three combinations agree up to the chiral crossover temperature, indicating again that a hadron resonance gas model is a valid description in the hadronic phase when additional states are included, before they start to deviate indicating the liberation of strangeness degrees of freedom in the QGP.

In a net strangeness neutral system, like in heavy ion collisions, the ratio \( \frac{\chi_{11}^S}{\chi_2^S} \) can be related to the strangeness chemical potential in terms of a Taylor expansion in \( \mu_B/T \) [4, 5], where the leading order only receives a small correction from the nonzero electric charge potential,

\[
\left( \frac{\mu_S}{\mu_B} \right)_{\text{LO}} \equiv s_1(T) = \frac{\chi_{11}^{BS}}{\chi_2^S} - \frac{\chi_{11}^{QS}}{\chi_2^S} \mu_Q/\mu_B,
\]

and the next-to-leading order correction is small in the relevant temperature region. Up to the chiral crossover temperature, the leading order results of the QM-HRG model agree with the lattice QCD results in Fig. 3(left), while the PDG-HRG model gives substantially lower values.

This has implications for the determination of the chemical freeze-out temperature, illustrated in Fig. 3(right) where the experimental freeze-out chemical potentials were obtained from the relative yields of strange anti-baryons to baryons for the NA57 experiment [6] and the STAR preliminary result [7]. Comparing the freeze-out chemical potentials to the leading order results for \( \mu_S/\mu_B \) in 3(left) determines the freeze-out temperature, \( T_f \). While the QM-HRG and lattice QCD results are in good agreement and give consistent values for \( T_f \), the freeze-out temperatures obtained from the PDG-HRG model are larger by about 8 MeV for the STAR data and 5 MeV for the NA57 data.
2. The melting of open charm hadrons

Due to their relation to chiral symmetry, deconfinement of light quark bound states happens at or close to the chiral crossover temperature, leading to sudden changes in bulk thermodynamic observables apparent in the behavior of fluctuations of conserved charges. For open strange hadrons, studying results of charge fluctuation observables containing strangeness, a description in terms of uncorrelated hadronic degrees of freedom breaks down in the chiral crossover region [9]. This is an indication that also strangeness gets dissolved at or close to $T_c$.

The situation of heavy quarks becomes more interesting as they are more related to the deconfinement aspects and less affected by chiral symmetry and at least some charmonium and bottomonium bound states are expected to dissolve at temperatures in the deconfined medium well above the chiral crossover region. In this section we will discuss the open charm sector which can be analyzed by charge fluctuation observable introduced in the previous section, adding a charm quark chemical potential.

In our lattice QCD results [8] the charm quark sector is treated within the quenched approximation, which is well justified in the temperature region analyzed here [10, 11]. We utilize the same gauge field configurations as in the previous section, generated with the HISQ
action and (2+1)-flavor with physical strange quark masses and almost physical light quark masses. To reduce discretization errors in the charm sector the so called $\epsilon$-term [12] is used for the charm contribution in the generalized susceptibilities of conserved charges,

$$\chi_{BQSC}^{klmn} = \frac{\partial^{(k+l+m+n)}[P(\hat{\mu}_B, \hat{\mu}_Q, \hat{\mu}_S, \hat{\mu}_C)/T^4]}{\partial\hat{\mu}_B^k \partial\hat{\mu}_Q^l \partial\hat{\mu}_S^m \partial\hat{\mu}_C^n} \bigg|_{\hat{\mu}=0}. \tag{5}$$

Using suitable combinations of cumulants of net charm fluctuations, $\chi_n^C$, and of correlations between net charm and net baryon number fluctuations, $\chi_{mn}^{BC}$, the open charm baryonic and mesonic sectors can be analyzed separately.

The ratio $\chi_{13}^{BC}/\chi_{22}^{BC}$ shown in Fig. 4(left) is unity in a hadron resonance gas and approaches a value of 3 in the infinite temperature non-interacting charm quark gas limit. The results suggest that above the crossover region, an uncorrelated gas of charmed baryons no longer provides an appropriate description of the net charm to net baryon correlations. The second ratio shown in Fig. 4(left), $\chi_{11}^{BC}/\chi_{13}^{BC}$, is unity in both limits and also the lattice QCD results are consistent with unity for all temperatures.

Fig. 4(right) shows ratios which are sensitive to the open charm meson sector. Also here it is obvious that a hadron resonance gas model description is only justified up to the crossover region.

The behavior of the correlations between net charm fluctuations and net baryon number fluctuations is similar to the behavior of corresponding correlations in the strangeness [9] as well as in the light quark sector [13]. Fig. 5 shows results for the three sectors. All the ratios should be unity in a gas of uncorrelated hadrons and approach their non-interacting quark gas limit at infinite temperatures. It is apparent that a hadron resonance gas model description breaks down just above the chiral crossover temperature not only for the light and open strange hadrons but also for the open charm hadrons.

3. The abundance of open charm hadrons

The results from suitable cumulants and correlations from conserved quantum numbers in the strangeness sector, as discussed in the previous sections, open the question about the importance of the inclusion of additional yet unobserved open charm mesons and charmed baryons in hadron resonance gas models and their contribution to the thermodynamics.
In Fig. 6 the partial pressures of open charm mesons and charmed baryons are shown for different HRG models, i.e. using all open charm resonances listed in the particle data table (PDG-HRG), including additional charm resonances calculated in a relativistic quark model (QM-HRG), the latter cut-off at mass 3 GeV (QM-HRG-3) and 3.5 GeV (QM-HRG-3.5). Due to the experimentally better known meson sector, the differences between the PDG-HRG and QM-HRG models are negligible up to the chiral crossover temperature, while in the baryonic sector the influence of predicted additional states becomes as large as 40% and the largest contributions come from states up to 3 GeV.

The HRG model predictions for the different open charmed baryon contents are shown in Fig. 7 for three ratios of charmed charge correlations and fluctuations that are sensitive to all charmed baryons (top), all charged charmed baryons (middle) and all strange charmed baryons (bottom). The lattice QCD results for those ratios show good agreement with a hadron resonance gas model that contains all open charm meson and baryon spectra calculated in a relativistic quark model [14, 15]. In contrast, the PDG-HRG model results are far below the lattice QCD data in the temperature range of the QCD crossover region. This observation provides evidence for a substantial contribution of experimentally so far unobserved charmed baryons to the pressure of a hadron resonance gas. Nevertheless the charm contribution to the total pressure is of course strongly suppressed relative to the contribution of the non-charmed sector.

4. Screening masses of quarkonia
The bulk thermodynamic charge fluctuations discussed in the previous sections provided information about the melting and abundance of open strange and open charm baryons. Due to their relation to conserved quantum numbers, these quantities are not sensitive to strange mesons ($s\bar{s}$) and charmonia ($c\bar{c}$). In this sector hadronic current-current correlation functions
are the appropriate tools to obtain spectral properties on the thermal modification of bound states in the medium.

In contrast to temporal correlation functions which are limited by the finite temporal extent, $1/T$, of the lattice, spatial correlation functions can be studied at larger separations and can directly be compared to the corresponding vacuum correlation functions to quantify modifications of the in-medium spectral functions. Although the relation to the spectral function, $\rho(\omega, p, T)$, is even more involved than in the temporal case as the spatial correlation functions are sensitive to the momentum dependence of spectral functions,

$$G(z, T) = \int_{-\infty}^{\infty} \frac{dp_z}{2\pi} \int_{0}^{\infty} \frac{d\omega}{2\pi} \rho(\omega, p_z, T),$$

the large distance behavior of correlation functions, $G(z, T) \sim \exp(-M(T)z)$, is dominated by an exponential decay characterized by the screening mass $M$. While at low temperatures, in the case of a bound state in the spectrum, the screening mass is equal to the pole mass of the ground state, at high temperatures when the mesonic excitations are completely melted, the screening mass becomes strongly temperature dependent. In the non-interacting limit it is related to the lowest non-zero Matsubara frequency [17],

$$M_{\text{free}} = \sqrt{m_{q_1}^2 + (\pi T)^2} + \sqrt{m_{q_2}^2 + (\pi T)^2}, \quad (7)$$

with the masses $m_{q_1}$ and $m_{q_2}$ of the quark and anti-quark of the corresponding meson.

Therefore a change of the temperature dependence of screening masses between those two limiting cases can be used as an indicator for thermal modifications and dissociation of charmonia and open charm mesons.

Fig. 8 shows results, obtained using the HISQ action [16], for $s\bar{s}$ mesons (top), $s\bar{c}$ (middle) and charmonium (bottom) for various states compared to the corresponding zero-temperature masses (solid lines) and non-interaction limit Eq. 7 (dashed line).

The screening masses for open charm mesons start to deviate from the vacuum masses already in the chiral crossover region and their temperature dependence is comparable to that in the strange meson sector. This is a further indication that open charm mesons start to melt in the vicinity of $T_c$ in agreement with the results of open quantum number fluctuations of the previous sections.
The results in the charmonium sector show a behavior compatible with a sequential melting pattern. While the $J/\Psi$ ($1^{−−}$) and $\eta_c$ ($0^{−+}$) screening masses remain almost identical to their vacuum pole masses up to around $1.1T_c$, the screening masses for $\chi_{c0}$ and $\chi_{c1}$ show thermal modifications already below $T_c$. At temperatures above two times $T_c$ all channels show a linear rise of the screening masses with temperature.

5. Heavy quark diffusion coefficients

Besides information on the medium modifications of bound states, also transport coefficients, in the case of heavy quarks these are heavy quark diffusion coefficients, are encoded in vector meson correlation and spectral functions. However due to the different contributions and different scales entering, it is more convenient to use an operator that is more sensitive to the transport contribution and does not contain any bound state contribution.

In the limit of heavy quarks, using Heavy Quark Effective Theory, a purely gluonic operator, the color-electric correlator can be derived [19, 20],

$$G_E(\tau) \equiv \frac{1}{3} \sum_{i=1}^{3} \frac{\langle \text{ReTr} \left[ U(\beta; \tau) gE_i(\tau, \vec{0}) U(\tau; 0) gE_i(0, \vec{0}) \right] \rangle}{\langle \text{ReTr}[U(\beta; 0)] \rangle}, \quad \beta = \frac{1}{T},$$

where $gE_i$ denotes the color-electric field, $T$ the temperature, and $U(\tau_2; \tau_1)$ a Wilson line in the Euclidean time direction.

In a recent study we have calculated the color-electric correlator (8) on large quenched lattices [18] and performed the continuum extrapolation for $G_E(\tau)$ at a temperature of about $1.5T_c$. Fig. 9 shows the results on the different lattices (left) and the continuum extrapolated correlator (right).

The correlator is related to the spectral function by

$$G_E(\tau) = \int_0^\infty \frac{d\omega}{\pi} \rho_E(\omega) \frac{\cosh[\omega(\frac{\tau}{T} - \tau)]}{\sinh[\frac{\omega}{T}]}.$$  

Figure 9. Left: Lattice data of the color-electric correlator after perturbative renormalization and the use of tree-level improved distances. Right: Continuum-extrapolated lattice data and examples of different interpolation results, as described in the text. The results have been normalized to the leading order correlator, $G_{\text{norm}}$. Taken from [18].
Figure 10. Left: Examples of model spectral functions, compared with the UV perturbative spectral function $\phi_{\text{UV}}^{(a)}$ and the result a Backus-Gilbert method (BGM) study, from [18].

Right: Results for the heavy quark momentum diffusion coefficient $\kappa$ based on different models and different fitting strategies. The grey band illustrates the final estimate based on models 2, 3a and BGM [18].

In the infrared regime ($\omega \ll T$), the heavy quark momentum diffusion coefficient can be defined as [19]

$$\kappa \equiv \lim_{\omega \to 0} \frac{2T \rho_E(\omega)}{\omega}.$$  \hspace{1cm} (10)

In contrast to the case of correlation and spectral functions of conserved currents where a transport peak is expected, the approach to this limit appears to be smooth and $\rho_E$ is rather a monotonically increasing function for small $\omega$,

$$\rho_{\text{IR}}^E = \frac{\kappa \omega}{2T}. \hspace{1cm} (11)$$

In the ultraviolet regime ($\omega \gg T$) due to asymptotic freedom, the spectral function can be computed in perturbation theory. We used various interpolations between the two limiting cases to perform a detailed analysis of the systematic uncertainties in extracting the heavy quark momentum diffusion $\kappa$ based on fits to the continuum extrapolated correlation function. In addition to these fits, we have also made use of a variant of the Backus-Gilbert method (BGM) [21, 22]. Some of the resulting correlation and spectral functions are shown in Fig. 9(right) and Fig.10(left) respectively.

The results of our full systematic analysis on the transport coefficient $\kappa$ are shown in Fig. 10(right). The grey band illustrates the central value,

$$\kappa/T^3 = 1.8 \ldots 3.4.$$  \hspace{1cm} (12)

In the non-relativistic limit, i.e. for a heavy quark mass $M \gg \pi T$ the heavy quark momentum diffusion $\kappa$ is related to the diffusion coefficient, $D = 2T^2/\kappa$, for which we obtain

$$DT = 0.59 \ldots 1.1.$$  \hspace{1cm} (13)
In this limit $\kappa$ is also related to the drag coefficient, $\eta_D = \kappa/(2MT)$. The latter can be interpreted as the kinetic equilibration time scale associated with heavy quarks, $\tau_{\text{kin}} = \eta_D^{-1}$. With our result for $\kappa$ (12) we obtain

$$\tau_{\text{kin}} = \frac{1}{\eta_D} = (1.8 \ldots 3.4) \left( \frac{T_c}{T} \right)^2 \left( \frac{M}{1.5 \text{ GeV}} \right) \text{fm/c}. \quad (14)$$

Close to $T_c$, charm quark kinetic equilibration appears therefore to be almost as fast as that of light partons, for which a time scale $\sim 1 \text{ fm/c}$ is generally considered.

Conclusions

Studying various observables of net strangeness and net charm fluctuations in comparison with predictions from hadron resonance gas models, we have found evidence that additional, experimentally so far unobserved strange and charm hadrons become thermodynamically relevant in the vicinity of the QCD crossover region. In the strange sector this leads to significant reductions of the chemical freeze-out temperature of strange hadrons. When including these additional states in hadron resonance gas models, the thermodynamics of open strange and open charm degrees of freedom in terms of an uncorrelated hadron gas gives a good description in the hadronic phase, but only up to the chiral crossover region. Deviations at higher temperatures suggest the liberation of strangeness degrees of freedom in the crossover region and that open charm hadrons start to dissolve already close to $T_c$. The analysis of screening masses are consistent with these findings for open charm mesons ($s\bar{c}$), but suggest a sequential melting pattern for charmonium ($c\bar{c}$) states in the QGP. We have determined a continuum estimate of the heavy quark momentum diffusion coefficient. It’s value can be used to serve as an indication that close to $T_c$, charm quark kinetic equilibration appears almost as fast as that for light partons in agreement with experimental results on the flow of charm quarks.

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