2.17 Thermal Shifts, Fluctuations, and Missing States

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Abstract

Thermal shifts and fluctuations at finite temperature below the deconfinement crossover from hadronic matter to the quark-gluon plasma provide a viable way to search for missing states with given quantum numbers in the hadronic spectrum. We analyze three realizations of the hadron resonance gas model in the light quark (uds) sector: the states from the Particle Data Group tables with or without width and from the Relativized Quark Model. We elaborate on the meaning of hadronic completeness and thermodynamical equivalence on the light of lattice QCD trace anomaly, heavy quark entropy shift and baryon,charge and strangeness susceptibilities.

1. Introduction

The concept of missing states in QCD is intimately related to the completeness of the hadronic spectrum. The issue was anticipated by Hagedorn in the mid 60's [1] when analyzing the mass-level density $\rho(M)$ and *predicting* the bulk of states at higher masses, which later on were experimentally confirmed. This also implies that the states may be *counted* one by one (and hence ordered) by, say, the cumulative number of states function,

$$N(M) = \sum_n g_n \theta(M - M_n)\,, \tag{1}$$

with g_n the total degeneracy and $\rho(M) = dN(M)/dM$. Updated analyses of the Hagedorn hypothesis may be found in [2, 3]. The function $N(M)$ assumes integer values, and the best mass resolution is $\Delta M = \min_n(M_{n+1} - M_n)$. For bound states, where the spectrum is discrete, this is a well defined procedure. In the continuum, this can only be done by putting the system in a box with finite but sufficiently large volume which acts as an infrared cut-off $V^{1/3}\Delta M \gg 1$. The ultraviolet cut-off is the maximum mass $M_{\max}$ in Eq. (1).

The commonly accepted reference for hadronic states is the Particle Data Group (PDG) table [4], a compilation reflecting a consensus in the particle physics community and which grades states *,**,***, and ****, according to the growing confidence in their existence, respectively. Global features of the hadronic spectrum may depend on whether we decide to promote or demote their significance, according to some theoretical prejudice. Of course, we expect the PDG hadronic states to have a one-to-one correspondence with colour neutral eigenstates of the QCD Hamiltonian; indeed, ground and some excited states have been determined on the lattice [5]. For hadronic states with only light (uds) quarks the maximum mass, $M_{\max}$, recorded by PDG is around 2.5 GeV for mesons and baryons, hence currently $N(M_{\max}) \sim 2.5 \times 10^3$. So far, the states listed by PDG echo the standard quark model classification for mesons ($\bar{q}q$) and baryons (qqq). Because of this feature, it will be pertinent to consider also the Relativized Quark Model (RQM) for mesons [6] and Baryons [7], as first done for $N(M)$ in [8] (Fig. 9). The remarkable coincidence $N_{\rm PDG}(M) \sim N_{\rm RQM}(M)$ up to $M_{\max}$ for *bot* mesons and baryons has been shown in Ref. [9]. The so-called "further states" may or may not be confirmed or expected and have not been clearly regarded by the PDG as identified, although they could be exotic tetraquarks, $\bar{q}q\bar{q}q$, pentaquarks, $\bar{q}qqqq$, glueballs gg, ggg or hybrids $\bar{q}qg$ [10].

In this contribution we analyze thermodynamic measures (various susceptibilities) which are sensitive to missing states. The setup corresponds to heating up the vacuum without dissolving its constituent hadrons into quarks and gluons and testing quark-hadron duality at temperatures below $T_c \sim 150$ MeV. Obviously, such a framework is inefficient for individual states, but becomes competitive if globally a relatively large number of states are missing. As reported in [11, 12] the Hagedorn conjectured behaviour of $N(M) \sim Ae^{M/T_H}$ for $M > M_{\max}$ may influence the results close to T_c, at temperatures above $T > 140$ MeV. According to [12], there is not much room for such states in the one-body observables, where they would spoil the agreement with the lattice data, unless suitable repulsion between states is simultaneously incorporated. Here will make no attempt to complete the spectrum beyond $M_{\max}$.

2. Prehistory of Missing States

The use of thermodynamical arguments to characterize the existence of missing states is a rather old subject which goes back to the early beginnings of the kinetic theory of gases and the equipartition theorem. In its most general form it states that every degree of freedom contributes to the mean energy with $\frac{1}{2}k_B T$.[1]. Therefore $\bar{E} = N\nu k_B T/2$, where ν is the total number of degrees of freedom. Generally, $\nu = \nu_{\rm translation} + \nu_{\rm vibration} + \nu_{\rm rotation}$ and the molar specific heat is $c_V/R = \nu/2$. A major obstacle at the time was pointed out by J. C. Maxwell in 1860 in connection to the specific heat of the diatomic gas such as, e.g., H_2, where a priori the total number of degrees of freedom is $\nu = 3_{\rm trans} + 2_{\rm vib} + 2_{\rm rot} = 7$. This would imply $c_V/R = 7/2$, whereas experimentally at room temperature one has $c_V/R \approx 5/2$. This is because the vibrational degrees of freedom are not active due to high excitation energy, and become visible only as the dissociation temperature of ~ 3200 K is approached. Likewise, as T is decreased, the rotational degrees of freedom are also frozen and below ~ 70 K, $c_V/R = 3/2$, as for the monoatomic molecules.

In modern terms the "freezing" of degrees of freedom is related to the quantization of energy levels for the Hamiltonian $H\Psi_n = E_n\Psi_n$ with energy eigenvalues above the temperature, $E_n > T$, contributing negligibly to the partition function

$$Z = {\rm Tr} e^{-H/T} = \sum_n e^{-E_n/T}. \qquad (2)$$

In QCD, the quantized energy levels are the masses of the existing hadronic states and, like in the Maxwell argument, the states which are not activated when $M_n > T$ do not contribute.

3. Completeness of the Hadron Spectrum

Completeness of the listed PDG states [4] is a subtle issue. On the one hand they are mapped into the $\bar{q}q$ and qqq quark model states. On the other hand, most reported states are not stable particles but resonances produced as intermediate steps in a scattering process.

With a finite lifetime τ_R, they are characterized by a mass distribution $\rho_R(M)$, with a central value M_R and a width $\Gamma_R \sim \hbar/\tau_R$. From a rigorous point of view resonances are poles of the *exact* amplitude in the second Riemann sheet in the complex s plane at $s = M^2 - iM\Gamma$. For multichannel scattering with N channels one has 2^N Riemann sheets, depending on which cuts have been crossed (see, e.g., [15, 16] for discussions in the meson-baryon $S = 0, -1$ sectors). Despite the rigor of these definitions, complex energies are not directly measured. An analytic continuation of a phenomenological and approximate scattering amplitude, taking into account a process dependent background, is needed and the arbitrariness grows with the width of the resonance [17] (see, e.g., for the specific 0^{++} case [18]). On average, most of the resonances listed by PDG [4] can be regarded as narrow, since one finds $\langle \Gamma_R/M_R \rangle = 0.12(8)$ *both* for mesons and baryons [19, 20], a fact numerically consistent

[1] The story around this principle illustrates many of the issues under discussion, including the contribution of an anonymous referee [13] D. Bernoulli [14] was the first who found in 1738 that the Boyle-Mariotte, Gay-Lussac, and Charles equations could be unified and understood by means of Newton's equations and in statistical terms. His work was forgotten, and only in 1845 J. J. Waterston submitted a paper to the Philosophical Transactions of the Royal Society (PTRS) which was rejected with a remark "The paper is nothing but nonsense, unfit even for reading before the Society". Hence this work was also ignored. Maxwell, in 1859, managed to publish the case of rigid molecules, and Boltzmann generalized it in 1868 to its modern form including rotational and vibrational degrees of freedom. Lord Rayleigh in 1895, found by chance Waterston's paper in the archives and decided to publish it in PTRS twelve years after Waterston's death with a commentary: "had he put forward his investigation as a development of Bernoulli a referee migh have hesitated to call it nonsense. It is probable that Waterston was unaquainted with his work.".

with the large N_c theoretical expectation $\Gamma_R/M_R = \mathcal{O}(N_c^{-1})$ [21]. In the Hamiltonian picture, resonances are identified as the so-called Gamow states and are not normalizable in the usual Hilbert space, as they are not conventional irreducible representations of the Poincarè group [22]. The completeness relation involves bound states and the continuum, which can be rewritten as a discrete sum of the Gamow states and a remainder [23].

The meaning of completeness is fairly clear within a given Hilbert space $\mathcal{H}$ with specified degrees of freedom when only bound states are possible. For instance, if we restrict ourselves to the meson $(\bar{q}q)$ or baryon (qqq) sectors, such as in RQM [6, 7], we can diagonalize the $\bar{q}q$ and qqq Hamiltonians with confining potentials in a given already complete basis, which is truncated but large enough that states with $M_n \leq M_{\max}$ converge. Thus we write

$$\mathcal{H}_{\rm RQM} = \mathcal{H}_{\bar{q}q} \oplus \mathcal{H}_{qqq} \oplus \mathcal{H}_{\bar{q}\bar{q}\bar{q}} \tag{3}$$

Within this framework, hadrons are stable, extended, and composite particles. This is explicitly illustrated by the virial relations in the massless quark limit [9] $M_{\bar{q}q} = 2\sigma\langle r\rangle_{\bar{q}q}$ and $M_{qqq} = N_c\sigma\langle r\rangle_{qq}$, which shows that hadrons are larger the heavier they become. Many of these states may decay by strong processes, such as $\rho \to 2\pi$ or $\Delta \to N\pi$, where a coupling to the continuum is needed by incorporating the $\mathcal{H}_{\bar{q}q\bar{q}q}$ and $\mathcal{H}_{\bar{q}qqqq}$ Fock state. As a result, the pole mass is shifted into the complex plane $M \to M + \Delta M - i\Gamma/2$. The mass-shift $\Delta M \sim \Gamma$ depends parametrically on the coupling to the continuum $\Delta M \sim \Gamma$ so that in the large N_c limit, $\Delta M/M = \mathcal{O}(N_c^{-1})$ [24].

On the lattice, hadrons are constructed as interpolating fields in a finite-volume box. Completeness proceeds along similar lines, with the important modification that resonances are characterized by volume-independent and real mass shifts. The connection to physical resonances in the complex energy plane requires also analytical extrapolation (for a review see, e.g., [25]).

4. Thermodynamic Equivalence

Be it the PDG [4], RQM [6, 7], or the lattice excited QCD [5], the partition function can be constructed from the (complete) energy localized colour neutral eigenstates, Eq. (2). The lattice at finite temperatures, or the ultrarelativistic heavy ions collisions, generate global colour neutral configurations which along the crossover are expected to delocalize. Most of the emerging physical quark-hadron duality picture has to do with the thermodynamical equivalence of different approaches.

According to the quantum virial expansion [26] one can compute the partition function from the knowledge of the S-matrix in the complete Hilbert space, i.e., involving all possible processes with any number of elementary particles in both the initial and final states, $n \to m$. In practice, hadrons have been taken as the building blocks in this approach, which for obvious practical reasons has never been taken beyond the $2 \to 2$ reactions, where the corresponding phase shifts are involved. In the case of narrow resonances one can replace the total contribution entering in terms of phase shifts by the resonance itself [27], whereby the resonance can be assumed to be elementary and point-like [28]. The result conforms to the Hadron Resonance Gas (HRG) as initially proposed by Hagedorn [1]. This provides the formal basis for modern HRG calculations using the PDG compilation. As mentioned above, most states entering the HRG are resonances with a given width, Γ. Therefore we will also consider the effect of smearing the mass distribution according to the replacement

$$\sum_R F(m_R^2) \to \int d\mu^2 F(\mu^2) \Delta_\Gamma(\mu^2 - m_R^2) \tag{4}$$

for an observable $F(\mu^2)$. [2]

However, the elementary constituents are both quarks and gluons. A different derivation proceeds along chiral quark-gluon models with a quantum and local Polyakov loop [33, 34]. [3] The action corresponds to creating, e.g., a quark at location $\vec{x}$ and momentum $\vec{p}$ in the medium

$$e^{-E(\vec{p})/T} \Omega(\vec{x})^\dagger, \tag{5}$$

where in the static gauge $\Omega(\vec{x}) = e^{igA_4(\vec{x})/T}$. Consequently, the total action can be separated into different quark and gluon sectors according to the low temperature partonic expansion around the vacuum [9, 37]

$$Z = Z_0 + Z_{\bar{q}q} + Z_{qqq} + Z_{\bar{q}\bar{q}\bar{q}} + \cdots \sim Z_{\rm RQM}. \tag{6}$$

Subsequent hadronization of $\bar{q}q$ and qqq states uses the cluster properties of the Polyakov loop correlator and group properties of the Haar measure, as well as the quantum, composite and extended nature of hadronic states. One appealing feature of this "microscopic" derivation of the HRG is the counting of states according to the quark model for the lowest Fock state components, but ambiguities arise when a given colour neutral multiquark state admits a separation into colour neutral irreducible subsystems [9, 38]. We take this result as our justification to use RQM. [4]

The fact that we use thermodynamic quantities to make a quantitative comparison does not sidestep the problem of discriminating different spectra. The best example is provided by a direct comparison of HRG using either PDG or RQM [6, 7] in terms of the trace anomaly, $\mathcal{A}(T) \equiv (\epsilon - 3P)/T^4$ which are hardly indistinguishable within the lattice QCD uncertainties from the WB [39] and HotQCD [40] collaborations (see Fig. 1 of Ref. [9]). As already mentioned the states with $M > M_{\rm max}$ with an exponential Hagedorn distribution are relevant below T_c [12] only at $T > 140$ MeV, and their contribution may be overcome with repulsive effects. Actually, the volume effects are expected to play a significant role; the excluded volume exceeds the total volume around $T \lesssim T_c$ (see Fig. 9 of Ref. [9]).

[2] Ideally the profile function should be determined from the scattering phase-shift [27], which displays cancellations [29, 30] and irrelevance of some weakly bound states [31] but it is not always available. Here we take a simple normalized Gaussian profile distribution. A Breit-Wigner representation works well around the resonance, but it has very long tails which do not faithfully represent the background. An upper bound for the error is to use the half-width rule [19, 32] according to which PDG masses are varied within half the width, i.e., taking $M_R \pm \Gamma_R/2$. We do not use this large N_c motivated prescription here as we feel that it largely overestimates the uncertainties for *all resonances* in the $N_c = 3$ world.

[3] This is unlike the more popular PNJL model [35, 36], where the quantum and local nature of $\Omega(\vec{x})$ is ignored, thus introducing an undesirable group coordinates dependence. In addition, in PNJL the Polyakov loop in the adjoint representation is not quenched, contradicting lattice calculations.

[4] Bound state masses are shifted when coupled to the continuum, so if we take a simple average estimate $\langle \Delta M/M \rangle_{\rm RQM} \sim \langle \Gamma/M \rangle_{\rm PDG} \sim 0.12(8)$. This roughly corresponds to take $5\% - 20\%$ uncertainty in T.

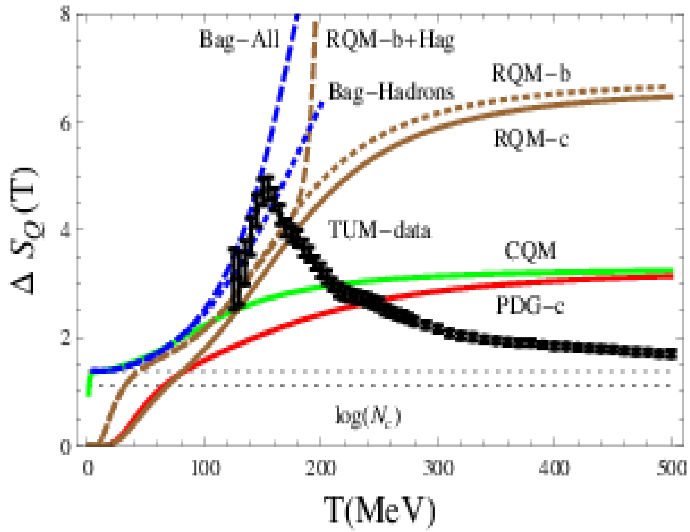

Figure 1: The entropy as a function of the temperature. We show results from various hadronic models: the bag model including all ($Q\bar{q}$, Qqq and $Q\bar{q}g$) states and just hadrons, the RQM with one c- or b-quark and the PDG states with one c-quark. The Hagedorn extrapolation of the b-spectrum is also displayed. We also plot the CQM with uds quarks and constituent mass $M = 300\ MeV$ and the bare $m_u = 2.5\ MeV$, $m_d = 5\ MeV$, $m_s = 95\ MeV$ masses. Horizontal lines mark $\Delta S_Q(0) = \log 2N_f$, with $N_f = 2$ the number of light degenerate flavours, and $\Delta S_Q(\infty) = \log(N_c)$. Lattice data for 2+1 flavours are taken from Ref. [46].

5. **Thermal Shifts**

The idea of thermal shifts is to study the change of thermodynamic quantities under the presence of local external sources. This looks very much like adding an impurity to a macroscopic system or adding a grain of salt to a bunch of snow. By looking a these thermal shift we may also assess a possible existence of missing states. An interesting hadronic example is provided by the free energy shift caused by a heavy quark placed in a hot medium with vacuum quantum numbers, which corresponds to a ratio of partition functions which can be identified with the Polyakov loop expectation value. This free energy shift is ambiguous and hence it is better to deal with the corresponding entropy shift and the specific heat, which are directly measurable quantities. A hadronic representation of Polyakov loop and its entropy has been analyzed [41, 42]. The implications of thermal shifts due to a heavy source or a heavy $Q\bar{Q}$ pair located at a fixed distance r at the hadronic level has recently been considered in [43–45].

Fig. 1 from Ref. [43] makes a good case for different categories of missing charm or bottom states. On the one hand the PDG is clearly insufficient to describe the entropy shift. So, we clearly miss higher mass states. Guided by the thermodynamic equivalence of PDG and RQM in the uds sector [9], we may complete the PDG spectrum using the RQM in the c- or b- sectors. As we see there is a big improvement and, moreover, the change when going from c to b is sufficiently small. Nonetheless, we have still missing states, a feature that is not mended when extending the spectrum a la Hagedorn. When a Bag model with the heavy source located at the center is considered for singly heavy hadrons $Q\bar{q}$, Qqq, and a hybrid $Q\bar{q}g$ the TUM lattice data are well reproduced.

6. **Fluctuations**

The connection between fluctuations and the abundance of hadronic resonances was pointed out by Jeon and Koch [47], who later [48] proposed it as a signal for the Quark-Gluon Plasma formation from the partition function (for pedagogical reviews see, e.g., [49, 50]). Implications for heavy ion collisions are reviewed in [51]. In Ref. [52], the event-by-event statistical analysis of ultrarelativistic heavy ions-collisions was compared to the HRG with a given chemical potential. Of course, any mismatch in this kind of analyses suggests missing resonances. Here we are concerned with the simplest vacuum zero density case. Actually, some authors have understood the significance of fluctuations as a possible hint of missing states [53].

Fluctuations of conserved charges, i.e., fulfilling $[Q_A, H] = 0$, are a way of selecting given quantum numbers [50] and become particularly simple in terms of the grand-canonical partition function which is given by

$$Z = \mathrm{Tr} e^{-(H-\sum_A \mu_A Q_A)/T} \qquad \Omega = -T \log Z. \tag{7}$$

with Ω the corresponding potential. One then gets

$$-\frac{\partial \Omega}{\partial \mu_A} = \langle Q_A \rangle_T, \quad -T\frac{\partial^2 \Omega}{\partial \mu_A \partial \mu_B} = \langle \Delta Q_A \Delta Q_B \rangle_T, \tag{8}$$

where $\Delta Q_A = Q_A - \langle Q_A \rangle_T$. In the uds sector the only conserved charges are the electric charge Q, the baryon charge B and the strangeness S, which is equivalent to the number of u, d, and s quarks. We consider the hot vacuum (no chemical potential) $\langle B \rangle_T = \langle Q \rangle_T = \langle S \rangle_T = 0$.

For $N_f = 2 + 1$, fluctuations have been computed on the lattice by the WB [54] and HotQCD [55] collaborations with the high temperature asymptotic limits

$$\chi_{BB}(T) = V^{-1}\langle B^2 \rangle_T \to \frac{1}{N_c} \tag{9}$$

$$\chi_{QQ}(T) = V^{-1}\langle Q^2 \rangle_T \to \sum_{i=1}^{N_f} q_i^2 \tag{10}$$

$$\chi_{SS}(T) = V^{-1}\langle S^2 \rangle_T \to 1, \tag{11}$$

where $(q_u, q_d, q_s, \dots) = (2/3, -1/3, -1/3, \dots)$. Higher order cumulants, such as skewness and kurtosis originally analyzed in Ref. [56], have also recently been computed more accurately [57], but we do not discuss them here.

In the hadron resonance model, the charges are carried by various species of hadrons, $Q_A = \sum_i q_A^{(i)} N_i$, where N_i is the number of hadrons of type i, hence

$$\langle \Delta Q_A \Delta Q_B \rangle_T = \sum_{i,j} q_A^{(i)} q_B^{(j)} \langle \Delta N_i \Delta N_j \rangle_T. \tag{12}$$

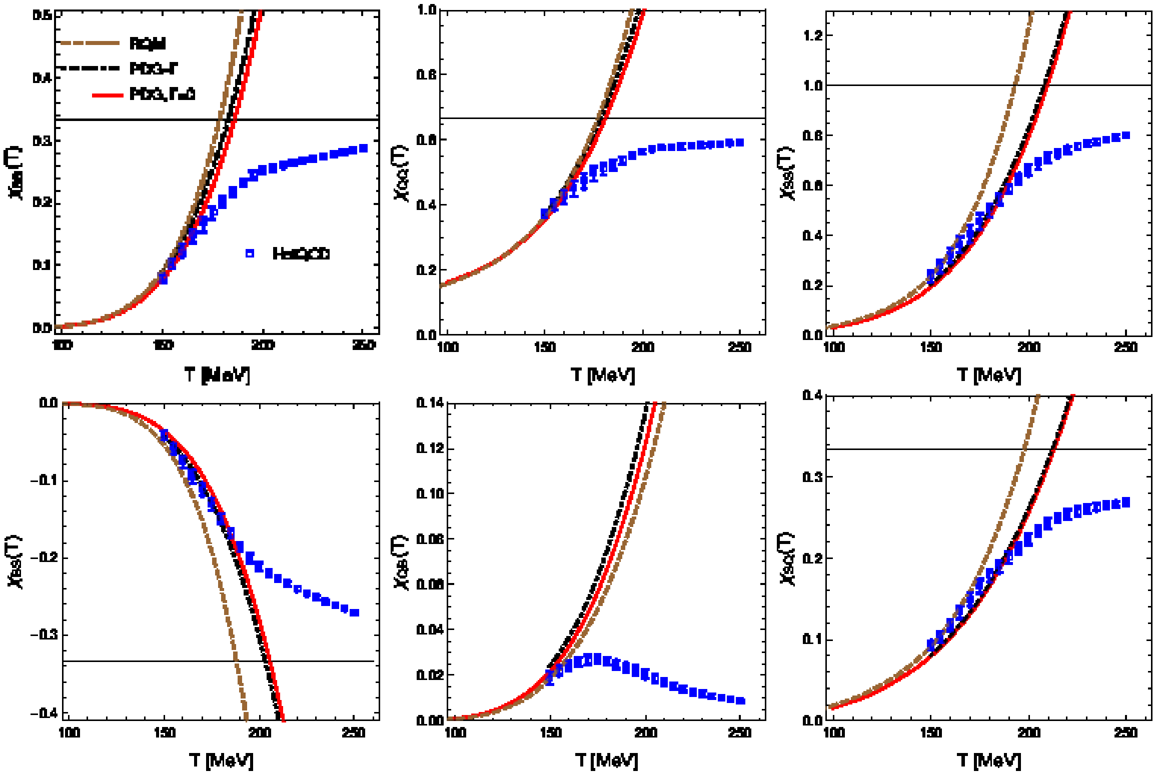

Figure 2: Baryon, charge and strangeness susceptibilities from HRG with the PDG, PDG(Γ) and RQM spectra, compared to the lattice HotQCD [55] data. WB data [54] are compatible with them so they are not plotted.

The average number of hadrons is

$$\langle N_i \rangle_T = V \int \frac{d^3k}{(2\pi)^3} \frac{g_i}{e^{E_{k,i}/T} + \eta_i}$$
$$= \frac{VT^3}{2\pi^2} \sum_{n=1}^{\infty} g_i \frac{(-\eta_i)^{n+1}}{n} \left(\frac{M_i}{T} \right)^2 K_2(nM_i/T)$$

where $E_{k,i} = \sqrt{M_i^2 + k^2}$, g_i is the degeneracy and $\eta_i = \mp 1$ for bosons/fermions respectively. In practice the Boltzmann approximation (i.e., just keeping $n = 1$) is sufficient. Regarding the fluctuations, since the different species are uncorrelated $\langle \Delta n_\alpha \Delta n_\beta \rangle_T = \delta_{\alpha\beta} \langle n_\alpha \rangle_T (1 - \eta_\alpha \langle n_\alpha \rangle_T)$, for the occupation numbers. Since $\langle n_\alpha \rangle_T \ll 1$,

$$\langle \Delta Q_A \Delta Q_B \rangle_T \approx \sum_i q_A^{(i)} q_B^{(i)} \langle N_i \rangle_T. \quad (13)$$

Our results for the susceptibilities are depicted in Fig. 2 where we show the HotQCD lattice data [55] (the earlier WB data [54] are compatible with them so they are not included in the figure to avoid cluttering.). We compare with the standard HRG model, denoted as PDG, the HRG including a Gaussian width profile, which we denote as PDG (Γ), and the RQM.

Our scheme here is to include *all* states from PDG, which as mentioned are mapped into the standard quark model classification of mesons as $\bar{q}q$ and baryons as qqq as the only hadronic states. This choice of states provides a visible effect in the SB correlator bringing it closer to the lattice data as compared to [53] where only $***\,*$ PDG states are considered. The inclusion of width effects is also generally quite sizeable and cannot be ignored, as it has routinely been done in many HRG comparisons in the past (see however [12, 32]). Nevertheless, there are other ways to include the width profile which will somehow blur the PDG(Γ) result, and a more systematic study, perhaps including also volume effects, would be most helpful.

The remarkable good agreement of the trace anomaly found between PDG and RQM [9] or the PDG(Γ) [12] compared with lattice QCD results from WB [39] and HotQCD [40] collaborations gets a bit spoiled in terms of the considered fluctuations, where these spectra may feature missing or exceeding states. For instance, a look at the BB correlation in Fig. 2 suggests that the RQM has too many baryonic states but not too many charged states. Therefore, the thermodynamic equivalence will depend on the quantum numbers, enhancing the relevance of a fluctuation analysis, as done here, in the discussion of quark-hadron duality.

7. Conclusions

In the present contribution we have revised the thermodynamical equivalence between the PDG, RQM, and lattice QCD for temperatures below the hadron-gas—quark-gluon-plasma crossover for the case of an entropy shift due to a heavy quark and fluctuations via Baryon, Charge and Strangeness susceptibilities as diagnostic tools for missing states.

The analysis of the entropy shift due to a heavy quark suggests that there are conventional (high mass) missing states in single charm, or bottom hadrons ($Q\bar{q}$ and Qqq) and it looks likely that a large number of hybrids ($Q\bar{q}g$) is also missing.

In the pure light uds sector, our perception on the missing states may change when finite width effects are placed into the calculation. This effectively corresponds to redistribute the mass spectrum weighted with an asymmetric Boltzmann factor. From that point of view the missing states effect could also be regarded as a missing mass effect. At this level the highest temperature of agreement for the trace anomaly seems to be $T \lesssim 150\ \mathrm{MeV}$ between either the HRG based on PDG, PDG (Γ) or RQM spectra and current QCD finite temperature calculations. However, the separate analysis in terms of B, Q, S fluctuations reveals a less obvious pattern regarding the verification of quark-hadron duality. While the HRG has arbitrated the lattice QCD discrepancies for the trace anomaly in the past, in the case of fluctuations we are now confronted with the opposite situation. Lattice data agree but are not universally reproduced by any of the three HRG realizations considered here. This may offer a unique opportunity to refine these models including other effects and which deserves further studies.

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