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QCD Level Density from Maximum Entropy Method

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We propose a method to calculate the QCD level density directly from the thermodynamic quantities obtained by lattice QCD simulations with the use of the maximum entropy method (MEM). Understanding QCD thermodynamics from QCD spectral properties has its own importance. Also it has a close connection to phenomenological analyses of the lattice data as well as experimental data on the basis of hadronic resonances. Our feasibility study shows that the MEM can provide a useful tool to study QCD level density.

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1. QCD level density

In this report, we discuss the QCD level density in a finite box with a size V. Denoting energy eigenstates of the QCD Hamiltonian \mathscr{H}_{QCD} by E_n , the energy-level density A(E,V) is defined by counting the number of states in the range of E to E + dE, i.e.,

$$A(E,V) \equiv \sum_{n} \delta(E - E_{n}) \quad \text{with} \quad \mathscr{H}_{QCD} |\Psi\rangle = E_{n} |\Psi\rangle.$$
(1.1)

Using this level density, the partition function is written as its Laplace transform;

$$\mathscr{Z}(\beta, V) = \operatorname{Tr}\left[e^{-\beta \mathscr{H}_{QCD}}\right] = \int_0^\infty A(E, V) e^{-\beta E} dE, \qquad (1.2)$$

where $\beta \equiv 1/T$ with T being the temperature of the system. Thermodynamic quantities such as the pressure, p, and the energy density, ε , are related to the partition function as

$$p(\boldsymbol{\beta}) = \frac{1}{V\boldsymbol{\beta}} \ln \mathscr{Z}(\boldsymbol{\beta}, V), \qquad \boldsymbol{\varepsilon}(\boldsymbol{\beta}) = -\frac{1}{V} \frac{\partial \ln \mathscr{Z}(\boldsymbol{\beta}, V)}{\partial \boldsymbol{\beta}}. \tag{1.3}$$

Eq.(1.2) together with Eq.(1.3) imply that every thermodynamic quantity is obtained from the information of the level density defined at zero temperature. Especially, Eq.(1.2) tells us that the properties of QCD phase transition at finite T, which is characterized by the non-analytic behavior of $p(\beta)$ in the thermodynamic limit, are already encoded in the QCD level density defined at T = 0.

The investigation of the level density in nuclear physics and in hadron physics has a long history: For example, Bethe studied the nuclear level density by evaluating the partition function of the Fermi gas [1]. By performing the inverse Laplace transform, he showed that $A \propto \exp(2\sqrt{cE})$ with *c* being a constant related to single-particle level density. Hagedorn studied hadronic level density and has derived an asymptotic formula for the state density of hadrons with a mass *m*,

$$\rho(m) \propto \frac{1}{m^a} \exp(m/T_H). \tag{1.4}$$

Here *a* and T_H are some constants and the latter is called the Hagedorn temperature [2]. Eq.(1.4) is derived from the celebrated bootstrap model in which the state density $\rho(m)$ and the energy-level density $A(E = m, V_0)$ in a fireball of size V_0 are identified for large *m*. The exponential growth of the hadronic state density, Eq.(1.4), agrees with experimental data up to 2 GeV at present and the agreement becomes better as new resonances are included [3]. Because of this success, the hadron resonance gas model as well as the Hagedorn's formula have been and is being widely used in QCD phenomenology. However, this model describes only the hadronic matter at temperature below T_H . If we try to calculate \mathscr{X} with Eq.(1.4) above T_H , the integral does not converge.

On the other hand, progresses in QCD thermodynamics has been obtained steadily by the first principle lattice simulations. The results show that ε and p increase rapidly near the transition temperature T_c and approach to the black-body formula, $\varepsilon \sim 3p \propto T^4$, for sufficiently high temperature. It has been also found that thermodynamics below T_c is well described by hadron resonance gas model as long as appropriate hadron masses relevant to lattice simulations are employed [4, 5]. Therefore, the time is now ripe to consider a unified and model-independent description of QCD thermodynamics on the basis of the QCD level density. In fact, detailed studies of the level density is particularly useful to identify the relevant degrees of freedom in hot QCD below and above T_c .





Figure 1: A schematic model for the pressure (left panel) and the energy density (right panel).

Now let us first pay attention to a close similarity between Eq.(1.2) and the spectral representation of the hadronic two-point correlation function, G, as a function of the imaginary time τ :

$$G(\tau) = \int_0^\infty R(\omega) e^{-\tau \omega} d\omega, \qquad (1.5)$$

where $R(\omega)$ is the spectral function and ω is the frequency. Formal correspondences, $\mathscr{Z} \leftrightarrow G$, $\beta \leftrightarrow \tau$, $E \leftrightarrow \omega$ and $A \leftrightarrow R$, are clear by comparing Eq.(1.2) with Eq.(1.5). Since the maximum entropy method (MEM) is known to be a powerful tool to extract the spectral function *R* from the lattice data *G* [6], the same technique is expected to be used to extract the level density A(E, V) from the lattice data of \mathscr{Z} .

2. A toy model

Before testing the idea of using MEM to extract the level density A(E,V), let us first discuss the general structure of A expected in simple cases where some analytic study is possible. First of all, the inverse Laplace transform (the Bromwich integral) of Eq.(1.2) reads

$$A(E,V) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \mathscr{Z}(\beta,V) e^{E\beta} d\beta = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{(p(\beta)V+E)\beta} d\beta,$$
(2.1)

where γ is a real number chosen so that all the singularities of $\mathscr{Z}(\beta, V)$ are to the left of it. In the leading order of the saddle point approximation, one readily finds

$$A(E,V) \propto \exp(s(\varepsilon)V),$$
 (2.2)

where $\varepsilon \equiv E/V$ is the energy density and $s(\varepsilon)$ is the entropy density.

Consider a simplest case of free massless particles where the pressure is given by $p(\beta) = (\sigma/3)T^4$. Then, by working out the Gaussian integral around the saddle point, one finds

$$A(E,V)|_{EV^{1/3} \gg 1} \sim \frac{1}{\sqrt{8\pi V}} \left(\frac{\sigma}{(E/V)^5}\right)^{1/8} \exp\left(\frac{4}{3}\sigma^{1/4}V(E/V)^{3/4}\right),$$
(2.3)



Figure 2: Left panel: A schematic picture of $s(\varepsilon) \propto \ln A(E, V)$ in a toy model as a function of $\varepsilon = E/V$. Right panel: The QCD level density A(E, V) in an arbitrary unit extracted from the lattice data.

which implies $\ln A \sim E^{3/4}$ at high excitation energies.

To examine a more realistic example with a phase transition, let us consider the bag equation of state in which we assume free massless pions (free massless quarks and gluons) below (above) T_c . In this case, the pressure of the system is given by

$$p(T) = \frac{T}{V} \ln \mathscr{Z} = \frac{\sigma_h}{3} T^4 \theta (T_c - T) + \left(\frac{\sigma_q}{3} T^4 - B\right) \theta (T - T_c), \qquad (2.4)$$

where *B* is the bag constant which is related the critical temperature as $T_c = [(3B)/(\sigma_q - \sigma_h)]^{1/4}$. σ_h and σ_q are proportional to the number of degrees of freedom in the hadronic phase and the quark-gluon plasma phase, respectively. A schematic sketch for p/T^4 and ε/T^4 is given in Fig. 1.

For the bag equation of state given in Eq.(2.4), the exponent $s(\varepsilon)$ in Eq.(2.2) turns out to be

$$\frac{4}{3}\sigma_{h}^{1/4}\varepsilon^{3/4} \quad [I], \qquad \frac{1}{3}\sigma_{h}T_{c}^{3} + \frac{\varepsilon}{T_{c}} \quad [II], \qquad \frac{4}{3}\sigma_{q}^{1/4}\left(\varepsilon - B\right)^{3/4} \quad [III].$$
(2.5)

Here the formulas [I], [II] and [III] are valid for $\varepsilon < \varepsilon_{c1}$, $\varepsilon_{c1} < \varepsilon < \varepsilon_{c2}$, and $\varepsilon > \varepsilon_{c2}$, respectively. Note that $\varepsilon_{c1} = \sigma_h T_c^4$ ($\varepsilon_{c2} = \sigma_q T_c^4 + B = \frac{1}{3} (4\sigma_q - \sigma_h) T_c^4$) is the energy density just below (above) the phase transition point as shown in the right panel of Fig. 1.

The behavior of the exponent $s(\varepsilon)$ given in Eq.(2.5) is illustrated in the left panel of Fig. 2. The level density shows the Hagedorn type behavior $\ln A \propto E$ in the phase transition region [II], while it shows softer behavior $\ln A \sim E^{3/4}$ in the high temperature region [III]. The exponent has a crossover from *E* to $E^{3/4}$ at $E = E_{c2} = \varepsilon_{c2}V$ at which the quark-gluon plasma starts to emerge.

3. Application of MEM

Let us now try to extract A(E,V) from lattice QCD data of the thermodynamic quantities. Following the idea of MEM, we minimize the "free-energy" functional Q(A) with respect to the level density A:

$$Q = \frac{\chi^2}{2} - \alpha S_{\rm inf}.$$
 (3.1)

Here, S_{inf} is the information entropy given by

$$S_{\rm inf} = \int (f - 1 - f \ln f) dE, \quad A(E, V) = A_{\rm asy}(E, V) \times f(E, V),$$
 (3.2)

where $A_{asy}(E, V)$ implies a "default model" representing the asymptotic behavior of A in the large E limit. In the present study, we adopt $A_{asy}(E, V) = (V^{1/3}/\sqrt{8\pi}) \exp\left(\frac{4}{3}\sigma^{1/4}V\varepsilon^{3/4}\right)$ which is proportional to the asymptotic form of A for a free quark-gluon gas. We adjust σ to reproduce ε/T^4 measured on the lattice at high temperature. For the likelihood function χ^2 , we have chosen

$$\chi^{2} = \sum_{i=1}^{n} \left(\frac{p_{i}^{\text{lat}} - \frac{1}{V\beta_{i}} \ln \int A(E, V) e^{-\beta_{i}E} dE}{\Delta p_{i}^{\text{lat}}} \right)^{2} + \sum_{i=1}^{n} \left(\frac{\varepsilon_{i}^{\text{lat}} - \frac{\int (E/V)A(E, V) e^{-\beta_{i}E} dE}{\exp(V\beta_{i}p_{i}^{\text{lat}})}}{\Delta \varepsilon_{i}^{\text{lat}}} \right)^{2}, \quad (3.3)$$

where p_i^{lat} and $\varepsilon_i^{\text{lat}}$ are the data obtained by lattice simulations at *n* discrete values of the inverse temperature β_i . Also, Δp_i^{lat} ($\Delta \varepsilon_i^{\text{lat}}$) denotes statistical error of the pressure (energy density).

We use the 2-flavor full QCD data with improved Wilson quarks generated on a $16^3 \times 4$ lattice [7]. The spatial size of the lattice in the physical unit is approximately $(4\text{fm})^3$, although the physical volume changes for different values of β_i . As a first step, we choose $V = 1 \text{ fm}^3$ in Eq.(3.3) by assuming small volume-dependence of the lattice data. We use the data for the pressure and energy density with $m_{PS}/m_V = 0.90$ in which there are "seven" independent data points (n = 7).

A(E,V) reconstructed by MEM is shown by the solid line in the right panel of Fig.2 in an arbitrary unit with the logarithmic scale. Dashed line is A_{asy} mentioned above. To set the scale in the horizontal axis, we assume $T_c \approx 175$ MeV. Also, we have chosen $\alpha = 1$ in the present MEM analysis: eventually it has to be eliminated by calculating the probability distribution $P[\alpha]$ [6]. As can be seen from the figure, the behavior of A(E,V) at high E is consistent with $A_{asy} \sim E^{3/4}$ (the dashed line), while A(E,V) decreases strongly around E = 9 - 10GeV and deviates substantially from A_{asy} at low energies. This rapid crossover of lnA is qualitatively consistent with what we have discussed using the toy model.

Now we briefly discuss some systematic uncertainty in the MEM analysis. Instead of utilizing both p_i^{lat} and $\varepsilon_i^{\text{lat}}$ as in Eq.(3.3), we have done MEM analyses by using p_i^{lat} only and by using $\varepsilon_i^{\text{lat}}$ only. In these cases, the crossover region has moved $\pm 20\%$ from that shown in the right panel of Fig. 2. Therefore, the systematic error due to different choices of χ^2 is still large at present as long as we take only seven data points. Nevertheless, we believe that MEM could become a useful tool to extract the QCD level density if large number of data points with high accuracy become available in the future.

4. Conclusions and outlook

To understand thermodynamic properties near the QCD phase transition, the knowledge of the energy-level density is quite useful. In this report, we proposed a new method to calculate the QCD level density and have made a feasibility test using lattice data. Although further systematic studies are necessary by increasing the number of data points, the direct calculation of the QCD level density seems to be possible using the maximum entropy method.

An extension of the present study to the system at non-zero baryon density is interesting to be explores in connection with recent progress of finite density lattice QCD. The grand partition function $\mathscr{Z}(\beta,\mu,V)$ can be separated into the canonical partition functions $\mathscr{Z}_N(\beta,V)$ for each fixed quark number *N* by the fugacity expansion as

$$\mathscr{Z}(\beta,\mu,V) = \sum_{N} e^{N\beta\mu} \mathscr{Z}_{N}(\beta,V) = \sum_{N} e^{N\beta\mu} \int_{0}^{\infty} A(E,N,V) e^{-\beta E} dE.$$
(4.1)

Then, by using the lattice data with several different values of β and μ , one may extract the level density A(E, N, V). Such an analysis will shed lights on colored composite states with non-zero baryon numbers above T_c such as the quark-gluon bound state and the diquark [8, 9]. If such states are important to thermodynamic quantities, they should also show up in the QCD level densities with N = 1 and N = 2.

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