Padé Improvement of the Free Energy in High Temperature QCD

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Abstract

Padé approximants (PA’s) are constructed from the perturbative coefficients of the free energy through $O(g^n)$ in hot QCD. Padé summation is shown to reduce the renormalization-scale dependence substantially even at temperature ($T$) as low as 250 MeV. Also, PA’s predict that the free energy does not deviate more than 10 % from the Stefan-Boltzmann limit for $T > 250$ MeV.

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Properties of quantum chromodynamics (QCD) at high temperature ($T$) acquire a lot of attention in relation to the physics of the early universe and of the relativistic heavy ion collisions \cite{1}. In non-abelian gauge theories, naive expectation, based on the asymptotic freedom, is that the perturbation theory works as far as the temperature is high enough \cite{2}. However, this may not be the case because of the infrared sensitivity in the high-order terms beyond $O(g^6)$ for the free energy with $g$ being the QCD coupling constant \cite{3}.

Another practical problem is the asymptotic nature of the perturbation series, which can be seen from the expansion recently established through $O(g^5)$ \cite{4}. If one takes the expansion literally, the perturbation theory works only for $T > 2 \text{ GeV}$ which is order of magnitude larger than the critical temperature ($T_c$) of the QCD phase transition. On the other hand, the lattice QCD simulations for energy density, pressure and entropy density show that they approach the Stefan-Boltzmann (SB) limit rather quickly above $T_c \simeq 150 \text{ MeV}$ \cite{6}.

This poses a question that whether one could reconcile the non-perturbative lattice result with the perturbative expansion in the region $T_c < T < 2 \text{ GeV}$ by making proper resummation of the perturbation series. From the experimental point of view, the highest temperature which one could access in the relativistic heavy-ion colliders are at most 300-500 MeV. Therefore, most of the future data reflect the physics in the above temperature interval.

If the perturbative expansion has an asymptotic nature, the truncated series shows a large fluctuation for medium/strong couplings by the change of the order of the truncation. Nevertheless, some information on the full result is reflected in the behavior of the fluctuation and the coefficients of the perturbative expansion. This is the place where resummation method such as the Padé approach could play a role \cite{7}. In fact, the Padé summation has been successfully applied to the perturbative QCD series in high energy processes: it ‘postdicts’ the known higher-order terms, and also removes the renormalization-scheme dependence \cite{8,9}.

In the following, we will apply the Padé approach for free energy of QCD at finite $T$ with vanishing chemical potential and quark masses. The general structure of the free energy
\( F(T, \mu) \) for massless \( n_f \)-flavors in \( \overline{\text{MS}} \) scheme through \( O(g^5) \) reads \[4,5\]

\[
R(\mu) \equiv \frac{F(T, \mu)}{F_{SB}(T)} = 1 + f_2 \bar{g}^2(\mu) + f_3 \bar{g}^3(\mu) + f_4(\mu/T, \ln \bar{g}) \bar{g}^4(\mu) + f_5(\mu/T) \bar{g}^5(\mu),
\]

where \( \mu \) is a renormalization-scale, \( \bar{g} \equiv g/2\pi \) and \( F_{SB} \) is the SB (classical) limit of the free energy. Since the explicit form of the coefficients \( f_i \) is given in \[4,5\], we will not recapitulate them here.

We plot \( R(\mu = 2\pi T) \) for \( n_f = 4 \) in Fig.1(a) as a function of \( \alpha_s(\mu = 2\pi T) \) with \( \alpha_s \equiv g^2/4\pi \) (see the discussions below for this choice of \( \mu \)). The solid lines in Fig.1(a) have a large fluctuation as one increases the order of the perturbation. \( \alpha_s(2\pi T) \) used in Fig.1(a) is shown in Fig.1(b), where we take the two-loop \( \beta \)-function with \( n_f = 4 \) for simplicity. Instead of expanding \( \alpha_s \) by \( 1/\ln(\mu/\Lambda) \), we calculated the running of \( \alpha_s \) numerically with an initial condition \( \alpha_s(\mu = 5\text{GeV}) = 0.21 \) obtained in the \( \overline{\text{MS}} \) scheme \[10\].

Before applying the Padé summation, let us first examine the renormalization-scheme dependence of \( R(\mu) \). Up to \( O(g^5) \) for the \( \beta \)-function, the scheme dependence is equivalent to the renormalization-scale dependence \[11\]. The solid line with ‘pert.’ in Fig.2 shows \( R(\mu) \) for \( n_f = 4 \) as a function of \( \mu \) at \( T = 250 \text{ MeV} \). This temperature is rather low but is still 1.7 times larger than \( T_c \). In Fig.2, \( R(\mu) \) shows a sizable \( \mu \) dependence and even becomes unstable (negative pressure) for low \( \mu \). \( R(\mu) \) keeps this substantial \( \mu \)-dependence unless \( T \) is extremely large.

The principle of minimum sensitivity (PMS) criterion \[11\] does not work in the above situation, since there is no solution of the stability condition \( dR(\mu)/d\mu = 0 \). The fastest convergence criterion (FAC) gives an unphysically large value \( \mu = 37.7\pi T \) (for \( n_f = 4 \) \[4\]). The criterion motivated by the Brodsky-Lepage-Mackengie (BLM) \[12\] suggests \( \mu = (0.95 \sim 4.4)\pi T \) but gives rise to a series reliable only for \( T > 2 \text{ GeV} \) \[4\]. Thus, any choice of \( \mu \) cannot solve the problem at hand, and we really need a summation of the series.

Perturbation series eq.(1) has two different features from that for high energy processes:

(i) Odd powers of \( \bar{g} \) appear.
(ii) There arises \( \ln \bar{g} \) in the coefficients. In fact, the coefficient \( f_4 \) depends linearly on \( \ln \bar{g} \).

Also, it is expected to appear at \( O(g^6) \) level \( [5] \).

Since the standard Padé approximants are based on the ratio of polynomials, (ii) is a new feature beyond the standard method in a strict sense. In this paper, we take a simple procedure that \( \ln \bar{g} \) is regarded as a part of the coefficients \( f_i \).

Let us write down the general form of the Padé approximants (PA’s)

\[
R^{[N/M]}(\mu) = \frac{1 + \sum_{n=1}^{N} c_n \bar{g}^n}{1 + \sum_{m=1}^{M} d_m \bar{g}^m}.
\]  

(2)

c_n and \( d_m \) are the functions of \( f_i \). Since we have 5 coefficients \( f_i \) (\( 1 \leq i \leq 5 \)), we can construct PA’s satisfying \( N + M \leq 5 \). For example, the highest PA’s are \([3/2], [2/3], [4/1]\) and \([1/4]\).

PA’s discussed above are the most “naive” Padé approximants (NPA’s). They have some unnatural feature from the physics point of view: NPA’s contain terms proportional to \( \bar{g} \) both in the numerator and the denominator. On the other hand, in eq.(1), we never have \( O(\bar{g}) \) term because of a trivial reason (the free energy has no external legs). Although NPA’s assure that their Tayler expansion by \( \bar{g} \) does not contain \( O(\bar{g}) \)-term by the condition \( c_1 = d_1 \), it is still unnatural that fictitious \( O(\bar{g}) \)-term play a crucial role to determine higher orders.

Therefore, one may also try alternative PA’s by assuming \( c_1 = d_1 = 0 \). In this “constrained” Padé Approximants (CPA’s), one can have PA’s one-step beyond, i.e. \( N + M \leq 6 \). For example, the highest CPA’s are \([4/2], [2/4] \) and \([3/3]\). It turns out that the coefficients \((c_i, d_i)\) in CPA’s are much simpler than those of NPA’s because of the condition \( c_1 = d_1 = 0 \). In particular, \((c_i, d_i)\) in NPA’s usually become complicated functions of \( \ln \bar{g} \), while they simple depend linearly on \( \ln \bar{g} \) in CPA’s.

Besides NPA’s and CPA’s, one can also start with the effective charge \( S(\mu) \equiv (R(\mu) - 1)/f_2 \). The corresponding PA’s for effective charge (EPA’s) read \( S^{[N/M]}(\mu) = \bar{g}^2 (1 + \sum_{n=1}^{N} c_n \bar{g}^n)/(1 + \sum_{m=1}^{M} d_m \bar{g}^m) \). In this case, \( N + M \leq 3 \) holds and highest PA’s are \([2/1]\) and \([1/2]\). However, one can show that \([2/1]-EPA \) and \([1/2]-EPA \) are equivalent to \([4/1]-NPA \) and \([3/2]-NPA \) respectively, so they are not independent from NPA.
We have tried all possible PA’s mentioned above and the following is a summary.

(a) \([3/2]-\text{NPA}, [2/3]-\text{NPA}, [4/2]-\text{CPA}, \) and \([2/4]-\text{CPA}\) give results qualitatively consistent with each other.

The solid (dashed) lines in Fig.2 show the \(\mu\) dependence of CPA’s (NPA’s) at \(T = 250\) MeV. The renormalization-scale dependence is reduced substantially compared to the original series (the solid line with ‘pert.’). This is one of the justifications that the Padé approximants point to the right direction. Similar \(\mu\) independence has been reported on PA’s for the Bjorken sum rules at high \(Q^2\) [8]. In the latter case, the approximate invariance of PA’s under the Euler transform is a key to the weak scale-dependence [9]. The similar argument is expected to hold at finite \(T\).

(b) \([4/1]-\text{NPA}\) and \([1/4]-\text{NPA}\) turn out to develop a pole in the denominator at \(\alpha_s \sim 0.04\) and 0.06, respectively. \([3/3]-\text{CPA}\) also has poles at \(\alpha_s \sim 0.12\) and \(\sim 0.3\). Whether they have real physical meaning or are the artifact of the approximation is not known.

(c) Low-order PA’s, namely \(N + M \leq 4\) for NPA’s, \(N + M \leq 5\) for CPA’s and \(N + M \leq 2\) for EPA’s, do not properly ‘postdict’ the existence of \(\ln \bar{g}\) in \(f_4\) or the absence of \(\ln \bar{g}\) in \(f_5\). This implies that every known information of \(f_i (i \leq 5)\) is required to construct proper PA’s.

Let us now focus on the successful cases in item (a) above. Because of the small \(\mu\) dependence of PA’s in (a), the choice of \(\mu\) is not a serious problem anymore as far as \(\mu > 1\text{GeV}\) for \(T > 250\text{MeV}\). The BLM scheme, which requires the leading \(n_f\) dependence to vanish, gives \(\mu \simeq 4.4\pi T\) (\(\mu \simeq \pi T\)) when it is applied to the coefficient \(f_4\) (\(f_5\)). Based on these observations together with the fact that \(2\pi T\) is the lowest non-zero Matsubara frequency for gluons, we adopt \(\mu = 2\pi T\) as a typical renormalization scale. To see the quantitative prediction of the Padé summation, we plot, in Fig.3, four different PA’s for \(R\) as a function of \(\alpha_s\) with \(\mu = 2\pi T\). All four curves turn out to have similar trend:
First of all, they do not deviate more than 10% from the SB limit even at $T = 250$ MeV. This is in contrast to 60% deviation of $R$ in eq.(1) (see Fig.1(a)). One should however note that such a small deviation does not necessarily imply that the system can be approximated by non-interacting gas of quarks and gluons. There could be still strong interactions, but various effects tend to cancel for free energy.

Secondly, PA’s for the pressure ($P = -\frac{\text{free energy}}{V}$) in Fig. 3 show that overall attraction (repulsion) occurs at high (low) $T$ by the quark-gluon interactions.

To compare PA’s with the original series, we plot the result of $[4/2]$-CPA by the dashed line in Fig.1(a) as an example. This shows the above two aspects explicitly.

Our resummation is solely based on the perturbative coefficients calculated through $O(g^5)$ where the non-perturbative magnetic-mass of $O(g^2T)$ does not play a role. Therefore, prediction of PA’s in this paper could be substantially modified in the strong coupling (low $T$) regime. Nevertheless, it will be interesting to estimate the $O(\bar{g}^6)$ coefficient by our PA’s. The formulas become particularly simple for the cases $[3/2]$-CPA and $[2/3]$-CPA, in which $f_6 = f_4 f_5 / f_3$ and $f_6 = f_2^3 + f_3^2 + (f_4 - f_2^2) / f_3$ are obtained, respectively. In both cases, $f_6$ has a proper structure, namely $a + b \ln \bar{g}$, since only $f_4$ depends linearly on $\ln \bar{g}$. This Padé prediction will work only for a part of $f_6$ which is insensitive to the physics of $O(g^2T)$.

One should also note that we have not attempted to study the convergence property of PA’s. This is because low-order PA’s do not ‘postdict’ the known perturbative coefficients and thus do not capture the essential features of the full result as we mentioned.

In summary, we have examined Padé approximants of the free energy of hot QCD. Naive PA’s as well as constrained PA’s reduce the renormalization-scale dependence substantially even at temperature as low as 250 MeV. After the Padé summation, the free energy takes a value close to the SB limit even at 250 MeV. Similar analyses with finite chemical potential and finite quark masses, which are more relevant to the data in relativistic heavy-ion collisions, remain as future problems [13].

After the submission of this work, the author was informed about a recent paper treating NPA’s in QCD and $\phi^4$ theory (B. Kastening, hep-ph/9708219). CPA’s and EPA’s are not
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[13] The Padé approximants based on the perturbation series through $O(g^4)$ at finite chem-
ical potential (with zero temperature) as well as a generalization of the analyses in the present paper will be given in a separate publication: T. Hatsuda in preparation.
**Fig.1:** (a) Normalized free energy $R(2\pi T)$ as a function of the running coupling $\alpha_s(2\pi T)$.\[ O(g^l) (l = 2, 3, 4, 5) \text{ shows } R \text{ summed up to the } l\text{-th order. The dashed line is the result of } [4/2] \text{ Padé approximants.} \] (b) $\alpha_s(2\pi T)$ as a function of $T$ numerically calculated with the two-loop $\beta$-function.

**Fig.2:** Renormalization-scale dependence of the normalized free energy $R(\mu)$. The solid line with ‘pert.’ corresponds to the perturbative evaluation up to $O(g^5)$. Others are the results after Padé summation.

**Fig.3:** Padé approximants of $R(2\pi T)$ as a function of $\alpha_s(2\pi T)$. 
Fig. 1 (b)

α_s(2πT) vs. T (GeV)
Fig. 2

\[ R(\mu) \]

\[ \mu \text{ (GeV)} \]

- [3/2]
- [2/3]
- [2/4]
- [4/2]

pert.

\[ T = 250 \text{ MeV} \]
