Revisiting the semi-classical approximation at high temperature

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Background story

Topological susceptibility $\chi(T)$ in QCD at high T

Interesting for axion physics

- 20 May 2015, Andreas Ringwald (DESY Hamburg), Ultralight Axion-Like Particles from Strings
- 5 October 2016, Sandor Katz (Eotvos), Axion cosmology from lattice QCD
- 12 February 2020, Tamas G Kovacs (Eotvos), Instanton interactions in high temperature QCD

Talks at our own Wednesday seminar series

Background story

Calculation of $\chi(T)$

- $T < T_c$: definitely non-perturbative, mostly lattice

- $T \to \infty$: semi-classical, perturbative

Comparison of lattice calculations with something else?
Only at very high temperature and only with semi-classical results.

Background story

Comparison of lattice results and semi-classical results at high T

Should be straighforward: semi-classical results (should be) well-known, reliable lattice results are available starting from 2015

One just needs to plot the 2 results and see

Semi-classical result involves $T = 0$ input and at $T > T_c$ a peculiar formula

Everybody uses these without ever checking

Let's check these $\rightarrow$ straightforward BSc thesis topic

Surprises along the way ...

Goal

Let's derive the best semi-classical formula
for $\chi(T)$ using the known ingredients
so we can compare with continuum lattice results

Outline

- Yang-Mills theory and QCD at finite temperature

- Semi-classical approach, instantons

- $\chi(T)$ within semi-classical approach

- Surprise 1: over-all prefactor in QCD case ($N_f \neq 0$)

- Surprise 2: temperature dependence $\rightarrow$ numerical integrals

Yang-Mills and QCD at finite temperature

$SU(N)$ gauge fields (gluons) + fermions (quarks)

In QCD: $SU(3)$, $\psi = (u, d, s, c, \ldots)$

$$S = \frac{1}{2g^2} \int d^4x \, \mathrm{Tr}\, F_{\mu\nu} F_{\mu\nu} + \int d^4x \sum_i \bar{\psi}_i (D + m_i) \psi_i$$

Euclidean signature, finite temperature field theory: $S^1 \times R^3$
circumference of S^1: $1/T$

Phase transition or cross-over at $T = T_c$

Calculations at finite temperature

Strong coupling at $T < T_c$ so perturbative calculations not reliable $\longrightarrow$ mostly lattice

Weak coupling at $T \to \infty$, perturbative calculations, semi-classical methods reliable, can compare with lattice

Topological charge

$$Q = \frac{1}{16\pi^2} \int d^4x \varepsilon_{\mu\nu\rho\sigma} \mathrm{Tr}\, F_{\mu\nu} F_{\rho\sigma}$$

Integer if appropriate boundary conditions $\rightarrow$ topological charge

In path integral need to sum over all Q

$$Z = \sum_Q \int \mathscr{D}_Q A \mathscr{D}\bar{\psi} \mathscr{D}\psi e^{-S}$$

$$Z = \ldots Z_{-2} + Z_{-1} + Z_0 + Z_1 + Z_2 + \ldots = Z_0 + 2Z_1 + 2Z_2 + \ldots$$

$Q = 1$: 1-instanton, $Q = 2$: 2-instanton, ...

Ordinary perturbation theory: expansion in g in $Q = 0$ sector

Semi-classical method: perturbative expansion in $Q \neq 0$ sector + tunnellings

Remember: reliable at $T \to \infty$

Topological susceptibility

$$\chi = \frac{\langle Q^2 \rangle}{V} = \frac{2}{V} \frac{Z_1 + 4Z_2 + 9Z_3 + \ldots}{Z_0 + 2Z_1 + 2Z_2 + 2Z_3 + \ldots}$$

$V = L^3/T$ space-time volume

Topological susceptibility

There should be a semi-classical formula to
1-loop, 2-loop, 3-loop, ... for $\chi(T)$

Should be reliable unambiguous prediction of QCD at $T \to \infty$

Lattice results could be compared at high temperature

$$\chi(T) \sim \frac{1}{T^{\beta_1 - 4 + N_f}} = \frac{1}{T^{11/3N + 1/3N_f - 4}}$$

$$\beta_1 = \frac{11}{3}N - \frac{2}{3}N_f$$

Main question: **constant of proportionality**

All ingredients are text book material

We all learnt about instantons from Laci Palla when we were students

Should be straightforward exercise

Let’s do the straightforward exercise! $\longrightarrow$ BSc thesis topic

Expectation: everything already done

We just need to understand all details

Which is basically literature search and some calculations
if not all details included in papers $\longrightarrow$ ideal for BSc

Results from literature

$$\chi = \frac{\langle Q^2 \rangle}{V} = \frac{2}{V} \frac{Z_1 + 4Z_2 + 9Z_3 + \ldots}{Z_0 + 2Z_1 + 2Z_2 + 2Z_3 + \ldots} = \frac{2}{V}\frac{Z_1}{Z_0} + \ldots$$

Last ... are suppressed because 2-instanton, 3-instanton, etc. are suppressed by $e^{-\frac{8\pi^2}{g^2}|Q|}$

$$\chi(T) = \frac{2}{V}\frac{Z_1}{Z_0}$$

Need path integral over 1-instanton moduli space and 1-loop fluctuations around 1-instanton

Results from literature

$$\chi(T) = \frac{2}{V}\frac{Z_1}{Z_0}$$

Position of instanton x_μ arbitrary $\longrightarrow$ factor V in integral

Size ϱ of instanton $\longrightarrow$ remaining $d\varrho$ integral

$$\frac{Z_1}{Z_0} = V \int_0^\infty d\varrho\, n(\varrho, T)$$

$n(\varrho, T)$: size distribution of instantons at T

Results from literature

$$n(\varrho, T) = n(\varrho) e^{-S(\varrho, T)}$$

Size distribution at T expressed from size distribution $n(\varrho)$ at $T = 0$

T-dependence from $S(\varrho, T)$, dimensionless, depends on $\lambda = \pi \varrho T$

$\longrightarrow$ Need two ingredients: $T = 0$ results and $T > 0$ modifications

Results from literature

Zero temperature 1-loop with light fermions, $m_i/T, m_i/\Lambda \ll 1$

$$n(\varrho) = C \left(\frac{16\pi^2}{g^2(\mu)}\right)^{2N} e^{-\frac{8\pi^2}{g^2(\mu)}} \frac{1}{\varrho^5} (\varrho\mu)^{\beta_1} \prod_{i=1}^{N_f} (\varrho m_i(\mu))$$

$g(\mu)$ running coupling, $m_i(\mu)$ running masses

Over-all constant coefficient C **is scheme-dependent**, because renormalization is defined in a particular scheme

Frequently used schemes: Pauli-Villars, MS, $\overline{\text{MS}}$, etc.

Results from literature $T = 0$

$$n(\varrho) = C \left(\frac{16\pi^2}{g^2(\mu)}\right)^{2N} e^{-\frac{8\pi^2}{g^2(\mu)}} \frac{1}{\varrho^5} (\varrho\mu)^{\beta_1} \prod_{i=1}^{N_f} (\varrho m_i(\mu))$$

Result for C in Pauli-Villars and $SU(2)$:

G. t Hooft, Phys. Rev. D 14, 3432 (1976)

Unfortunately C incorrect, but only trivial mistake (factors of π), corrected later in erratum

Erratum: [Phys. Rev. D 18, 2199 (1978)]

Pauli-Villars $SU(2)$ result correct

Results from literature $T = 0$

$$n(\varrho) = C \left(\frac{16\pi^2}{g^2(\mu)}\right)^{2N} e^{-\frac{8\pi^2}{g^2(\mu)}} \frac{1}{\varrho^5} (\varrho\mu)^{\beta_1} \prod_{i=1}^{N_f} (\varrho m_i(\mu))$$

Result for C in Pauli-Villars and $SU(N)$

C. W. Bernard, Phys. Rev. D 19, 3013 (1979).

General $SU(N)$ in Pauli-Villars correct

Results from literature $T = 0$

$$n(\varrho) = C \left(\frac{16\pi^2}{g^2(\mu)}\right)^{2N} e^{-\frac{8\pi^2}{g^2(\mu)}} \frac{1}{\varrho^5} (\varrho\mu)^{\beta_1} \prod_{i=1}^{N_f} (\varrho m_i(\mu))$$

More frequently used schemes: MS and $\overline{\text{MS}}$

Need to convert C to these schemes

$$C_1 = C_2 \left(\frac{\Lambda_2}{\Lambda_1}\right)^{\beta_1}$$

Need to know Λ-parameter ratios

Results from literature $T = 0$

Needed: $\Lambda_{PV}/\Lambda_{\mathrm{MS}}$, first given in original

G. t Hooft, Phys. Rev. D 14, 3432 (1976)

Unfortunately incorrect (not in Erratum either...)

Correct result

$$\frac{\Lambda_{\mathrm{PV}}}{\Lambda_{\mathrm{MS}}} = e^{\frac{1}{2}(\log(4\pi)-\gamma)+\frac{1}{22}}$$

A. Hasenfratz and P. Hasenfratz, Phys. Lett. 93B, 165 (1980)

Confirmed in G. t Hooft, Phys. Rept. 142, 357 (1986)

Results from literature $T = 0$

Note: incorrect Λ-parameter ratios in

P. Weisz, Phys. Lett. 100B, 331 (1981)

R. F. Dashen and D. J. Gross, Phys. Rev. D 23, 2340 (1981)

Results from literature $T = 0$

In any case, MS result correct since Hasenfratz-Hasenfratz 1980

Most frequently used: $\overline{\text{MS}}$

Conversion MS $\to$ $\overline{\text{MS}}$ should be straightforward

$$\frac{\Lambda_{\overline{\text{MS}}}}{\Lambda_{\text{MS}}} = e^{\frac{1}{2}(\log(4\pi)-\gamma)} \qquad \frac{\Lambda_{\text{PV}}}{\Lambda_{\overline{\text{MS}}}} = e^{\frac{1}{22}}$$

W. A. Bardeen, A. J. Buras, D. W. Duke and T. Muta, Phys. Rev. D 18, 3998 (1978)

And we have seen

$$C_1 = C_2 \left(\frac{\Lambda_2}{\Lambda_1}\right)^{\beta_1}$$

Results from literature $T = 0$

Explicitly reported in $\overline{\text{MS}}$

A. Ringwald and F. Schrempp, Phys. Lett. B 438, 217 (1998) [hep-ph/9806528]

Unfortunately incorrect, never corrected before

$$C = \frac{e^{c_0 + c_1 N + c_2 N_f}}{(N-1)!(N-2)!}$$

c_0 and c_1 correct, but c_2 reported incorrectly

Problem: MS $\to \overline{\text{MS}}$ conversion involves β_1 which depends on N_f, conversion used pure Yang-Mills β_1: c_2 incorrect

Mismatch: $\frac{1}{33} = \frac{2}{3} \cdot \frac{1}{22}$ where $\frac{2}{3}$ from N_f-dependence of β-function, $\frac{1}{22}$ from MS-$\overline{\text{MS}}$ Λ-parameter ratio

Results from literature $T = 0$

Wrong $\overline{\text{MS}}$ results used in all lattice - semi-classical comparisons

Furthermore, another wrong c_2 reported in

S. Moch, A. Ringwald and F. Schrempp, Nucl. Phys. B 507, 134 (1997) [hep-ph/9609445]

I. I. Balitsky and V. M. Braun, Phys. Rev. D 47, 1879 (1993)

First correct $\overline{\text{MS}}$ result

$$C_{\overline{\text{MS}}} = \frac{e^{c_0 + c_1 N + c_2 N_f}}{(N-1)!(N-2)!}$$

$$\begin{aligned}
c_0 &= \frac{5}{6} + \log 2 - 2\log\pi && = -0.76297926 \\
c_1 &= 4\zeta'(-1) + \frac{11}{36} - \frac{11}{3}\log 2 && = -2.89766868 \\
c_2 &= -4\zeta'(-1) - \frac{67}{396} - \frac{1}{3}\log 2 && = 0.26144360
\end{aligned}$$

Ringwald-Schrempp: $c_2 = 0.291746$

Moch-Ringwald-Schrempp, Balitsky-Braun: $c_2 = 0.153$

First correct $\overline{\text{MS}}$ result

$$n(\varrho) = C_{\overline{\text{MS}}} \left(\frac{16\pi^2}{g^2(\mu)}\right)^{2N} e^{-\frac{8\pi^2}{g^2(\mu)}} \frac{1}{\varrho^5} (\varrho\mu)^{\beta_1} \prod_{i=1}^{N_f} (\varrho m_i(\mu))$$

Finally $T = 0$ instanton size distribution in $\overline{\text{MS}}$ at 1-loop

Once $C_{\overline{\text{MS}}}$ okay, (partial) 2-loop result from literature can be taken over

Results in literature $T > 0$

$$n(\varrho, T) = n(\varrho) e^{-S(\lambda)} \qquad\qquad \lambda = \pi \varrho T$$

$$S(\lambda) = \frac{1}{3}\lambda^2(2N + N_f) + 12A(\lambda)\left(1 + \frac{N - N_f}{6}\right)$$

D. J. Gross, R. D. Pisarski and L. G. Yaffe, Rev. Mod. Phys. 53, 43 (1981)

$$12A(\lambda) = \frac{1}{16\pi^2}\left[\int_{S^1\times R^3}\left(\frac{\partial_\mu \Pi \partial_\mu \Pi}{\Pi^2}\right)^2 - \int_{R^4}\left(\frac{\partial_\mu \Pi_0 \partial_\mu \Pi_0}{\Pi_0^2}\right)^2\right]$$

Results in literature $T > 0$

$$12A(\lambda) = \frac{1}{16\pi^2}\left[\int_{S^1\times R^3}\left(\frac{\partial_\mu \Pi \partial_\mu \Pi}{\Pi^2}\right)^2 - \int_{R^4}\left(\frac{\partial_\mu \Pi_0 \partial_\mu \Pi_0}{\Pi_0^2}\right)^2\right]$$

Where Π_0 from 1-insanton solution on R^4 and Π is from Harrington-Sheppard 1-instanton solution on $S^1 \times R^3$

$$\begin{aligned}
\Pi_0(t,r) &= 1 + \frac{\varrho^2}{t^2 + r^2} \\
\Pi(\tau,r) &= 1 + \sum_{n=-\infty}^{\infty}\left(\Pi_0\left(\tau + \frac{n}{T}, r\right) - 1\right) = \\
&= 1 + \frac{\pi\varrho^2 T}{r}\frac{\sinh(2\pi r T)}{\cosh(2\pi r T) - \cos(2\pi\tau T)}
\end{aligned}$$

$-\infty < t < \infty$ and τ periodic, $A(0) = 0$ from subtraction

Results in literature $T > 0$

Because of spherical symmetry, $A(\lambda)$ is a 2-dimensional integral and $A(0) = 0$

Analytically not possible, numerical form from Gross-Pisarski-Yaffe:

$$12A_{GPY}(\lambda) = -\log\left(1 + \frac{\lambda^2}{3}\right) + \frac{12\alpha}{\left(1 + \gamma\lambda^{-3/2}\right)^8}$$

$$\alpha = 0.01289764 \qquad\qquad \gamma = 0.15858$$

Claimed absolute numerical uncertainty: $6 \cdot 10^{-4}$

Once $A(\lambda)$ is known, the full $\chi(T)$ is known semi-classically

Above A_{GPY} used in **all** works

Why the specific form? Why the powers 3/2 and 8?

New results for $A(\lambda)$

Main motivation was to understand the peculiar form of $A(\lambda)$

In Gross-Pisarski-Yaffe no details are given

Technically: difference of two 2D integrals, both are divergent, difference finite

We do three things:

- Evaluate numerically to high precision
- Obtain analytic $\lambda \ll 1$ and $\lambda \gg 1$ series
- Fit numerical result with simple function

New results for $A(\lambda)$

Evaluate numerically to high precision

$$12A(\lambda) = \frac{1}{16\pi^2}\left[\int_{S^1\times R^3}\left(\frac{\partial_\mu \Pi \partial_\mu \Pi}{\Pi^2}\right)^2 - \int_{R^4}\left(\frac{\partial_\mu \Pi_0 \partial_\mu \Pi_0}{\Pi_0^2}\right)^2\right]$$

$$\begin{aligned}
\Pi_0(t,r) &= 1 + \frac{\varrho^2}{t^2+r^2} \\
\Pi(\tau,r) &= 1 + \sum_{n=-\infty}^{\infty}\left(\Pi_0\left(\tau + \frac{n}{T}, r\right) - 1\right) = \\
&= 1 + \frac{\pi\varrho^2 T}{r}\frac{\sinh(2\pi r T)}{\cosh(2\pi r T) - \cos(2\pi\tau T)}
\end{aligned}$$

New results for $A(\lambda)$

In first term, do integral over S^1 via residue theorem, rescale r by $1/(2\pi T)$

In second term, do integral over $-\infty < t < \infty$, rescale r by ϱ

$$12A(\lambda) = \frac{1}{2} \int_0^\infty dr\, r^2 \, (I(r) - I_0(r))$$

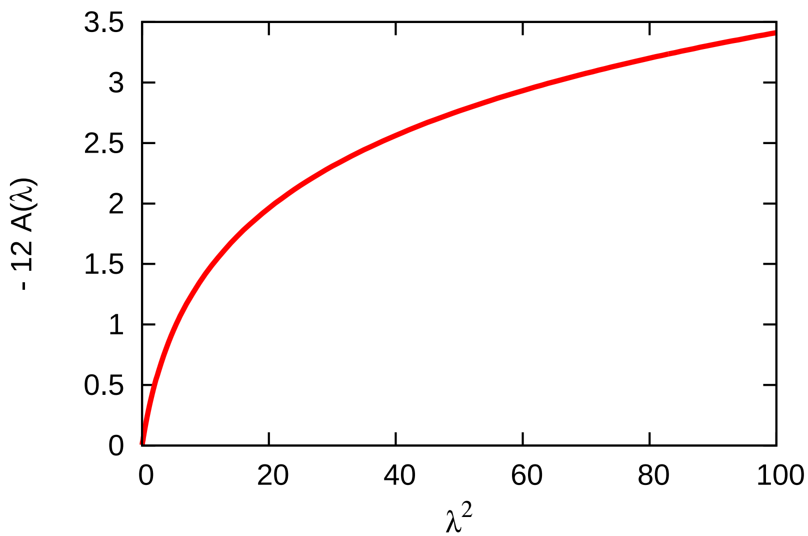
$I(r)$ and $I_0(r)$ analytically

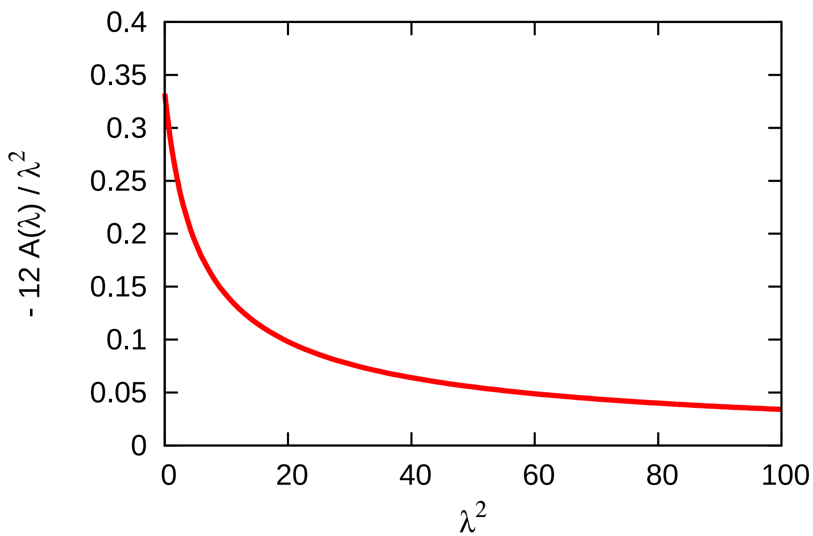
r-integrals separately divergent, difference finite

New results for $A(\lambda)$

Numerical evaluation of r-integrals: trapezoid or Simpsons on $(0, 8)$, semi-analytic or $(8, \infty)$ $\rightarrow$ absolute precision $O(10^{-6})$

Essential: $O(100)$ significant digits because of large cancellations between $I(r)$ and $I_0(r)$ and also inside $I(r)$ for small λ





New results for $A(\lambda)$ - asymptotics

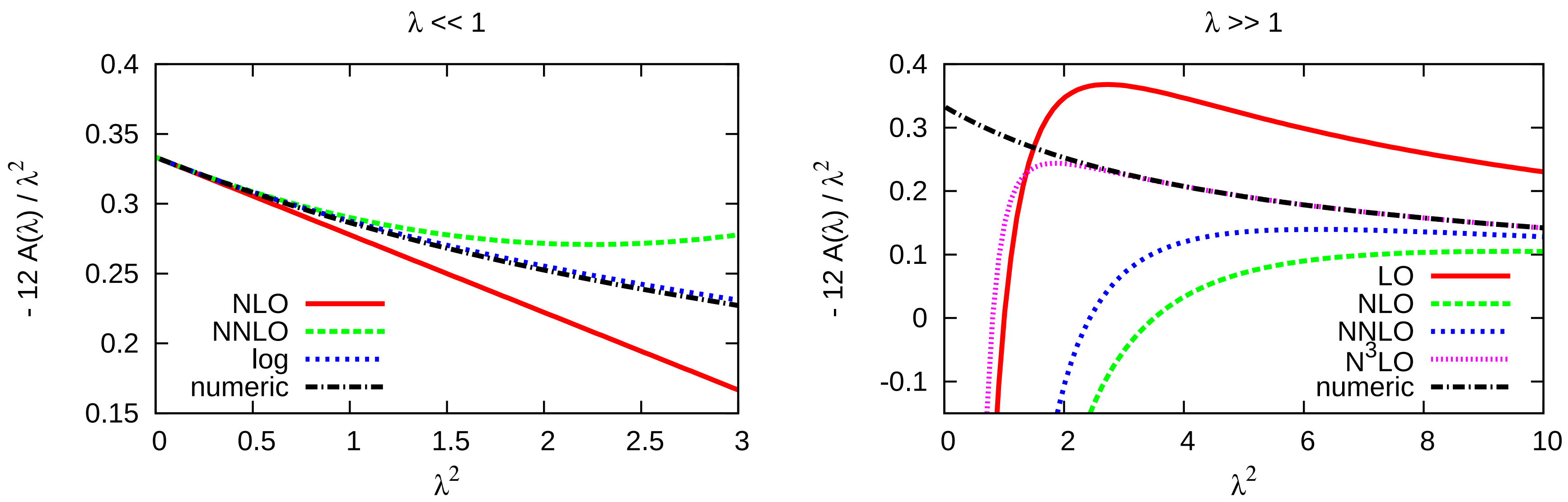
Small λ asymptotics - log still a bit mysterious

$$12A(\lambda) = -\frac{1}{3}\lambda^2 + \frac{1}{18}\lambda^4 - \frac{1}{81}\lambda^6 + O(\lambda^7) = -\log\left(1 + \frac{\lambda^2}{3}\right) + O(\lambda^7)$$

Large λ asymptotics

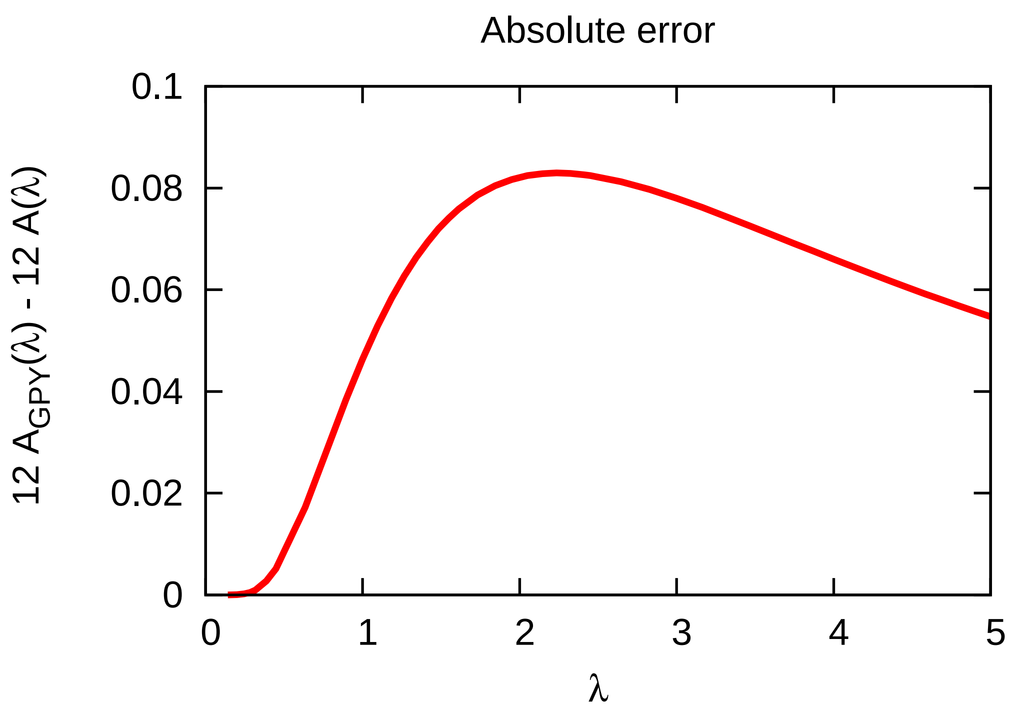
$$\begin{aligned} 12A(\lambda) &= -\log(\lambda^2) + C_1 - \frac{\log(\lambda^2)}{\lambda^2} - \frac{C_2}{\lambda^2} + O\left(\frac{1}{\lambda^3}\right) \\ C_1 &= 2\left(\frac{1}{3} - \frac{\pi^2}{36} - \gamma + \log\pi\right) = 1.25338375 \\ C_2 &= 1 + \log 2 + \frac{\pi^2}{36} + \gamma - \log\pi = 1.39978864 \end{aligned}$$

New results for $A(\lambda)$ - asymptotics



These look good - let's compare with Gross-Pisarski-Yaffe

New results for $A(\lambda)$ - comparison with GPY



$8 \cdot 10^{-2}$, two orders of magnitude worse than claimed

GPY: 2D integral numerically

New results for $A(\lambda)$ - useful parametrization

$$-12A_{param}(\lambda) = p_0 \log(1 + p_1\lambda^2 + p_2\lambda^4 + p_3\lambda^6 + p_4\lambda^8)$$

$$p_0 = 0.247153244, \quad p_1 = 1.356391323$$

$$p_2 = 0.675021523, \quad p_3 = 0.145446632, \quad p_4 = 0.008359667$$

Absolute precision $2 \cdot 10^{-4}$

Biggest deviation from GPY: $\lambda = O(1)$ because of large cancellations inside $I(r)$ $\rightarrow$ the most sensitive region for ϱ-integral in $\chi(T)$ $\rightarrow$ potentially large effect

Absolute and relative precision

Absolute precision on $A(\lambda) \rightarrow$

Relative precision on $n(\varrho, T) \sim e^{-12A(\lambda)\left(1+\frac{N-N_f}{6}\right)} \rightarrow$

Relative precision on $\chi(T)$

Discrepancy A_{GPY} vs. our A_{param} in $\chi(T)$:

- $SU(3)$ $N_f = 0, 2, 3, 4$: 10%, 7%, 6%, 4%
- $SU(10)$ pure Yang-Mills: 22%
- $SU(20)$ pure Yang-Mills: 40% (scales with N)

Accounting for $T = 0$ and $T > 0$ discrepancies in QCD

$T = 0$ from $C_{\overline{\mathsf{MS}}}$: approx 5% (correct smaller)

$T > 0$ from $A(\lambda)$: approx 5% (correct larger)

But in opposite directions ... nearly cancel

Eventually very small effect in QCD

But at least now the semi-classical result is fully correct

Actual comparison at high temperature

$SU(3)$ pure Yang-Mills at $T/T_c = 4.1$

Lattice (continuum): $\log\left(\frac{\chi(T)}{T_c^4}\right) = 12.47(21)$ from 1806.01162

Semi-classical: $\log\left(\frac{\chi(T)}{T_c^4}\right) = 13.80(10)(40)$

Using 5-loop running, 2-loop χ. First error: residual μ-dependence, second (dominant) error: $T_c/\Lambda_{\overline{\mathrm{MS}}}$ error (from lattice)

Within 3σ

Actual comparison at high temperature in QCD (4 flavors) at $T = 2000\, MeV$

PDG: $\Lambda_{\overline{\mathsf{MS}}} = 292(16)\, MeV$ approx 5% error

Lattice (continuum): $\log\left(\frac{\chi(T)}{MeV^4}\right) = 3.99(68)$
from S. Borsanyi et al., Nature 539, no. 7627, 69 (2016) [arXiv:1606.07494 [hep-lat]]

Semi-classical: $\log\left(\frac{\chi(T)}{MeV^4}\right) = 1.15(3)(46)$

Within 3.5σ

For higher temperature, deviation decreasing

For better agreement: higher loop $\chi(T) \rightarrow$ difficult

Summary

- Obtained $n(\varrho, T)$ at high temperature semi-classically
- Needed to correct $T = 0$ results in literature
- Needed to correct $T > 0$ 1-loop fluctuation determinant
- Correctly include experimental error on $\Lambda_{\overline{\mathrm{MS}}}$
- Makes $\chi(T)$ comparison with lattice possible
- Exactly **zero** new or original idea :)
- Nevertheless interesting outcome from simple BSc thesis topic

Thank you for your attention!