Finite Temperature Sum Rules in Lattice Gauge Theory

Harvey B. Meyer
Center for Theoretical Physics
Massachusetts Institute of Technology
Cambridge, MA 02139, U.S.A.
meyerh@mit.edu

Abstract
We derive non-perturbative sum rules in SU(N) lattice gauge theory at finite temperature. They relate the susceptibilities of the trace anomaly and energy-momentum tensor to temperature derivatives of the thermodynamic potentials. Two of them have been derived previously in the continuum and one is new. In all cases, at finite lattice spacing there are important corrections to the continuum sum rules that are only suppressed by the bare coupling $g_0^2$. We also show how the discretization errors affecting the thermodynamic potentials can be controlled by computing these susceptibilities.
1 Introduction

Sum rules in continuum QCD at zero temperature were introduced by Novikov et al. \[1\] and a lot of hadron phenomenology was subsequently based on them. A few years later Michael derived sum rules for SU(\(N\)) pure gauge theories in lattice regularization \[2, 3, 4\], which were only recently generalized to Wilson lattice QCD in \[5\]. Since sum rules are relations that hold non-perturbatively, the lattice regularization provides a framework in which their derivation proceeds in a particularly rigorous way: it only involves operations on multi-dimensional integrals.

On the lattice the simplest identities relate zero-momentum three-point functions to the spectrum of the theory. By comparing the sum rules to continuum relations \[6\], one realizes \[7, 8\] that they relate the normalization of a particular discretization of the trace anomaly and the energy-momentum tensor to anisotropy coefficients. The latter are derivatives of the bare lattice parameters with respect to physical parameters such as the lattice spacing in hadronic units or the ratio of spatial and temporal lattice spacings. Indeed this normalization is non-trivial since translation invariance is broken down to a discrete group at finite lattice spacing.

Ellis et al. derived finite-temperature sum rules in pure gauge theories \[9\] and in full QCD \[10\]. In this paper we rederive the SU(\(N\)) gauge theory sum rules, focusing on those concerning two-point functions of the trace anomaly and the energy-momentum tensor, in lattice regularization. We find that they have important corrections to the continuum versions, which are only suppressed by one power of the bare coupling \(g_0^2\). From the point of view of Monte-Carlo simulations, where thermodynamics calculations are performed around \(g_0 \approx 1\), they can thus not be neglected. We also derive a new sum rule involving only the traceless part of the energy-momentum tensor, and we relate the results obtained to contact terms in the two-point functions of the Hamiltonian.

The \(p = 0\) two-point function of the trace anomaly, in other words its susceptibility, is related to the rate of change of \((\epsilon - 3P)/T^4\) with temperature \[9\] (\(\epsilon\) is the energy density and \(P\) the pressure). Because the bulk viscosity is related to this two-point function by a Kubo formula \[11\], it was argued recently \[12\] that the bulk viscosity rises sharply just above the deconfining temperature \(T_c\). Direct calculations of the two-point functions at \(p = 0\) and general \(\omega = p_0\) have confirmed the existence of this effect \[13\]. In the context of such calculations, the sum rule can be used to constrain the reconstruction of the spectral function \(\rho(\omega)\).

Another application of these considerations to finite-temperature Monte Carlo simulations is to compute directly the leading lattice spacing dependence of the thermodynamic potentials. This idea has the most potential of being useful in the context of full QCD simulations, where the computational cost is high and grows with a large power of the inverse lattice spacing.

Decomposing the energy-momentum tensor \(T_{\mu\nu}\) into a traceless part \(\theta_{\mu\nu}\) and a scalar part \(\theta\) via \(T_{\mu\nu} = \theta_{\mu\nu} + \frac{1}{4}\delta_{\mu\nu}\theta\), the explicit Euclidean expressions are

\[
\theta(x) \equiv \beta(g)/(2g) F_{\rho\sigma}(x) F_{\rho\sigma}(x) \quad \quad \theta_{\mu\nu}(x) \equiv \frac{1}{4} \delta_{\mu\nu} F_{\rho\sigma}^a F_{\rho\sigma}^a - F_{\mu\alpha}^a F_{\nu\alpha}^a.
\] (1)

The beta-function is defined by \(q d\bar{g}/dq = \beta(g) = -\bar{g}^3(b_0 + b_1 \bar{g}^2 + \ldots)\) and \(b_0 = 11N/(3(4\pi)^2), b_1 = 34N^2/(3(4\pi)^4)\) in the SU(\(N\)) pure gauge theory. The gauge action reads \(\frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a\) in
this notation. If $(\ldots)_T$ denotes the thermal average at temperature $T$,
\[
\epsilon - 3P = (\theta)_T - (\theta)_0, \quad \epsilon + P = \frac{4}{3}(\theta_{00})_T.
\] (2)

In section 2 we introduce our notation, review the relations relevant to thermodynamics and introduce new anisotropy coefficients. In section 3 we derive the sum rules on the lattice. In section 4 we take the extreme continuum limit, $g_0^2 \ll 1$ and compare our results to those of [9]. Section 5 describes the possibility of computing the leading discretization errors affecting $\epsilon$ and $P$ in numerical simulations, and section 6 contains concluding remarks.

2 Thermodynamics and the energy-momentum tensor

We consider a Euclidean lattice of spatial extent $N_\sigma$ sufficiently large that the thermodynamics limit has been reached. The time-extent $N_\tau = L_0/a$ fixes the temperature $T = 1/L_0$. Thermal averages are denoted by $\langle \ldots \rangle$. The temperature dependence is made explicit by $\langle \ldots \rangle_T$ to distinguish this average from the average $\langle \ldots \rangle_0$ on a zero-temperature lattice.

The contents of this section is mostly a review of the early lattice thermodynamics articles [14, 15], with the exception of subsection 2.4. We however emphasize a lot more the role of $\theta_{00}$ and $\theta$, since they are the operators of interest in the sum rules.

2.1 Isotropic lattice

We start from the Wilson action [18] for SU($N$) gauge theories:
\[
S_g = \beta \sum_x \sum_{\mu<\nu} S_{\mu\nu}(x),
\] (3)
\[
S_{\mu\nu}(x) = \frac{1}{N} \text{Re Tr} \left\{ 1 - U_{\mu}(x)U_{\nu}(x + a\hat{\mu})U^{-1}_{\mu}(x + a\hat{\nu})U^{-1}_{\nu}(x) \right\}
\] (4)
and $\beta \equiv \frac{2N}{g_0^2}$. It is useful to consider two separate sets of parameters:

bare parameters: \quad $\beta$, $N_\tau$

physical parameters: \quad $a(\beta)$, $T(\beta, N_\tau)$

where $1/T = L_0 = N_\tau a(\beta)$. With the notations
\[
S_\pm = S_\sigma \pm S_\tau, \quad S_\sigma = \sum_{k<l} S_{kl}, \quad S_\tau = \sum_k S_{0k},
\] (7)
we use the following discretizations:
\[
\Theta(x) = Z^+(\beta) \ S_+, \quad \Theta_{00}(x) = Z^- (\beta) \ S_-, \quad (8)
\]
with
\[
Z^+(\beta) = \frac{d\beta}{d\log a}, \quad Z^- (\beta) = \beta Z(\beta).
\] (9)

The presence of the normalization factor $Z(\beta) = 1 + O(1/\beta)$ must be expected, since $\int d^3x \theta_{00}(x)$ is not a Noether charge, due to the lack of continuous translation invariance on the lattice. A precise expression can be given for $Z(\beta)$ in terms of derivatives with respect
to the anisotropy, see Eq. 29 and also Eq. 58. For a parametrization of $Z(\beta)$ in the case of SU(3) based on the data of [17], see [16] (Eq. 6). The continuum limit takes the form

$$F_+(\beta, N_\tau) \equiv N_\tau^4((\Theta)_T - \langle \Theta \rangle_0) \xrightarrow{a \to 0} \frac{\epsilon - 3P}{T^4} \equiv f_+(T)$$

$$F_-(\beta, N_\tau) \equiv \frac{4}{3} N_\tau^4\langle \Theta_{00} \rangle \xrightarrow{a \to 0} \frac{\epsilon + P}{T^4} \equiv f_-(T),$$

where the leading corrections are $O(a^2)$.

### 2.2 Anisotropic lattice

On the anisotropic lattice with spatial lattice spacing $a_\sigma$ and temporal lattice spacing $a_\tau$, the action reads

$$S_g = \sum_x \beta_\sigma S_\sigma(x) + \beta_\tau S_\tau(x).$$

(12)

The two separate sets of parameters are:

bare parameters: $\beta_\sigma, \beta_\tau, N_\tau$

(13)

physical parameters: $a_\sigma(\beta_\sigma, \beta_\tau), \xi(\beta_\sigma, \beta_\tau), T(\beta_\sigma, \beta_\tau, N_\tau)$

(14)

where

$$\xi \equiv a_\sigma/a_\tau$$

$$1/T = L_0 = N_\tau a_\tau = N_\tau a_\sigma \xi^{-1}.$$ (15)

Obviously, $\xi = 1$ when $\beta_\sigma = \beta_\tau$.

We use the following discretizations:

$$\xi^{-3} \Theta(x) = Z^+_{\sigma}(\beta_\sigma, \beta_\tau)S_\sigma + Z^+_{\tau}(\beta_\sigma, \beta_\tau)S_\tau,$$

(17)

$$\xi^{-3} \Theta_{00}(x) = Z^-_{\sigma}(\beta_\sigma, \beta_\tau)S_\sigma - Z^-_{\tau}(\beta_\sigma, \beta_\tau)S_\tau,$$

(18)

where at the symmetric point $\xi = 1$,

$$Z^+_{\sigma}(\beta, \beta) = Z^+_{\tau}(\beta, \beta) = Z^+(\beta), \quad Z^-_{\sigma}(\beta, \beta) = Z^-_{\tau}(\beta, \beta) = Z^-(\beta).$$

(19)

The continuum limit $a_\sigma \to 0$ is taken at fixed $\xi$. The factor $Z^\pm_{\sigma, \tau}$ are such that, for instance, $\langle \sum_x \Theta_{00}(x) \rangle \to \langle \int d^4x \theta_{00}(x) \rangle$. The continuum limit of thermodynamic potentials is obtained according to

$$F_+(\beta_\sigma, \beta_\tau, N_\tau) \equiv N_\tau^4\xi^{-3}((\Theta)_T - \langle \Theta \rangle_0) \xrightarrow{a_\sigma \to 0} \frac{\epsilon - 3P}{T^4} \equiv f_+(T)$$

$$F_-(\beta_\sigma, \beta_\tau, N_\tau) \equiv \frac{4}{3} N_\tau^4\xi^{-3}\langle \Theta_{00} \rangle \xrightarrow{a \to 0} \frac{\epsilon + P}{T^4} \equiv f_-(T),$$

(21)

where the leading corrections are $O(a^2_\sigma)$.
2.3 Thermodynamics and normalization of θ and θ

In this section we relate the normalization factors $Z^\pm$ to derivatives of the bare parameters with respect to physical parameters. We start from the thermodynamic relations

$$\epsilon = -\frac{1}{3} \frac{\partial \log Z}{\partial L}, \quad p = \frac{1}{L^3} \frac{\partial \log Z}{\partial L}$$

(22)

where

$$\log Z(\beta_\sigma, \beta_\tau, N_\sigma, N_\tau) = \log Z(\beta_\sigma, \beta_\tau, N_\sigma, N_\tau) - \frac{N_\tau}{N_\tau^{\text{ref}}} \log Z(\beta_\sigma, \beta_\tau, N_\sigma, N_\tau^{\text{ref}}).$$

(23)

The subtraction, which sets the free energy $F = -T \log Z$ to zero at a reference temperature $T_\text{ref} = 1/(N_\tau^{\text{ref}} a_\tau)$, is necessary in quantum field theory. On a $\xi = 1$ lattice a common choice is $N_\tau^{\text{ref}} = N_\sigma$, which implies that $T_\text{ref} = 0$ in the thermodynamic limit. We can combine the equations

$$\frac{\partial \log Z}{\partial \log a_\sigma} = 0 \quad \text{and} \quad \frac{\partial \log Z}{\partial \log \xi} = 0$$

into

$$(\epsilon - 3P)a^3_{\sigma, \tau} = \frac{\partial \beta_\sigma}{\partial \log a_\sigma} \langle S_\sigma \rangle_{T=0} + \frac{\partial \beta_\tau}{\partial \log a_\sigma} \langle S_\tau \rangle_{T=0}$$

(24)

$$\frac{\xi^3 (\epsilon + P) a^3_{\sigma, \tau}}{4} = -\left( \frac{\partial \beta_\sigma}{\partial \log \xi} + \frac{1}{4 \partial \log a_\sigma} \right) \langle S_\sigma \rangle - \left( \frac{\partial \beta_\tau}{\partial \log \xi} + \frac{1}{4 \partial \log a_\sigma} \right) \langle S_\tau \rangle$$

(25)

From here we read off the normalization factors of $\Theta$ and $\Theta_{00}$:

$$\xi^3 Z^+ = \frac{\partial \beta_\sigma}{\partial \log a_\sigma}, \quad \xi^3 Z^+ = \frac{\partial \beta_\tau}{\partial \log a_\sigma},$$

(26)

$$\xi^3 Z^- = -\frac{\partial \beta_\sigma}{\partial \log \xi} - \frac{1}{4 \partial \log a_\sigma}, \quad \xi^3 Z^- = \frac{\partial \beta_\tau}{\partial \log \xi} + \frac{1}{4 \partial \log a_\sigma}.$$ 

(27)

Since, by Euclidean symmetry, $Z^-_{\sigma, \tau} = Z^+_{\tau, \sigma}$, we have the equalities

$$\frac{\partial (\beta_\sigma + \beta_\tau)}{\partial \log \xi} \equiv \frac{1}{2 \partial \log a}$$

(28)

$$\frac{\partial (\beta_\tau - \beta_\sigma)(a_\sigma, \xi)}{\partial \log \xi} \equiv 2 \beta Z(\beta).$$

(29)

We discuss a different choice of bare parameters often used in numerical simulations in appendix A.

2.4 Derivatives of $Z^\pm_{\sigma, \tau}$ at $\xi = 1$

At $\xi = 1$, $(\partial \beta_\sigma + \partial \beta_\tau)$ becomes $d/d\beta$. Using

$$\left( \frac{\partial \log a_\sigma}{\partial \log \xi}, \frac{\partial \log a_\sigma}{\partial \beta_\sigma}, \frac{\partial \log a_\tau}{\partial \beta_\sigma} \right) \xi \equiv \frac{1}{2 \beta Z(\beta)} \left( \frac{\partial \beta_\sigma}{\partial \log a_\sigma}, \frac{\partial \beta_\tau}{\partial \log a_\sigma}, \frac{\partial \beta_\sigma}{\partial \log a_\sigma} \right).$$

(30)
one easily obtains the relations
\[
\frac{1}{2} \left( \frac{\partial}{\partial \beta_\sigma} - \frac{\partial}{\partial \beta_\tau} \right) (Z_\sigma^+ + Z_\tau^+) \xi = 1 = 3 \frac{d\beta}{d\log a} \frac{1}{\beta Z(\beta)},
\]
\[
\frac{1}{2} \left( \frac{\partial}{\partial \beta_\sigma} - \frac{\partial}{\partial \beta_\tau} \right) (Z_\sigma^+ - Z_\tau^+) \xi = 1 \frac{d\beta}{d\log a} \frac{\partial(\beta Z(\beta))}{\beta Z(\beta)}.
\]
(31)

We shall need these relations in the next section. Similarly we introduce the quantities
\[
\lambda_{00}^+(\beta_\sigma, \beta_\tau) \equiv \frac{1}{2} \left( \frac{\partial}{\partial \beta_\sigma} - \frac{\partial}{\partial \beta_\tau} \right) (Z_\sigma^+ - Z_\tau^+).
\]
(32)

At $\xi = 1$ they evaluate to
\[
\lambda_{00}^+(\beta) = 3 - \frac{1}{2} \frac{d\beta}{d\log a} \left[ \frac{1}{\beta} + \frac{dZ}{Zd\beta} \right] + \frac{1}{2} \frac{d^2(\beta_\sigma - \beta_\tau)}{d(\log \xi)^2},
\]
(33)

\[
\beta Z(\beta) \lambda_{00}^-(\beta) = \frac{1}{2} \left[ - \frac{1}{8} \frac{d^2\beta}{d(\log a)^2} + \frac{d^2(\beta_\sigma + \beta_\tau)}{d(\log \xi)^2} \right].
\]
(34)

These derivatives thus depend on second derivatives with respect to $\xi$. In appendix B we obtain the leading order values of $\lambda_{00}^+(\beta)$ in $g_0^2$.

3 Derivation of the sum rules

We now derive the sum rules, neglecting $O(a^2)$ discretization errors, but without using perturbative approximations to normalization factors such as $\frac{d\beta}{d\log a}$ and $Z(\beta)$.

3.1 Derivation on the isotropic lattice

We consider a renormalization group invariant (RGI) quantity $f(a, T)$, which is obtained as the continuum limit of a function $F(\beta, N_\tau)$ of the bare parameters. The renormalization group equation $a \partial f/\partial a = 0$ implies
\[
T \partial f/\partial T = - \frac{d\beta}{d\log a} \frac{\partial F}{\partial \beta}.
\]
(35)

We have used
\[
adN_\tau/da = -N_\tau \quad \text{and} \quad N_\tau \partial F/\partial N_\tau = -T \partial_T f.
\]
In particular, we can apply this equation to $F_\pm(\beta, N_\tau)$, since they are RGI quantities (see Eq. 10, 11). For the case of $F_+$, we obtain
\[
a^{-4} \langle \sum_x \Theta(x)\Theta(0) \rangle_T^+ - a^{-4} \langle \sum_x \Theta(x)\Theta(0) \rangle_0^+ = T^5 \partial_T \frac{\epsilon - 3P}{T^4} \left( \frac{d\beta}{d(\log a)^2} \right) \frac{1}{d\beta/d\log a} (\epsilon - 3P).
\]
(36)

This sum rule was first derived in [9] in the continuum, in which case the second term on the right-hand side is absent. Indeed, the factor multiplying $(\epsilon - 3P)$ behaves asymptotically as $2b_1 g_0^4$ at small bare coupling. Consider next the case of $F_-$; the sum rule reads
\[
\frac{4}{3a^4} \langle \sum_x \Theta(x)\Theta_{00}(0) \rangle_T^+ = T^5 \partial_T \frac{\epsilon + P}{T^4} + \frac{d\beta}{d\log a} \frac{\partial(\beta Z(\beta))}{Z(\beta)\beta} (\epsilon + P).
\]
(37)

Note that the left-hand side vanishes by Euclidean symmetry at $T = 0$. The factor multiplying $(\epsilon + P)$ in the second term on the right-hand side vanishes in the continuum limit as $(-2b_0 g_0^4)$. 

5
3.2 Derivation on the anisotropic lattice

For any RGI quantity \( f(a_\sigma, \xi, T) \), \( a_\sigma \partial_{a_\sigma} f = 0 \) and \( \xi \partial_\xi f = 0 \) respectively imply

\[
\frac{T}{T} \frac{\partial f}{\partial T} = \begin{pmatrix}
-1 \\
1
\end{pmatrix},
\begin{pmatrix}
\frac{\partial^2 \beta_\sigma}{\partial \log a_\sigma} & \frac{\partial \beta_\sigma}{\partial \log \xi} \\
\frac{\partial \beta_\sigma}{\partial \log a_\sigma} & \frac{\partial^2 \beta_\sigma}{\partial \log \xi}
\end{pmatrix}\begin{pmatrix}
\frac{\partial F}{\beta_\sigma} \\
\frac{\partial F}{\beta_\sigma}
\end{pmatrix}
\]

(38)

We have used

\( a_\sigma \partial_{a_\sigma} N_\tau = -N_\tau \) and \( N_\tau \partial \log a_\sigma = -T \partial_\tau f \).

From now on we evaluate the expression at the isotropic point \( \beta_\sigma = \beta_\tau \). The determinant of the matrix is then

\[
\Delta = 2 \beta Z(\beta) \frac{d \beta}{d \log a}.
\]

(39)

Taking suitable linear combinations, we obtain the two equations

\[
-T \frac{\partial f}{\partial T} = \frac{d \beta}{d \log a} \left( \frac{\partial F}{\beta_\sigma} + \frac{\partial F}{\beta_\tau} \right),
\]

(40)

\[
-\frac{3}{4} T \frac{\partial f}{\partial T} = \beta Z(\beta) \left( \frac{\partial F}{\beta_\sigma} - \frac{\partial F}{\beta_\tau} \right).
\]

(41)

The first relation is equivalent to Eq. 35 derived on the isotropic lattice, since \( \frac{d}{dx} f(x,x) = (\partial_y + \partial_z) f|_{y,z=x} \) for a general function of two variables \( y, z \). We therefore focus on the second relation in the following.

The observables \( f_\pm \) are RGI quantities. Consider first \( f_+(T) \). Using Eq. 31 and the thermodynamic relations \( T \partial_T p = \epsilon + P \) and \( (\epsilon - 3P)/T^4 = T \partial_T (p/T^4) \), Eq. 41 leads to Eq. 37 derived on the isotropic lattice.

We now apply Eq. 41 to \( f_-(T) \). We obtain a new sum rule,

\[
a^4 \langle \sum_x \Theta_{00}(x) \Theta_{00}(0) \rangle_T - \beta Z(\beta) \lambda_{00}(\beta) a^{-4} \langle S_+ \rangle_T = \frac{3}{4} \lambda_{00}^+(\beta)(\epsilon + P) + \left( \frac{3}{4} \right)^2 T^5 \partial_T \left( \frac{\epsilon + P}{T^4} \right).
\]

(42)

The quantities \( \lambda_{00}^+(\beta) \) are defined in Eq. 32. Since the right-hand side of Eq. 42 manifestly has a finite continuum limit, this equation implies that the short-distance quartic divergence of the integrated correlator is compensated by the quartic divergence \( a^{-4} \) of the expectation value of the trace anomaly,

\[
\langle \beta S_+ \rangle_T = \frac{3}{2} d_A \left( 1 + O(g_0^2) \right) \quad (d_A \equiv N^2 - 1).
\]

(43)

3.3 Contact terms in two-point functions of the Hamiltonian

The \( \langle \theta \theta \rangle, \langle \theta_0 \theta_0 \rangle \) and \( \langle \theta_0 \theta_0 \rangle \) correlators are related at vanishing spatial momentum because the Hamiltonian operator \( \int d^3 x T_{00} \) has simple correlation functions:

\[
(\int d^3 x \ T_{00}(x,0) \ O)_T = T^2 \partial_T \langle O \rangle_T + A_O(T) \ \delta(x_0)
\]

(44)

for any local operator \( O \). The delta function arises because the Hamiltonian operator applied on transfer-matrix eigenstates with energies at the cutoff scale does not yield the
expected matrix elements; for instance off-diagonal matrix elements are expected to appear in general.

The sum rules (Eq. 36 37 42) determine the contact terms \( A_{θ_00} \) and \( A_θ \):

\[
A_{θ_{00}} = \frac{λ_{θ_{00}}(g_0)Z(g_0)}{g_0^2 d g_0^2 / d \log a} (θ)_T + 3 \left( \frac{1}{4} λ_{θ_{00}}(g_0) + \frac{g_0^2 d g_0^2}{16 d \log a} \left[ 1 - \frac{g_0^2 d Z}{Z d g_0^2} \right] - 1 \right) (ε + P), \quad (45)
\]

\[
A_θ = \left( \frac{1}{4} \frac{d^2 g_0^2}{d (\log a)^2} \frac{1}{d g_0^2 / d \log a} - 1 \right) (ε - 3P) + 3 \frac{g_0^2 d g_0^2}{4 d \log a} \left[ 1 - \frac{g_0^2 d Z}{Z d g_0^2} \right] (ε + P)
+ \frac{1}{4} \langle f d^4 x \ θ(x)θ(0) \rangle_0. \quad (46)
\]

The contact term of \( ⟨T_{θ_{00}}T_{θ_{00}}⟩ \) is then given by \( A_{T_{θ_{00}}} = A_{θ_{00}} + \frac{1}{4} A_θ \). Note that the contact terms have a quartically divergent contribution, plus finite, temperature-dependent contributions.

4 Sum rules in the continuum

Taking the bare coupling \( g_0^2 \ll 1 \) in Eq. (36 37 42) yields the following continuum sum rules:

\[
\langle f d^4 x \ θ(x)θ(0) \rangle_0^c = T^5 ∂_T \frac{ε - 3P}{T^4}, \quad (47)
\]

\[
\langle f d^4 x \ θ(x)θ(0) \rangle_0^c = \frac{3}{4} T^5 ∂_T \frac{ε + P}{T^4}, \quad (48)
\]

\[
\langle f d^4 x \ θ_{00}(x)θ_{00}(0) \rangle_0^c + \frac{λ_{θ_{00}}(g_0)}{2g_0^2 d g_0^2 / d \log a} (θ)_T = \frac{3}{4} λ_{θ_{00}}^+(ε + P) + (\frac{3}{4})^2 T^5 ∂_T \frac{ε + P}{T^4}. \quad (49)
\]

The coefficients \( λ_{θ_{00}}^± \) are now to be taken at \( g_0 = 0 \), where they are pure, finite numbers. We compute these numbers in appendix B, see Eq. (67) and (74). The calculation of \( λ_{θ_{00}}^+ \) suggests that the latter is independent of the regularization used. If true, this would mean that the regularization dependence cancels entirely between the two terms on the left-hand side of this equation. It would be useful to derive Eq. (49) in a different regularization to confirm this.

The difference of relation (49) between finite and zero-temperature gives

\[
\langle f d^4 x \ θ_{00}(x)θ_{00}(0) \rangle_0^c - \langle f d^4 x \ θ_{00}(x)θ_{00}(0) \rangle_0^c + \frac{λ_{θ_{00}}(g_0)}{2g_0^2 d g_0^2 / d \log a} (θ)_T = \frac{3}{4} λ_{θ_{00}}^+(ε - 3P) + (\frac{3}{4})^2 T^5 ∂_T \frac{ε + P}{T^4}.
\]

This relation shows that even after subtraction of the quartic divergence, a temperature-dependent logarithmic divergence remains in the susceptibility of \( θ_{00} \).

5 Sum rules and cutoff effects on \( ε \) and \( P \)

The idea to remove the leading cutoff effects on physical quantities by using lattice sum rules was proposed in [5]. Here we show that it can be applied to thermodynamic potentials. Consider for instance \( (ε - 3P)/T^4 \). On a \( ξ = 1 \) lattice, this quantity is obtained by taking the \( N_τ \to \infty \) limit of

\[
φ(N_τ) ≡ F_+(β(N_τ), N_τ), \quad (50)
\]
where $\beta(N_\tau)$ is tuned so that $(N_\tau a)$ is constant and $F_\pm$ was defined in Eq. (10). Following the steps of section 3, we can evaluate

$$\frac{d\varphi}{d \log N_\tau} = \frac{\partial F_+}{\partial \log N_\tau} - \frac{d\beta}{d \log a} \frac{\partial F_+}{\partial \beta}$$

$$= \frac{\partial F_+}{\partial \log N_\tau} - \frac{\partial^2 \beta}{(\partial \log a)^2} \varphi(N_\tau) + N_\tau^4 \langle \sum_x \Theta(x) \Theta(0) \rangle _T - 0 \quad (51)$$

Thus the cutoff effects can be evaluated in Monte-Carlo simulations at fixed $\beta$. The first term is itself unambiguous only up to $O(a^2)$ if a *symmetric* difference scheme is used, and $O(a)$ if not [5]. It requires performing a simulation at a second value of $N_\tau$. Thus in total three simulations are required (for instance with the number of points in the time direction set to $N_\tau$, $N_\tau + 1$, and $N_\sigma$ for the zero-temperature subtractions). Choosing a different couple ($\beta(N'_\tau), N'_\tau$) tuned to the same temperature requires four simulations in total and provides essentially the same information (unless $N'_\tau$ is much larger than $N_\tau$, but in practice, typical values are $N_\tau = 6$ and $N'_\tau = 8$). If one follows both strategies, one can check how close $\varphi(N'_\tau)$ is from

$$\varphi(N_\tau) + \frac{1}{2} \frac{d\beta}{d \log N_\tau} \left(1 - (N_\tau/N'_\tau)^2\right).$$

If $N_\tau$ is large enough, $\varphi$ is in the regime where $O(a^2)$ effects dominate over higher order cutoff effects and $\varphi(N'_\tau)$ will be numerically consistent with this expression. In general, this provides a way of testing whether $\varphi$ is in this regime without having to perform simulations at $N''_\tau > N'_\tau$. Since the cost of finite-temperature calculations grows with a high power of $N_\tau$, this information is very precious.

### 6 Conclusion

We have derived finite temperature sum rules, valid at finite lattice spacing up to $O(a^2)$ corrections. The main results are Eq. (36, 37, 42), and, for the reader interested in continuum results, Eq. (47, 49).

As an application of these considerations, we have proposed a way to check whether thermodynamics calculations are performed in the regime where the $O(a^2)$ cutoff effects dominate over higher order cutoff effects, using only two values of $N_\tau$.

Further sum rules can be obtained for other RGI quantities. Equations (35) and (40, 41) can for instance be applied to renormalized Polyakov or Wilson loops in order to study thermal contributions to quark masses, and the static potential relevant to $J/\psi$ suppression [20]. Finally the sum rules can be generalized to full QCD with commonly used quark actions.

This work was supported in part by funds provided by the U.S. Department of Energy under cooperative research agreement DE-FG02-94ER40818.
A A different choice of bare parameters

Although the set of bare parameters \((\beta_\sigma, \beta_\tau)\) is most convenient to derive sum rules, in numerical practice, it is more convenient to parametrize these parameters as

\[
\beta_\sigma = \frac{\beta}{\xi_0}, \quad \beta_\tau = \beta \xi_0.
\] (52)

In order to take the continuum limit at fixed anisotropy \(\xi\), the first task of the lattice practitioner is to establish the lines of constant \(\xi\) in the \((\beta, \xi_0)\) plane, so that \(\xi_0\) can thereafter be viewed as a function of \((\beta, \xi)\). Secondly the relation between \(\beta\) and \(a_\sigma\) must be worked out at fixed anisotropy \(\xi\). After this preparatory work, the set of variables used in practice is \((\beta, \xi)\).

The expression (26) can thus be written as

\[
\frac{\partial \beta_\sigma(a_\sigma, \xi)}{\partial \log a_\sigma} = \frac{1}{\xi_0} \frac{\partial \beta(a_\sigma, \xi)}{\partial \log a_\sigma} \left[ 1 - \frac{\beta}{\xi_0} \frac{\partial \xi_0(\beta, \xi)}{\partial \beta} \right] \] (53)

\[
\frac{\partial \beta_\tau(a_\sigma, \xi)}{\partial \log a_\sigma} = \xi_0 \frac{\partial \beta(a_\sigma, \xi)}{\partial \log a_\sigma} \left[ 1 + \frac{\beta}{\xi_0} \frac{\partial \xi_0(\beta, \xi)}{\partial \beta} \right]. \] (54)

Similarly, using

\[
\frac{\partial \beta(a_\sigma, \xi)}{\partial \log \xi} = -\frac{\partial \beta(a_\sigma, \xi)}{\partial \log a_\sigma} \frac{\partial \log a_\sigma(\beta, \xi)}{\partial \log \xi} = -\frac{\partial \beta(a_\sigma, \xi)}{\partial \log a_\sigma} \frac{\partial \log \xi_0(\beta, \xi)}{\partial \log \xi} \frac{\partial \log a_\sigma(\beta, \xi)}{\partial \log \xi_0(\beta, \xi)},
\]

we obtain

\[
\frac{\partial \beta_\sigma(a_\sigma, \xi)}{\partial \log \xi} = -\frac{\beta}{\xi_0} \frac{\partial \log \xi_0(\beta, \xi)}{\partial \log \xi} \times \left[ 1 + \frac{\partial \beta(a_\sigma, \xi)}{\partial \log a_\sigma} \frac{\partial \log \xi_0(\beta, \xi)}{\partial \log \xi_0(\beta, \xi)} \left( \frac{1}{\beta} - \frac{\partial \log \xi_0(\beta, \xi)}{\partial \beta} \right) \right].
\] (55)

\[
\frac{\partial \beta_\tau(a_\sigma, \xi)}{\partial \log \xi} = \frac{\xi_0 \beta}{\xi_0} \frac{\partial \log \xi_0(\beta, \xi)}{\partial \log \xi} \times \left[ 1 - \frac{\partial \beta(a_\sigma, \xi)}{\partial \log a_\sigma} \frac{\partial \log \xi_0(\beta, \xi)}{\partial \log \xi_0(\beta, \xi)} \left( \frac{1}{\beta} + \frac{\partial \log \xi_0(\beta, \xi)}{\partial \beta} \right) \right].
\] (56)

These expressions suggest how to determine \(\partial \beta_\sigma(a_\sigma, \xi)/\partial \log \xi\) non-perturbatively. Since, by Euclidean symmetry, \(Z_\sigma^{\xi=1} = Z_\tau\) and \(\frac{\partial \xi_0(\beta, \xi)}{\partial \beta} \equiv 0\), we have the equalities

\[
\frac{\partial \beta(a_\sigma, \xi)}{\partial \log \xi} \equiv \frac{1}{4d \log a} \frac{d \beta}{d \log a}, \] (57)

\[
Z(\beta) \equiv \frac{\partial \xi_0(\beta, \xi)}{\partial \xi}.
\] (58)

B Leading-order computation of \(\lambda_{00}^\pm\)

In this appendix we calculate the coefficients \(\lambda_{00}^\pm(\beta)\) defined in Eq. 52. Using the standard notation \(\hat{p}_\mu = 2 \sin(p_\mu/2)\), we define the dimensionless integrals

\[
I_\sigma(\xi_0^2, N_\tau) = \frac{1}{N_\tau} \sum_{p_0} \int_{-\pi}^{\pi} \frac{d^3 p}{(2\pi)^3} \frac{\hat{p}_0^2}{\xi_0^2 p_0^2 + \sum_k p_k^2}
\] (59)
\[ I_\tau(\xi_0^2, N_\tau) = \frac{1}{N_\tau} \sum_{p_0} \int_{-\pi}^{\pi} \frac{d^3p}{(2\pi)^3} \frac{\xi_0^2 p_0^2}{\xi_0^2 p_0^2 + \sum_k p_k^2} \]  

(60)

The variable \(p_0\) takes the values \(2\pi k/N_\tau\) for \(0 \leq k < N_\tau\). One finds that \(I_\sigma(1, \infty) = I_\tau(1, \infty) = 1/4\) and

\[ 3 \frac{\partial I_\sigma}{\partial \xi_0^2}(\xi_0^2 = 1, \infty) = -\frac{1}{4} + \int_{-\pi}^{\pi} \frac{d^4p}{(2\pi)^4} \frac{p_0^4}{(p_0^2 + \sum_k p_k^2)^2} = -0.154933 \ldots \]  

(61)

B.1 \(\lambda_{00}^-\)

Notice first that \(\lambda_{00}^-(\beta)\) can be rewritten

\[ \lambda_{00}^-(\beta) = \frac{1}{2} Z^-(\beta) \left( \frac{\partial}{\partial \beta_\sigma} - \frac{\partial}{\partial \beta_\tau} \right) \log \left( \frac{Z^-_{\sigma}}{Z^-_{\tau}} \right). \]  

(62)

The matrix elements of \(\theta_{00}\) on physical states are RGI quantities. On a \(\xi = 1\) lattice,

\[ \langle \Omega|\theta_{00}|\Omega \rangle = 0, \]  

(63)

as a consequence of the Euclidean symmetry on an \(N_\sigma = N_\tau = \infty\) lattice. Therefore Eq. 63 must be satisfied also on a \(\xi \neq 1\) lattice. This condition determines the ratio \(Z^-_{\sigma}/Z^-_{\tau}\):

\[ \frac{Z^-_{\sigma}}{Z^-_{\tau}} = \frac{\langle S_\tau \rangle_0}{\langle S_\sigma \rangle_0}. \]  

(64)

At leading order on an \(N_\tau \times \infty^3\) lattice,

\[ \frac{\beta_\tau}{d_A}(S_\tau)_T \left[ I_\tau(\xi_0^2, N_\tau) + I_\sigma(\xi_0^2, N_\tau) \right] = \frac{3}{2} - 3I_\sigma(\xi_0^2, N_\tau), \]  

(65)

\[ \frac{\beta_\sigma}{d_A}(S_\sigma)_T = 3I_\sigma(\xi_0^2, N_\tau) (T = (a_\tau N_\tau)^{-1}), \]  

(66)

which leads to

\[ \lambda_{00}^- = 1 + 8 \frac{\partial I_\sigma}{\partial \xi_0^2}(\xi_0^2 = 1, \infty) = 0.586844 \ldots \]  

(67)

B.2 \(\lambda_{00}^+\)

A second physics condition (in addition to Eq. 64) is necessary in order to fix \(Z^-_{\sigma}\) and \(Z^-_{\tau}\) separately and therefore to determine \(\lambda_{00}^+\). We impose the condition

\[ \frac{N_\tau^4}{\xi^3}(\Theta_{00})_T = \frac{3}{4} (\epsilon + P)/T^4 \]  

(68)

This leads to the expressions

\[ Z^-_{\sigma} = \left[ \frac{3}{4} \frac{\epsilon + P}{d_AT^4} \right] \frac{\beta_\tau}{N_\tau^4 W_T(\xi_0^2)} (\beta_\tau S_\tau/d_A)_0 \]  

\[ Z^-_{\tau} = \left[ \frac{3}{4} \frac{\epsilon + P}{d_AT^4} \right] \frac{\beta_\sigma}{N_\tau^4 W_T(\xi_0^2)} (\beta_\sigma S_\sigma/d_A)_0 \]  

(69)
where
\[ W_T(\xi^2_0) \equiv \langle \beta_\tau S_\tau/d A \rangle_0 \langle \beta_\sigma S_\sigma/d A \rangle_T - \langle \beta_\tau S_\tau/d A \rangle_T \langle \beta_\sigma S_\sigma/d A \rangle_0. \] (70)

Cutoff effect due to finite \( N_\tau \) can be removed by taking the limit \( N_\tau \to \infty \). Expressions Eq. 69 in principle allow for a non-perturbative determination of \( Z^-_{\sigma,\tau} \), but at tree level we shall use the Stefan-Boltzmann expression \( \pi^2 d_A/15 \) for the right-hand side of Eq. 68. In that approximation we have
\[ W_T(\xi^2_0) \overset{LO}{=} \frac{9}{2} \left[ I_\sigma(\xi^2_0, N_\tau) - I_\sigma(\xi^2_0, \infty) \right]. \] (71)

For \( \xi^2_0 = 1 \), we know that both \( Z^-_\sigma \) and \( Z^-_\tau \) are equal to \( \beta \) at leading order. Thus
\[ \lim_{N_\tau \to \infty} N_\tau^4 W_T(1) = \frac{\pi^2}{20}. \] (72)

Because \( \lim_{N_\tau \to \infty} N_\tau^4 W_T(\xi^2_0) \) is a continuum limit, \( \hat{p} \) can be replaced by \( p \) and one then finds that
\[ \lim_{N_\tau \to \infty} N_\tau^4 W_T(\xi^2_0) = \xi^3_0 \lim_{N_\tau \to \infty} N_\tau^4 W_T(1) = \frac{\pi^2 \xi^3_0}{20}. \] (73)

One then straightforwardly obtains
\[ \lambda^+_{00} = 6. \] (74)

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