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Finite volume effects in thermal field theory

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ABSTRACT: We analyze the effect of a finite volume on the thermodynamic potentials of a relativistic quantum field theory defined on a hypertorus at vanishing chemical potential. Using the symmetries of the Euclidean partition function, we interpret the thermodynamic observables as the expectation value of the energy-momentum tensor in the same theory living on a $\beta \times L^2$ volume. In the case where the screening correlation lengths in the thermal system are finite, we obtain a closed formula for the leading finite volume effects in terms of the smallest screening mass. This formula can be used to estimate, and possibly correct for, the leading finite volume effects in lattice calculations of QCD thermodynamics.

KEYWORDS: Lattice QCD, Thermal Field Theory

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1 Introduction

The description of relativistic quantum systems at finite temperature plays a central role in cosmology, astrophysics, plasma physics and in the physics of heavy-ion collisions. In the latter context, the thermodynamics of Quantum Chromodynamics (QCD) is being studied intensively by lattice Monte-Carlo methods [1-5] and by analytic [6, 7] and semi-analytic methods [8]. The lattice calculations have to control both the discretization errors and the finite volume effects. References [9-11] address the question of how to reduce the former uncertainties. Here we address in some generality the finite-volume corrections to the energy density, entropy density and pressure calculated on a hypertorus of dimensions L^3 . At the same time, the method we follow provides a complementary point of view on the thermodynamics of the quantum field theory. This alternative interpretation might find some use in approximate analytic treatments such as the variational method [12, 13].

Finite size effects in gauge theories have been studied before at weak coupling [14, 15]. In [16], an elegant calculation is presented that yields the finite-size effects for noninteracting gauge bosons. For non-Abelian gauge theories at extremely high temperatures, these finite-volume effects are indeed expected to be the leading ones in the regime $1/q \gg$ $LT \gg 1$ (L is the linear box size, T is the temperature and g is the gauge coupling). In that regime, the effects of electric and magnetic screening [17] are absent. However, at any finite temperature the asymptotic $LT \to \infty$ finite-size effects must be exponentially

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suppressed by the finite, non-perturbative spatial correlation length. In other words the finite-size corrections to the thermodynamic potentials are bound to be $O(e^{-cg^2TL})$, where c is a number of order unity. At a few times the deconfining temperature T_c , the screening masses are known to some extent from four-dimensional calculations, both in SU(3) gauge theory [18, 19] and in full QCD [20]. And at much higher temperatures, the dimensional reduction approach allows one to predict the temperature evolution of these correlation lengths [21]. Choosing L large compared to the longest of these correlation lengths should therefore ensure that finite-size effects are small.

In this paper we first reinterpret the finite-volume effects by using symmetry properties of the Euclidean partition function and of the stress-energy tensor. We point out that there is a generic dynamical regime, where the leading finite size effects can be expressed completely in terms of the gap in the spatial screening spectrum and its derivative with respect to temperature. This is possible because $T_{\mu\nu}$ plays the dual role of stress-energy and energy-momentum tensor: on the one hand its thermal expectation value gives the energy density and pressure, on the other hand its diagonal matrix elements on an individual state yield its energy and momentum. Since the screening gap can be calculated on the lattice relatively easily, the formula we derive allows one to estimate the finite-size effects in practice, and possibly to correct for them.

In section 2 we describe the thermodynamic potentials as expectation values of elements of the energy-momentum tensor and the dual interpretation of these matrix elements. In section 3 we exploit this interpretation further to estimate the leading finite-size effects on the thermodynamic potentials. Numerical applications to QCD are presented in section 4, and we finish with some concluding remarks (section 5).

2 Thermodynamic observables and their dual interpretation

We consider a relativistic theory in four space-time dimensions without chemical potentials in Matsubara's Euclidean formalism. Euclidean expectation values are denoted by $\langle . \rangle$. At zero temperature and in infinite spatial volume, the system has a full SO(4) symmetry group corresponding to the Lorentz group in Minkovsky space. As a consequence of translation invariance, the theory possesses a conserved, symmetric energy-momentum tensor $T_{\mu\nu}$. We will sometimes consider separately its traceless part and its trace θ , using the notation

$$T_{\mu\nu} = \theta_{\mu\nu} + \frac{1}{4}\theta\delta_{\mu\nu}, \qquad \qquad \theta_{\mu\mu} \equiv 0.$$
(2.1)

The conserved charges measure energy and momentum, respectively, i.e. for a common eigenstate of these operators, we have

$$\int d^3x \, \hat{T}_{00}(x) |\Psi\rangle = E |\Psi\rangle, \qquad (2.2)$$

$$\int d^3x \, \hat{T}_{0k}(x) |\Psi\rangle = P_k |\Psi\rangle \,. \tag{2.3}$$

The partition function is $Z = \sum_{n} e^{-\beta E_n}$ in terms of the eigenvalues of $\int d^3x \hat{T}_{00}$, where $\beta \equiv 1/T$ is the inverse temperature. The pressure, energy density and entropy density are

obtained from Z according to

$$p = T \left(\frac{\partial \log Z}{\partial V}\right)_T + \text{cst}, \qquad e = \frac{T^2}{V} \left(\frac{\partial \log Z}{\partial T}\right)_V + \text{cst}, \qquad s = \frac{1}{V} \left(\frac{\partial (T \log Z)}{\partial T}\right)_V.$$
(2.4)

We will exclusively be considering volumes $V = L^3$, with periodic boundary conditions in all four directions for bosons, and antiperiodic boundary conditions in all four directions for fermions. The energy density and pressure are defined up to an additive constant, which we choose such that both vanish at $\beta = L$. This is the standard choice in Monte-Carlo simulations. We have $(e - 3p)(\beta, L) = \langle \theta \rangle_{\beta \times L^3} - \langle \theta \rangle_{L^4}$, $(e + p)(\beta, L) = \frac{4}{3} \langle \theta_{00} \rangle_{\beta \times L^3}$ and, in the limit $L \to \infty$, $s = \beta(e + p)$. We remark that one can define different operators that play the role of energy-momentum tensor and lead to the same conserved charges [22]. But due to translation invariance, the Euclidean expectation values of the canonical and the Belinfante energy-momentum tensor are identical, since they differ only by a total derivative term [23].

In [24], using exact lattice QCD sum rules [25–27] we showed that if $|\Psi\rangle$ is a state of definite energy *E* living in a periodic box $L_1 \times L_2 \times L_3$,

$$\langle \Psi | \int d^3x \,\hat{\theta}_{00}(x) |\Psi\rangle = \frac{3}{4} \left[1 - \frac{1}{3} \sum_{k=1}^3 L_k \frac{\partial}{\partial L_k} \right] E \,, \tag{2.5}$$

$$\langle \Psi | \int d^3 x \,\hat{\theta}(x) | \Psi \rangle = \left[1 + \sum_{k=1}^3 L_k \frac{\partial}{\partial L_k} \right] E \,, \tag{2.6}$$

and one can similarly show that

$$\langle \Psi | \int d^3 x \, \hat{\theta}_{33}(x) | \Psi \rangle = -\frac{1}{4} \left[1 - 4L_3 \frac{\partial}{\partial L_3} + \sum_{k=1}^3 L_k \frac{\partial}{\partial L_k} \right] E \,. \tag{2.7}$$

The states are normalized such that $\langle \Psi | \Psi \rangle = 1.^1$ Strictly speaking, these equations hold when taking the difference between two states. Note however that for $|\Psi_0\rangle =$ the vacuum state in infinite volume, $\langle \Psi_0 | \hat{\theta}_{00} | \Psi_0 \rangle = \langle \Psi_0 | \hat{\theta}_{33} | \Psi_0 \rangle = 0$ by Euclidean symmetry. Therefore the energy appearing on the right-hand-side of eq. (2.5) and (2.7) can be thought of as the energy of the state $|\Psi\rangle$ relative to the infinite-volume vacuum $|\Psi_0\rangle$. For the operator θ , due to its mixing with the unit operator one must always consider differences of matrix elements. Finally, we expect relations eq. (2.5)–(2.7) to be true in other relativistic theories as well.

2.1 Interchanging the coordinate axes

Let us consider the expectation value of the operator θ_{00} . Since $\theta_{kk} \equiv -\theta_{00}$, in a $\beta \times L^3$ box we have $\langle \theta_{ij} \rangle = -\frac{\delta_{ij}}{3} \langle \theta_{00} \rangle$. We now want to reinterpret the axis labels.² The axis $\hat{3}$ will play the role of Euclidean time (with extent L), while the short $\hat{0}$ axis assumes the role of a spatial direction (with extent β). In the expectation values below, we always indicate the dimensions of the lattice (in the order $\hat{0}, \hat{1}, \hat{2}, \hat{3}$).

¹In the infinite volume limit, one recovers from eq. (2.5)–(2.7) the Minkovsky-space result $\langle \Psi | T_{\mu\nu} | \Psi \rangle = P_{\mu}P_{\nu}/M$ for covariantly normalized one-particle states, $\langle \Psi | \Psi \rangle = (E/M)L^3$.

²The idea of interchanging the coordinate axes in this way is of course not new, see for instance [28].

In this new system of coordinates, the operator θ_{33} plays the role of the 00 component of the same tensor,

$$\langle \theta_{00} \rangle_{\beta \times L^3} = -3 \langle \theta_{33} \rangle_{\beta \times L^3} = -3 \langle \theta_{00} \rangle_{L \times (L^2 \beta)}.$$
(2.8)

Next we apply formula (2.5) on the energy eigenstates of the $\beta \times L \times L$ system. Note that for a homogeneous state, by which we mean $E \propto L_1 L_2 L_3$, this expression vanishes. However, we will apply this on the lowest-energy state of the $\beta \times L \times L$ system. We write the energy levels of that system \tilde{E}_0 , \tilde{E}_1 , \tilde{E}_2 etc. ordered by increasing energy. We expect the energy per unit volume to have a finite limit when $L \to \infty$,

$$\tilde{e}_0(\beta) = \lim_{L \to \infty} \left(\frac{\tilde{E}_0(\beta)}{\beta L^2} - \frac{\tilde{E}_0(L)}{L^3} \right) \,. \tag{2.9}$$

The energy density $\tilde{e}_0(\beta)$ is thus measured relative to the infinite-space vacuum. In this section we take the limit $L \to \infty$ in eq. (2.8) and assume that therefore the expectation value of a local operator is equal to its expectation value in the ground state of energy \tilde{E}_0 . A sufficient condition for this is that there should be a spectral gap between \tilde{E}_1 and \tilde{E}_0 . By combining eq. (2.5) and eq. (2.8), we learn that the entropy density of the thermal system corresponds to

$$s = \frac{4\beta}{3} \langle \theta_{00} \rangle_{\beta \times \infty^3} = \beta^2 \frac{\partial \tilde{e}_0(\beta)}{\partial \beta}.$$
 (2.10)

Similarly, using eq. (2.6) one easily finds that

$$e - 3p = 4\tilde{e}_0(\beta) + \beta \frac{\partial \tilde{e}_0(\beta)}{\partial \beta}$$
(2.11)

By taking a linear combination of the last two equations, we also obtain the 'dual' interpretation of the pressure of the thermal system

$$p = -\tilde{e}_0(\beta). \tag{2.12}$$

For instance, in a regime where the system behaves in a scale-invariant way, $s = cT^3$ and e - 3p = 0, the corresponding dual ground-state energy is given by

$$\tilde{e}_0(\beta) = -\frac{c}{4\beta^4}.$$
(2.13)

We remark that finite-temperature phase transitions are mapped into quantum phase transitions in this interpretation [29]. The vacuum energy $\tilde{e}_0(\beta)$ has a non-analyticity at a critical value of β equal to $1/T_c$. This non-analyticity is typically due to an avoided level-crossing.

3 Finite-volume effects on the thermodynamic potentials

We can exploit the dual interpretation of the partition function further to study the finitevolume effects on the thermal system. Through a chain of relations, we successively relate the expectation value of the energy-momentum tensor on a $\beta \times L^3$ lattice to the same expectation value on a $\beta \times \infty^3$ lattice. This allows us to arrive at a formula for the finitevolume correction to the thermodynamic potentials. Starting with the thermal expectation value of θ_{00} , we successively write

$$-\frac{1}{3}\langle\theta_{00}\rangle_{\beta\times L^{3}} = \langle\theta_{33}\rangle_{\beta\times L^{3}} = \langle\theta_{00}\rangle_{L\times(L^{2}\times\beta)} = \langle\theta_{00}\rangle_{\infty\times(L^{2}\times\beta)} + \mathcal{K}_{1}$$

$$= \langle\theta_{11}\rangle_{L\times(\infty\times L\times\beta)} + \mathcal{K}_{1} = \langle\theta_{11}\rangle_{\infty\times(\infty\times L\times\beta)} + \mathcal{K}_{1} + \mathcal{K}_{2}$$

$$= \langle\theta_{00}\rangle_{\infty\times(\infty\times L\times\beta)} + \mathcal{K}_{1} + \mathcal{K}_{2} = \langle\theta_{22}\rangle_{L\times(\infty\times\infty\times\beta)} + \mathcal{K}_{1} + \mathcal{K}_{2}$$

$$= \langle\theta_{22}\rangle_{\infty\times(\infty\times\infty\times\beta)} + \mathcal{K}_{1} + \mathcal{K}_{2} + \mathcal{K}_{3} = -\frac{1}{3}\langle\theta_{00}\rangle_{\beta\times\infty^{3}} + \mathcal{K}_{1} + \mathcal{K}_{2} + \mathcal{K}_{3} .$$

$$(3.1)$$

A spectral representation for the \mathcal{K}_i is obtained in appendix A, for instance

$$\mathcal{K}_1 = \frac{1}{\beta L^2 Z \, e^{\tilde{E}_0 L}} \sum_{n \ge 1} \left(\langle \tilde{\Psi}_n | \int d^3 x \, \hat{\theta}_{00}(x) | \tilde{\Psi}_n \rangle - \langle \tilde{\Psi}_0 | \int d^3 x \, \hat{\theta}_{00}(x) | \tilde{\Psi}_0 \rangle \right) e^{-(\tilde{E}_n - \tilde{E}_0)L} \,, \quad (3.2)$$

where the $|\tilde{\Psi}_n\rangle$ and \tilde{E}_n are the eigenstates and energy levels of the $\beta \times L^2$ system. We can use eq. (3.1) to produce an expression for the finite-volume effects on the entropy density:

$$s = \frac{4\beta}{3} \langle \theta_{00} \rangle_{\beta \times \infty^3} = \frac{4\beta}{3} \langle \theta_{00} \rangle_{\beta \times L^3} + 4\beta (\mathcal{K}_1 + \mathcal{K}_2 + \mathcal{K}_3) \,. \tag{3.3}$$

Following the same steps as for the entropy density, we can obtain an expression for the leading finite-volume effects on the interaction measure. This case is slightly simpler, because the trace-anomaly operator is a Lorentz scalar:

$$\langle \theta \rangle_{\beta \times L^3} = \langle \theta \rangle_{L \times (L^2 \times \beta)} = \langle \theta \rangle_{\infty \times (L^2 \beta)} + \mathcal{J}_1$$

$$= \langle \theta \rangle_{L \times (\infty \times L \times \beta)} + \mathcal{J}_1 = \langle \theta \rangle_{\infty \times (\infty \times L \times \beta)} + \mathcal{J}_1 + \mathcal{J}_2$$

$$= \langle \theta \rangle_{L \times (\infty \times \infty \times \beta)} + \mathcal{J}_1 + \mathcal{J}_2 = \langle \theta \rangle_{\infty \times (\infty \times \infty \times \beta)} + \mathcal{J}_1 + \mathcal{J}_2 + \mathcal{J}_3$$

$$= \langle \theta \rangle_{\beta \times \infty^3} + \mathcal{J}_1 + \mathcal{J}_2 + \mathcal{J}_3 .$$

$$(3.4)$$

A definition for the \mathcal{J}_i based on the spectral representation is given in appendix B. We can apply the same reasoning to the L^4 system, sending the extent of each direction in turn to infinity. There are then four correction terms (\mathcal{I}_{μ}) instead of three. Therefore we obtain

$$e - 3p = \langle \theta \rangle_{\beta \times \infty^3} - \langle \theta \rangle_{\infty^4} = \langle \theta \rangle_{\beta \times L^3} - \langle \theta \rangle_{L^4} - (\mathcal{J}_1 + \mathcal{J}_2 + \mathcal{J}_3) + (\mathcal{I}_0 + \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3).$$
(3.5)

3.1 The case of finite and discrete screening masses

The general formulas (3.3) and (3.5) can be used together with the spectral definition of the $\mathcal{I}_{\mu}, \mathcal{J}_i, \mathcal{K}_i$ to predict the finite volume effects on the thermodynamic potentials. In the following, we make a qualitative assumption on the spectrum of the theory on a $\beta \times L^2$ hypertorus with $L \gg \beta$, which is in particular relevant to QCD at finite temperature.

We consider the case where the low-lying screening masses are *discrete* energy levels of the $\beta \times L^2$ system. That is to say,

$$Lm \equiv L(\tilde{E}_1 - \tilde{E}_0) \gg 1 \tag{3.6}$$

and the next energy levels are simply that same excitation with non-zero momentum in the 'transverse' dimensions of size L,

$$\omega(\mathbf{k}_{\perp}) = \sqrt{m^2 + \mathbf{k}_{\perp}^2}, \qquad \mathbf{k}_{\perp} = \frac{2\pi}{L}(n_1, n_2), \qquad n_i \in \mathbf{Z}.$$
(3.7)

This lightest screening excitation can potentially have a ν -fold degeneracy. The next screening mass is assumed to be separated by a gap from the lowest one, $(m_2 - m)L \gg 1$. In that situation, the \mathcal{K}_i and \mathcal{J}_i can be evaluated in a simple fashion, since they receive contributions only from one-'particle' states. We use particle in quotes because the lowest excitations have only two components of momentum; higher up in the screening spectrum one expects states with an additional energy of order $1/\beta$.

We expect the scenario described above to apply in asymptotically free and conformal non-Abelian gauge theories. For every relativistic theory, the appropriate regime must be studied in order to correctly predict the leading finite-volume effects. As a counterexample to the above scenario, it is well-known that magnetic fields are not screened in an Abelian plasma.

Since we are interested in the leading finite-volume effects, in the remainder of this section we write equations that hold up to terms of order $\max(e^{-2mL}, e^{-m_2L})$. In appendix A, we calculate the corrections $\mathcal{K}_{i=1,2,3}$ under these assumptions and find:

$$\mathcal{K}_{1} = \frac{\nu e^{-mL}}{2\pi\beta L^{3}} \left[2 + 2mL + \frac{3}{4}m^{2}L^{2} - \frac{mL^{2}}{4}\beta\partial_{\beta}m(\beta) \right]$$
(3.8)

$$\mathcal{K}_{2} = \mathcal{K}_{3} = -\frac{\nu e^{-mL}}{2\pi\beta L^{3}} \left[1 + mL + \frac{1}{4}m^{2}L^{2} + mL^{2}\frac{\beta\partial_{\beta}m}{4} \right]$$
(3.9)

Plugging these expressions into eq. (3.3), we obtain our final formula

$$s - \frac{4\beta}{3} \langle \theta_{00} \rangle_{\beta \times L^3} = \frac{m\nu \, e^{-mL}}{2\pi L} \left[m(\beta) - 3\beta \partial_\beta m(\beta) \right] + \dots$$
(3.10)

It shows that the knowledge of the longest spatial correlation length 1/m as a function of temperature $T = 1/\beta$ allows one to compute the leading finite-volume corrections.

The corrections \mathcal{I}_{μ} and \mathcal{J}_k are computed in appendix B under the same assumptions formulated above. The zero-temperature volume corrections \mathcal{I}_{μ} are assumed to be due to ν_0 degenerate states of mass m_0 . We find to leading order

$$\mathcal{J}_1 = \mathcal{J}_2 = \mathcal{J}_3 = \frac{m \, e^{-mL}}{2\pi\beta L} \left[m + \beta \partial_\beta m \right] \tag{3.11}$$

$$\mathcal{I}_0 = \mathcal{I}_1 = \mathcal{I}_2 = \mathcal{I}_3 = \frac{\nu_0 m_0^3}{2\pi^2 L} K_1(m_0 L), \qquad (3.12)$$

where K_1 is the modified Bessel function, m_0 is the mass gap of the theory on the hypertorus of size L^3 , and ν_0 is its degeneracy. For instance, in isospin-symmetric QCD there would be $\nu_0 = 3$ pions. The final formula for the leading finite-volume effects on e - 3p follows,

$$e - 3p = \langle \theta \rangle_{\beta \times L^3} - \langle \theta \rangle_{L^4} - \frac{3m\nu \, e^{-mL}}{2\pi L} \left[m/\beta + \partial_\beta m \right] + \frac{2\nu_0 m_0^3}{\pi^2 L} \, K_1(m_0 L) + \dots \quad (3.13)$$

Combining eq. (3.13) and (3.10) with the thermodynamic identity Ts = e + p, we find that the pressure p is the thermodynamic quantity with the simplest finite-volume effect:

$$p = -\frac{1}{3} \left(\langle T_{kk} \rangle_{\beta \times L^3} - \langle T_{kk} \rangle_{L^4} \right) + \frac{m^2 \nu \, e^{-mL}}{2\pi L \beta} - \frac{m_0^3 \nu_0}{2\pi^2 L} \, K_1(m_0 L) + \dots$$
(3.14)

When the zero-temperature finite-volume corrections are negligible, the pressure computed in finite volume is lower than in the thermodynamic limit. Note that in eq. (3.14) the pressure p(L) is assumed to be obtained directly from the expectation value of T_{kk} . If p/T^4 is obtained with the so-called 'integral method' (see for instance [30]), i.e. by integrating $(e-3p)/T^4$ over temperature starting at T = 0, one should go back to eq. (3.13) to compute the finite-volume effects.

4 Applications

We give two examples where we expect the formulas derived above to apply.

4.1 Confined phase of SU(N) gauge theory

We first consider the pure SU(N) gauge theory (see [31] for a review of its properties). Below the deconfining temperature T_c , the center symmetry associated with the direction of length β is unbroken. Correspondingly, the expectation value of the Polyakov loop vanishes even in the infinite spatial-volume limit. However, for N = 2 and 3 the correlation length associated with the sector of non-zero winding number³ becomes very long as the critical temperature is approached from below. In fact, in the case of SU(2) gauge theory, it even diverges with the 3d Ising exponent [32]. For SU(3), the correlation length becomes very long but remains finite. In [33], it was found that

$$m(\frac{1}{T_c})/T_c = 0.53(4).$$
 (4.1)

We can use the reinterpretation of the partition function to estimate the leading finitevolume effects on the pressure. At zero-temperature, the lightest state is the scalar glueball, so $\nu_0 = 1$. Given its large mass, $M_G/T_c \approx 5.3$ [34, 35], it is not difficult to ensure that the \mathcal{I}_{μ} corrections are negligible by making the box size L large enough. We therefore have

$$\frac{p(T_c, L = \infty)}{T_c^4} = \frac{p(T_c, L)}{T_c^4} + \delta, \qquad (4.2)$$

with

$$\delta = \frac{m^2}{T_c^2} \frac{e^{-(m/T_c) \cdot LT_c}}{2\pi LT_c} = (0.0013, \ 0.00031) \quad \text{for} \quad LT_c = (4, \ 6). \tag{4.3}$$

In fact, the value of $p(T_c)/T_c^4$ is not known precisely, but is most likely on the order of 0.02, based on available numerical data [36], or on the pressure exerted by the known spectrum of glueballs [37, 38], assuming that they are non-interacting. Therefore the correction at $LT_c = 4$ is not negligible if one aims at a precision of one percent on the pressure.

³For SU(3), the sector of winding number 2 is equivalent to the sector with winding number -1, which by charge conjugation has the same correlation length as the +1 sector. Therefore there are only two sector to discuss (winding 0 and +1).

In order to predict the finite volume correction to the entropy density, we need an estimate of the derivative of m with respect to $\beta = 1/T$. For a first idea of the order of magnitude involved, we can use the Nambu-Goto formula [39–41] for $m(\beta) = \sigma_{\text{eff}}(\beta)\beta$ with

$$\frac{\sigma_{\text{eff}}(\beta)}{\sigma} = \left[1 - \frac{2\pi}{3} \frac{1}{\sigma\beta^2}\right]^{\frac{1}{2}},\qquad(4.4)$$

where σ is the string tension at T = 0, to estimate the derivative of the screening mass with respect to β . The finite-volume effect is proportional to

$$m(m - 3\beta\partial_{\beta}m) = -2(m^2 + \pi\sigma).$$
(4.5)

In particular, this quantity is negative, so the 'effective' entropy density computed in finite volume decreases towards the infinite-volume limit (the sign is opposite to the volume correction on the pressure). When m becomes small near T_c , the magnitude of the finite volume effect on s is about $\frac{\sigma e^{-mL}}{L}$. We can do a numerical application in the SU(3) case. For $LT_c = 4$, using the value of $m(\beta)$ given in eq. (4.1) and $T_c/\sqrt{\sigma} \approx 0.64$ [35], we get $\frac{\sigma e^{-mL}}{LT_c^3} \approx 0.08$. Since s/T_c^3 itself is about 0.2 [36, 42] (approaching from the confined phase), this is a large effect indeed. A box size of $LT_c = 9$ is required to reduce this finite-size effect to one percent. This corresponds to a length L of about 6fm.

It would be interesting to know in what range of quark masses this large finite-volume effect persists in full QCD, even though the center symmetry responsible for the existence of the light mode is broken in the presence of quarks. In the case of two light flavors, the phase transition corresponds to the restoration of chiral symmetry; it becomes second order in the chiral limit. Therefore, at small quark masses we again expect a long correlation length in the vicinity of T_c and potentially large volume effects. In practice, it is important for the applicability of the finite-volume formulas that the exponent mL be large, as otherwise corrections that are formally higher order can be important.

4.2 In the deconfined phase

Let us consider the SU(3) gauge theory in the deconfined phase. Above T_c , we know that the smallest screening mass corresponds to a state invariant under all symmetries of the theory in a $\beta \times L^2$ box [18, 19] and its value is [43]

$$\beta m(\beta) = 2.62(16), \qquad 2.83(16), \qquad 2.88(10)$$

$$(4.6)$$

respectively at the temperatures $1.24T_c$, $1.65T_c$ and $2.20T_c$. Due to these large values of the screening mass, the volume correction to the pressure appears to be negligible already for LT = 4, $\delta p/T^4 \approx 8 \cdot 10^{-6}$. Recall that the Stefan-Boltzmann pressure is $p_{\rm SB}/T^4 = 8\pi^2/45 \simeq 1.75$ for N = 3, $N_{\rm f} = 0$.

In the strongly coupled, large-N, $\mathcal{N} = 4$ Super-Yang-Mills theory the screening masses have been calculated by AdS/CFT methods [44, 45]. They turn out to be significantly larger than in QCD, so that finite-volume effects would be even smaller for the same value of LT.

At asymptotic temperatures in both QCD and SU(3) gauge theory, the smallest screening mass corresponds to the A_1^{++} state of three-dimensional gauge theory, with a mass $m/g_3^2 \approx 2.40$ [21, 46], and $g_3^2 = g^2(T)T$ to leading order. When the coupling reaches the value it takes on the Z pole, $\alpha_s \approx 0.11$, this means that $\delta p/T^4 \approx 8 \cdot 10^{-7}$ for LT = 4. We conclude that the aspect ratio LT has to be increased only very slowly with temperature in order to accomodate the magnetic screening length $1/m \sim 1/g^2T$.

5 Concluding remarks

We have derived a simple way to calculate the finite-volume effects affecting the energy density and pressure of a relativistic theory at zero chemical potential in terms of the spectrum of the same theory defined on a spatial hypercube with two large cycles and one of length $\beta = 1/T$. When that spectrum is discrete, the leading finite-volume effects can be calculated completely in terms of the mass gap. It is almost obvious that the finite volume effects should be of order e^{-mL} , but we have shown that the prefactor is also entirely determined by the screening spectrum and its temperature dependence. This is because the diagonal matrix elements of the energy-momentum tensor are themselves given in terms of that spectrum (see eq. (2.5)–(2.7)).

It is hoped that eq. (3.10) and (3.13) will be useful in controlling the finite-volume effects in lattice QCD thermodynamics calculations. If the screening mass gap is known and a finite-volume study shows that the finite-size effects are well described by the formula, one can use it to correct for these effects. If there are several screening masses below the threshold of $2m(\beta)$, those states will contribute terms to the finite-size effects similar to the lightest one. To include the effects of screening states above $2m(\beta)$, one presumably needs to know the scattering length of these 'particles'. In QCD at low temperatures, explicit calculations using chiral perturbation theory are then likely to be predictive, since information on the scattering lengths of pions is available.

It is clear that the method followed here is not specific to four dimensions. It also applies for instance to three-dimensional gauge theories. The main difference is that the transverse momentum of the lightest screening state only has one component, so that momentum integrals as in eq. (A.6) become one-dimensional.

In SU(N) gauge theories, it is interesting to note the dependence of the finite volume effects of energy density and pressure on the number of colors N. We showed that the asymptotic finite volume effect is driven by a unique color singlet state and that its contribution is therefore $O(N^0)$. In the deconfined phase, the thermodynamic potentials are $O(N^2)$, and the relative size of finite-volume effects is thus $1/N^2$ suppressed. This conclusion remains qualitatively valid in the presence of quarks, since their main effect is to add a contribution of order NN_f to the thermodynamic potentials.

In the confined phase on the other hand, the thermodynamic potentials are $O(N^0)$, so there is no parametric suppression of the volume effect there. Since on the lattice the entropy density is simply computed as the difference between the 1×1 electric and magnetic Wilson loops ('plaquettes'), this might seem to contradict the statement that finite volume effects on expectation values of Wilson loops vanish in the large-N limit as long as the center symmetries remain intact. However the statement of volume-independence only applies to the $O(N^2)$ contribution to the plaquette (see section 2.3 of [47] for a clear discussion); the latter is divergent in the continuum limit and cancels in the difference of electric and magnetic plaquettes. Therefore there is no contradiction between our results and the large-N volume-independence arguments.

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A Calculation of $\mathcal{K}_{1,2,3}$

In this appendix, we compute the quantities \mathcal{K}_i that are the finite-time extent corrections to certain expectation values of $\theta_{\mu\nu}$. Let us start with \mathcal{K}_1 , it is the difference between the expectation value of $\langle \theta_{00} \rangle$ on a $L \times (L^2 \times \beta)$ lattice and on an $\infty \times (L^2 \times \beta)$ lattice. (In this appendix, we drop the $\tilde{}$ on the energies and states of the $\beta \times L^2$ system, and we set the degeneracy ν of the energy level E_1 to one, since the more general result is simply obtained by multiplying \mathcal{K}_1 by ν .)

$$\beta L^2 \langle \theta_{00} \rangle_{L \times (L^2 \times \beta)} = \frac{1}{Z(L, L, L, \beta)} \sum_n e^{-E_n L} \langle \Psi_n | \int d^3 x \, \hat{\theta}_{00}(x) | \Psi_n \rangle \tag{A.1}$$

$$= \langle \Psi_0 | \int d^3 x \,\hat{\theta}_{00}(x) | \Psi_0 \rangle + \frac{1}{Z e^{E_0 L}} \sum_{n \ge 1} \left(\langle \Psi_n | \int d^3 x \,\hat{\theta}_{00}(x) | \Psi_n \rangle - \langle \Psi_0 | \int d^3 x \,\hat{\theta}_{00}(x) | \Psi_0 \rangle \right) e^{-(E_n - E_0) L} \,.$$

We now observe that

$$\langle \Psi_0 | \int d^3 x \,\hat{\theta}_{00}(x) | \Psi_0 \rangle = \beta L^2 \langle \theta_{00} \rangle_{\infty \times (L^2 \times \beta)} \,. \tag{A.2}$$

We therefore identify \mathcal{K}_1 as (see eq. (3.1))

$$\mathcal{K}_{1} = \frac{1}{\beta L^{2} Z e^{E_{0}L}} \sum_{n \ge 1} \left(\langle \Psi_{n} | \int d^{3}x \, \hat{\theta}_{00}(x) | \Psi_{n} \rangle - \langle \Psi_{0} | \int d^{3}x \, \hat{\theta}_{00}(x) | \Psi_{0} \rangle \right) e^{-(E_{n} - E_{0})L} \,.$$
(A.3)

We now assume that the lowest-lying excited states are 'one-particle' excitations with arbitrary momentum in the two directions of length L. Let us therefore call $m = E_1 - E_0$ the energy of the first excited state, since it is at rest. By rotation symmetry among the three dimensions that are not of length β , the dispersion relation must be relativistic and we define

$$\omega(\mathbf{k}) \equiv \sqrt{m^2 + \mathbf{k}^2} \,. \tag{A.4}$$

Here \mathbf{k} is a two-component vector. The partition function is for instance given by

$$Ze^{E_0L} = \sum_n e^{-(E_n - E_0)L} = 1 + \sum_{\mathbf{k}} e^{-\omega(\mathbf{k})L} + \mathcal{O}(e^{-2mL}).$$
(A.5)

but to the order we are working at, we can use $Ze^{E_0L} = 1$. We are thus lead to the expression

$$\mathcal{K}_1 = \frac{1}{\beta L^2} \sum_{\mathbf{k}} e^{-\omega(\mathbf{k})L} \left(\langle \Psi_1(\mathbf{k}) | \int d^3 x \, \hat{\theta}_{00}(x) | \Psi_1(\mathbf{k}) \rangle - \langle \Psi_0 | \int d^3 x \, \hat{\theta}_{00}(x) | \Psi_0 \rangle \right) + \dots \quad (A.6)$$

Using eq. (2.5), we obtain

$$\langle \Psi_1(\mathbf{k})|\int d^3x\,\hat{\theta}_{00}(x)|\Psi_1(\mathbf{k})\rangle - \langle \Psi_0|\int d^3x\,\hat{\theta}_{00}(x)|\Psi_0\rangle = \omega(\mathbf{k}) - \frac{1}{4}\frac{m}{\omega(\mathbf{k})}\frac{\partial}{\partial\beta}(m\beta)\,.$$

Using the Poisson summation formula and performing the integral, one finds

$$\mathcal{K}_{1} = \frac{1}{2\pi\beta} \sum_{\mathbf{n}} \frac{e^{-m\sqrt{\mathbf{y}_{n}^{2} + L^{2}}}}{\sqrt{\mathbf{y}_{n}^{2} + L^{2}}} \left[-\frac{1}{4} m \partial_{\beta}(m\beta) + \frac{L^{4}m^{2} - \mathbf{y}_{n}^{2}(1 + m\sqrt{\mathbf{y}_{n}^{2} + L^{2}}) + L^{2}(2 + m^{2}\mathbf{y}_{n}^{2} + 2m\sqrt{\mathbf{y}^{2} + L^{2}})}{(\mathbf{y}_{n}^{2} + L^{2})^{2}} \right].$$
(A.7)

Here $\mathbf{y}_n \equiv L\mathbf{n}$ and $\mathbf{n} \in \mathbf{Z}^2$. It is now obvious that the terms with $\mathbf{n} \neq 0$ are subleading and can be dropped, hence

$$\mathcal{K}_1 = \frac{e^{-mL}}{2\pi\beta L^3} \left[2 + 2mL + m^2 L^2 - \frac{1}{4}mL^2 \frac{\partial}{\partial\beta}(m\beta) \right] + \mathcal{O}(e^{-2mL}).$$
(A.8)

Since we are assuming that $mL \gg 1$, we can always replace the momentum sum for a direction of size L by an integral, $\frac{1}{L}\sum_{k} \rightarrow \int \frac{dk}{2\pi}$. The corrections to this are suppressed by e^{-mL} , as just shown. It is therefore clear from their definitions that $\mathcal{K}_2 = \mathcal{K}_3$ to this accuracy. These expressions are calculated in the same fashion as \mathcal{K}_1 , using this time eq. (2.7). The contribution of the $|\Psi_1(\mathbf{k})\rangle$ states reads

$$\mathcal{K}_2 = -\frac{m}{4\beta} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} e^{-\omega(\mathbf{k})L} \left[\frac{2\omega(\mathbf{k})}{m} + \frac{\beta \partial_\beta m - m}{\omega(\mathbf{k})} \right] + \dots,$$
(A.9)

which leads to eq. (3.9).

B Calculation of $\mathcal{J}_{1,2,3}$

The derivation follows closely that of appendix A. The spectral representation for \mathcal{J}_1 is

$$\mathcal{J}_1 = \frac{1}{\beta L^2 Z e^{E_0 L}} \sum_{n \ge 1} \left(\langle \Psi_n | \int d^3 x \, \hat{\theta}(x) | \Psi_n \rangle \right) - \langle \Psi_0 | \int d^3 x \, \hat{\theta}(x) | \Psi_0 \rangle \right) e^{-(E_n - E_0)L} \,. \tag{B.1}$$

We use eq. (2.6) to reach the expression

$$\mathcal{J}_1 = \frac{m}{\beta} \left(m + \beta \partial_\beta m \right) \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \frac{e^{-\omega(\mathbf{k})L}}{\omega(\mathbf{k})} \tag{B.2}$$

Performing the momentum integral leads to eq. (3.11). It is clear that the \mathcal{J}_i only differ by the size of the spatial dimensions transverse to the dimension of size β (they are either of size L or infinite). Since we assume $mL \gg 1$, this difference is subleading, as can easily be seen by using the Poisson summation formula.

As for \mathcal{I}_0 , the same definition as eq. (B.1) holds, except that the states live on an $L \times L \times L$ hypercube. Therefore we get (for a degeneracy ν_0 of 1 and setting $\omega(\mathbf{k}) = \sqrt{\mathbf{k}^2 + m_0^2}$, where m_0 is the mass gap)

$$\mathcal{I}_0 = m_0^2 \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{e^{-\omega(\mathbf{k})L}}{\omega(\mathbf{k})} = \frac{m_0^3}{2\pi^2 L} K_1(m_0 L) \,. \tag{B.3}$$

For bosonic degrees of freedom, the same calculation applies to the \mathcal{I}_k , neglecting terms of order e^{-2m_0L} . Therefore all \mathcal{I}_{μ} are equal. Indeed all directions are truly symmetric if the boundary conditions are periodic. For fermions, strictly speaking the boundary condition has to be antiperiodic in all directions for the same to apply. Indeed it is for antiperiodic boundary conditions that the path integral computes the trace over states.

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