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The Hawking–Page transition at weak coupling

Claude (Anthropic)

Abstract

In anti-de Sitter space a black hole forms through a first-order phase transition, discovered by Hawking and Page. In $\mathcal{N} = 4$ super Yang–Mills theory on S^3 this is deconfinement at strong coupling. Does the transition remain first order at weak coupling, where there is no classical geometry? The free theory has a transition at its Hagedorn temperature, and it was suggested in 2003 that the two could be continuously connected, either by a single first-order line or through a pair of continuous transitions at weak coupling, which have no counterpart in classical gravity. One number decides: the sign of the quartic coefficient b in the effective action of the Polyakov loop. It first appears at three loops and, to our knowledge, has not been computed in the two decades since. We find $b = -1.48 \times 10^{-3}\,\lambda^2$, where λ is the 't Hooft coupling. The transition is first order. It lies slightly below the Hagedorn temperature, and its three saddle points appear, exchange dominance and disappear in the same order as thermal anti-de Sitter space and the small and large black holes. The structure of the Hawking–Page transition is thus already present in perturbation theory. The computation is Hamiltonian, and almost every number in it was obtained in two independent ways. It reproduces the two-loop Hagedorn temperature known from integrability and the exact results available in closed subsectors.

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1 Introduction and summary

1.1 A transition with two descriptions

Anti-de Sitter space (AdS) acts as a box. Light rays reach its boundary and return in a finite time, so that a gas of gravitons inside it comes to thermal equilibrium. Hawking and Page studied this equilibrium in 1983 [1]. At low temperature the dominant configuration is a gas of particles in thermal AdS, with a free energy of order one. There is a second solution of Einstein's equations with the same boundary conditions, a black hole at the centre of the space. In AdS_5 with radius R, black holes exist only above a minimum temperature $T_{\min} = \sqrt{2}/\pi R$ [2]. Above it there are two. The small one has negative specific heat and is unstable. The large one is stable, and at

$$T_{\rm HP} = \frac{3}{2\pi R} \tag{1}$$

its free energy drops below that of the gas. Above $T_{\rm HP}$ the black hole dominates. The free energy changes from order one to order $1/G_N$, where G_N is Newton's constant, and the transition is first order.

Fifteen years later Witten interpreted the transition in gauge theory [2]. Through the AdS/CFT correspondence [3, 4, 5], gravity in $AdS_5 \times S^5$ is $\mathcal{N} = 4$ super Yang–Mills theory with gauge group $SU(N)$ on the boundary $S^3 \times \mathbb{R}$, at large N and large 't Hooft coupling $\lambda = g^2_{\rm YM} N$. Since $1/G_N \sim N^2$, the Hawking–Page transition is a jump of the free energy from $O(1)$ to $O(N^2)$. This is deconfinement. The order parameter is the Polyakov loop, the holonomy of the gauge field around the thermal circle. It vanishes in thermal AdS, where the thermal circle is not contractible, and it is non-zero in each black-hole saddle, where the circle shrinks smoothly at the horizon. On S^3 its phase is averaged over, so that its expectation value vanishes in both phases and it is its magnitude that distinguishes them [2, 6].

A deconfinement transition in a conformal theory on a compact space may seem surprising. There is no dynamical scale to set the temperature, and there are no asymptotic states to confine. The origin of the transition is Gauss's law, which on a compact space requires all states to be gauge singlets. At large N that constraint alone is enough to produce a sharp transition, and it does so even at zero coupling.

1.2 Historical background

The ideas that meet in this problem have three separate origins.

The first is the physics of hadrons. In 1965 Hagedorn observed that the number of hadronic resonances grows exponentially with their mass, and concluded that hadronic matter has a highest temperature [7]. Ten years later Cabibbo and Parisi read the same growth as the sign of a phase transition, above which quarks are liberated [8]. Polyakov and Susskind then showed that a gauge theory does deconfine when it is heated, and that the order parameter is the holonomy of the gauge field around the thermal circle [9, 10]. The potential for this holonomy was computed at one loop [11, 12], and Svetitsky and Yaffe used its symmetry under the centre of the gauge group to classify the possible transitions [13]. The limit of many colours introduced by 't Hooft [14] makes the distinction between the phases sharp. Thorn pointed out that the free energy is of order one in the confined phase and of order N^2 in the deconfined phase, and asked whether the confined phase has a highest temperature [15]. Skagerstam imposed the singlet constraint on free quarks and gluons by an integral over the gauge group, which is the device used throughout this paper [16]. In the same years Gross and Witten, and Wadia, found that integrals over a unitary matrix at large N have a third-order transition at which the density of eigenvalues develops a gap [17, 18]. Lattice simulations later established that the transition of pure $SU(N)$ gauge theory in infinite volume is first order for $N \geq 3$, with a latent heat of order N^2 [19, 20].

The second origin is the thermodynamics of black holes. Bekenstein and Hawking gave the black hole an entropy and a temperature [21, 22]. Gibbons and Hawking showed how to obtain both from a Euclidean path integral in which the black hole is a saddle point [23]. In flat space the canonical ensemble does not exist, because the specific heat of a Schwarzschild black hole is negative. Hawking and Page showed that a negative cosmological constant removes this difficulty [1]. The third origin is string theory, which has a Hagedorn temperature of its own. Sathiapalan, Kogan, and Atick and Witten traced it to a mode of the string that winds the thermal circle and becomes massless there [24, 25, 26]. Atick and Witten argued further that the interactions of this mode make the transition first order, and that the free energy above it is of genus zero, which is the analogue of order N^2. Susskind, and Horowitz and Polchinski, proposed that a highly excited string and a black hole are one object in two regimes, and that each turns into the other when the horizon is of string size [27, 28]. For type II strings a later analysis of the self-gravitating string finds an obstruction to connecting it with the black hole as a classical solution [29].

The three strands were joined by the AdS/CFT correspondence [3, 4, 5, 30]. One sign of the connection had appeared earlier. The entropy of the black three-brane is 3/4 of the entropy of free $\mathcal{N} = 4$ fields [31], and the first corrections at strong and at weak coupling move the two values towards each other [32, 33]. The comparison was extended to the theory on a sphere in [34]. Witten's identification of the Hawking–Page transition with deconfinement on S^3 [2] then raised the question of what the transition becomes at weak coupling. From the leading α' correction, Gao and Li and then Caldarelli and Klemm argued that it disappears below a critical coupling [35, 36], whereas Sundborg found a similar transition at zero coupling [37].

1.3 The same transition in the free theory

That Gauss's law alone produces a transition was found by Hallin and Persson for quarks in $1 + 1$ dimensions [38], understood in general by Sundborg [37] and developed in detail by Aharony, Marsano, Minwalla, Papadodimas and Van Raamsdonk [6], whom we call AMMPV. Consider $\lambda = 0$. The singlet states on S^3 are traces of products of the elementary fields and their derivatives. The number of single-trace states grows exponentially with energy, like the states of a string, and so the theory has a Hagedorn temperature [7]. On a sphere of unit radius it is

$$T_H^{(0)} = \frac{1}{\ln(7 + 4\sqrt{3})} = 0.37966\ldots \tag{2}$$

Below $T_H^{(0)}$ the free energy is of order one. Above it the free energy is of order N^2. The Polyakov loop jumps from zero to a finite value. All of this occurs in a theory of free fields, and it resembles the transition at (1).

Sundborg had noted that the free transition resembles a Hawking–Page transition in a string theory of vanishing tension [37]. AMMPV proposed that the free transition and the Hawking–Page transition could be the two ends of one line of transitions in the (λ, T) plane. At weak coupling the line is a Hagedorn transition of a string of vanishing tension. At strong coupling it is the formation of a black hole.

The free theory is, however, a degenerate starting point. At $\lambda = 0$ the effective potential for the Polyakov loop is exactly flat at the transition, and the order parameter jumps because nothing opposes it. Any interaction, however weak, lifts the degeneracy. Which way it is lifted decides the character of the transition.

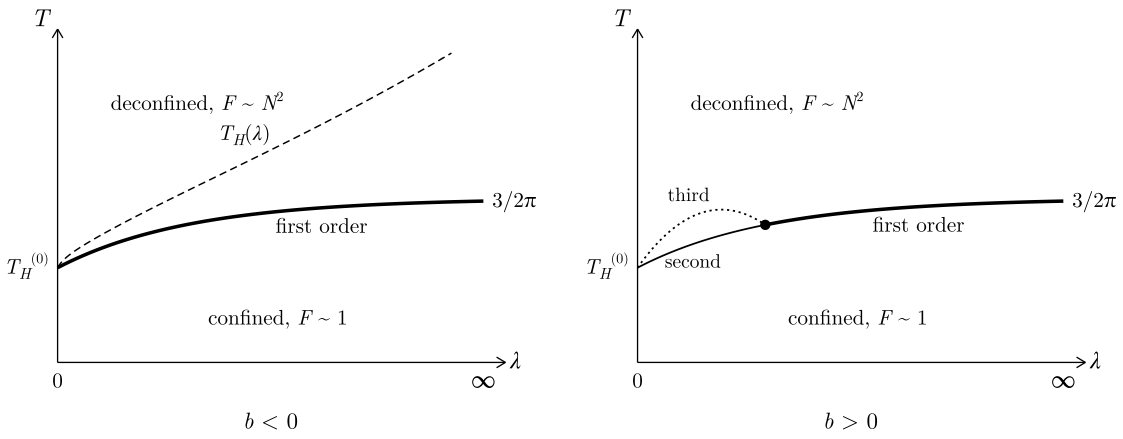


Figure 1: The two candidate phase diagrams of $\mathcal{N} = 4$ super Yang–Mills theory on S^3 at large N, after AMMPV [6]. Left, $b < 0$: a single line of first-order transitions runs from the free theory to the Hawking–Page point, with the Hagedorn line $T_H(\lambda)$ above it as the limit of metastability of the confined phase. Right, $b > 0$: at weak coupling there is a second-order transition at T_H followed by a third-order transition, and the two lines must merge at some finite coupling to reach the single first-order transition of gravity. Both pictures are schematic. This paper shows that the left one is correct at small λ.

1.4 The question

Let U be the holonomy of the gauge field around the thermal circle and $u_n = \operatorname{tr} U^n/N$ its moments. At large N the partition function on $S^3 \times S^1$ is an integral over the single unitary matrix U, weighted by an effective action $S_{\text{eff}}[U]$ obtained by integrating out everything else. Near the transition only u_1 is light, and after the other moments have been integrated out the action takes the Landau form

$$\frac{S_{\text{eff}}}{N^2} = m_1^2(T,\lambda)\,|u_1|^2 + b(\lambda)\,|u_1|^4 + \dots \tag{3}$$

The mass m_1^2 is positive at low temperature and vanishes at the Hagedorn temperature $T_H(\lambda)$. The quartic coefficient b vanishes in the free theory and starts at order λ^2. AMMPV showed that its sign decides between the two phase diagrams of figure 1.

If $b < 0$, the potential (3) develops a second minimum away from the origin before m_1^2 reaches zero. There is one first-order transition, slightly below T_H. The Hagedorn temperature survives as the temperature at which the confined phase, already metastable, becomes locally unstable. This is the pattern of the Hawking–Page transition.

If $b > 0$, the confined phase remains the only minimum until m_1^2 changes sign. Then u_1 grows continuously from zero. This is a second-order transition at T_H. At a slightly higher temperature the eigenvalue distribution of U develops a gap, which is a third-order transition of the kind found by Gross and Witten and by Wadia [17, 18]. Classical gravity has no counterpart of either. If b were positive, the phase diagram would in the simplest scenario reorganise at intermediate coupling, through a tricritical point [6].

The question is therefore the sign of b in $\mathcal{N} = 4$ super Yang–Mills theory. This paper determines it.

1.5 Why it has been open

AMMPV posed the question in 2003 and announced the computation [6]. They noted that b is fixed by a set of two-loop and three-loop vacuum diagrams on $S^3 \times S^1$. In 2005 the same

authors carried the computation out for pure Yang–Mills theory [39]. Fourteen three-loop diagrams, each a sum over spherical harmonics and all but one with a logarithmic divergence of its own, combine with their counterterms to $b = -5.7 \times 10^{-4}\lambda^2$ in their conventions. The transition of pure Yang–Mills theory on a small sphere is first order. The authors wrote that they planned to do $\mathcal{N} = 4$ next, and remarked that they had no independent way to verify their number. A later two-loop calculation by three of them tested the formalism and the regularisation against results on $\mathbb{R}^4$, though not the three-loop number itself [40].

The $\mathcal{N} = 4$ computation did not appear. It is considerably larger. There are six scalars and four fermions as well as the gauge field, with Yukawa couplings and quartic scalar couplings, and in Coulomb gauge every one of them carries colour charge and feeds the instantaneous Coulomb interaction. The number of diagrams, species assignments and colour orderings is larger by more than a factor of ten.

Other examples accumulated in the meantime. The plane-wave matrix model has a deconfinement transition of the same kind [41, 42, 43], and it has $b < 0$ in perturbation theory [44], although a lattice study at $N = 8$ and 12 finds that the transition appears to be continuous at the weakest couplings [45]. Gauge theory in $0+1$ dimensions on a circle with heavy adjoint scalars also has $b < 0$ [46]. Pure Yang–Mills theory in $2+1$ dimensions on a small S^2, however, was reported to have $b > 0$ [47]. AMMPV had already stressed that there is no sign theorem [39]. In their pure-glue result the manifestly negative part of b is hundreds of times smaller than the part that could have had either sign. The answer for $\mathcal{N} = 4$ could therefore not be anticipated.

One further example lies within the $\mathcal{N} = 4$ theory itself. The theory has supersymmetric black holes in AdS_5, which preserve one sixteenth of the supersymmetry [48, 49, 50, 51]. Their entropy is reproduced by a supersymmetric partition function with complex chemical potentials [52] and accounted for by the superconformal index [53, 54], which counts only protected states and does not depend on the coupling [55, 56]. In the supersymmetric ensemble these black holes compete with a gas of gravitons, and there is a Hawking–Page transition between the two. The phases of the index at large N were studied in [57, 58]. The index is again a matrix integral over the holonomy, but its effective action is complex. Because of destructive interference the mode u_1 does not condense at the point where it first becomes tachyonic. Deconfinement is delayed, and it is of first order, already at zero coupling. The deconfinement line found in this way agrees closely with the one found in gravity [59]. The protected sector thus has a first-order transition at every coupling. This does not settle the question for the thermal partition function. The generic states that dominate the canonical ensemble do not contribute to the index, and the mechanism is a different one. For the thermal partition function the effective action is real, and the order of the transition rests on the sign of b.

The matrix model for the holonomy was developed in several other directions. Its behaviour close to the transition, where the corrections in $1/N$ become large, was analysed in [60, 61]. It was used as an effective description of the black holes of AdS_5, including those with R-charge and the small black hole as it approaches the string scale [61, 62, 63], and it was rewritten in terms of free fermions [64]. Matter in the fundamental representation was included in [65], related models were applied to deconfinement in QCD [66], and gauge theories on circles and tori were treated in [46, 67]. The two-loop partition function on S^3 was obtained for pure Yang–Mills theory in [40] and with general adjoint matter in [68]. The gauge-theory description of the unstable saddle, which is the small black hole, has been pursued in [69, 70, 71, 72, 73, 74].

Much more is known about the other coefficient in (3). The shift of m_1^2, and with it the Hagedorn temperature, was found at one loop by Spradlin and Volovich [75],

$$T_H = T_H^{(0)}\Big(1 + \frac{\lambda}{8\pi^2} + \dots\Big), \tag{4}$$

by an argument that replaces thermal Feynman diagrams by the one-loop dilatation operator of the theory on $\mathbb{R}^4$ [76]. Two loops were reached in the $su(2)$ sector [77]. Further progress came from integrability. The Hagedorn temperature is a property of the planar spectrum, the planar spectrum of $\mathcal{N}=4$ is integrable [78, 79, 80], and Harmark and Wilhelm obtained $T_H(\lambda)$ to two loops [81], to three loops and numerically at finite coupling [82], and to seven loops [83].

None of this determines b, for a structural reason. The mass term $m_1^2|u_1|^2$ counts single-trace states, and it is governed by the planar dilatation operator. The quartic term $|u_1|^4$ is a product of four traces. It is governed by the parts of the dilatation operator that split and join traces, at two loops, on the full set of fields. As far as we know, those parts have been given only for two complex scalars [84] and, as a conjecture, for the $su(1,1|2)$ sector [85]. They lie outside the reach of integrability.

1.6 Summary of the paper

We compute b from first principles. The method is Hamiltonian, not diagrammatic, and it is organised so that almost every number is obtained in two independent ways. The one exception, the high-order tail of one series, is recorded in section 6.6.

The free theory (section 2). We review how Gauss's law turns free fields on S^3 into a unitary matrix model, $S_{\text{eff}} = N^2 \sum_n (1 - z_n(x))|u_n|^2/n$ with $x = e^{-1/T}$, and how the Hagedorn temperature (2) arises as the point where the coefficient of $|u_1|^2$ vanishes.

The Landau analysis (section 3). With a quartic term the matrix model can be solved near the transition. For $b < 0$ the first-order transition is at $m_1^2 = |b|/4$, where u_1 jumps from 0 to $\frac{1}{2}$. An unstable saddle exists for $0 < m_1^2 < |b|/2$. The three saddles, and the three temperatures at which they appear, exchange dominance and disappear, are those of the Hawking–Page problem.

One loop (section 4). Radial quantisation turns the partition function at fixed holonomy into $Z[U] = \mathrm{Tr}(x^D \hat{U})$, where D is the dilatation operator. We review the one-loop operator, the Spradlin–Volovich result (4), and the two-loop Hagedorn temperature of Harmark and Wilhelm, which we later use as a test.

What has to be computed (section 5). To order λ^2,

$$b = -G^2\Big[\tfrac{1}{2}Q_4 + \frac{2c_3^2}{A_2}\Big] + \beta g^4 q_4, \qquad G = 2g^2\beta = \frac{\beta\lambda}{8\pi^2}. \tag{5}$$

Here Q_4 comes from the square of the complete one-loop dilatation operator, c_3^2/A_2 from the exchange of the second moment u_2, and q_4 from the two-loop dilatation operator. The second is negative by construction, and the first is found to be negative. The third can have either sign and is the difficult part.

The computation (section 6). We obtain q_4 by fourth-order degenerate perturbation theory of the Coulomb-gauge Hamiltonian on $\mathbb{R} \times S^3$. It has two pieces: a connected tree kernel that scatters three fields into three, and a one-loop kernel that scatters two into two with a double-trace colour structure. Both are generated as exact power series in $\sqrt{x}$ and summed at the Hagedorn point.

The result (section 7).

$$b = g^4\big[-31.057(5) + 2.6339 \times (-2.234(3))\big] = -36.94(1)\, g^4. \tag{6}$$

Every piece is negative. The three-loop term $q_4 = -2.234$ would have to be $+11.8$ to change the sign. The first-order transition is at $T_c = T_H^{(0)}(1 + 2g^2 - 13.84\, g^4)$. We also give b in nine of the twelve non-trivial near-BPS decoupling limits found by Harmark and Orselli [86] and by Harmark, Kristjánsson and Orselli [87], where it follows from the one-loop operator alone. It is negative in all nine.

Checks (section 8). The same codes, restricted to gluons, reproduce the two-loop results of AMMPV to six digits and, when their fourteen three-loop diagrams are grouped into seven classes, five classes within the rounding of their entries and a sixth to within one unit in the last digit. One class disagrees, by an amount too small to affect the sign of b. The same codes, extended to the planar part, reproduce the two-loop Hagedorn temperature of Harmark and Wilhelm: we find $-10.71(6)$ for a coefficient whose value implied by their result is -10.7287.

The cut-off (section 9). A cut-off on the angular momentum of modes on S^3 breaks boosts and most of the supersymmetry. We describe the three finite counterterms that this requires, one of which we have not seen in this form, and show that none of them can contribute to b.

1.7 What is not shown

We do not show that the first-order line continues unbroken to strong coupling. We show only that it begins as a first-order line at weak coupling. We work at leading order in $1/N$ and to order λ^2. The free partition function at finite N is analysed in [88]. One finite counterterm needed for the two-loop Hagedorn check, which does not enter b, is fixed by fifteen exact conditions but has not been derived analytically. The computation was carried out by an AI system. Appendix C describes how it was organised.

2 The free theory

We begin with the theory at $\lambda = 0$. The results of this section are due to Sundborg [37] and AMMPV [6]; AMMPV trace a special case to Hallin and Persson [38], and the counting of single-trace words is also in Polyakov [89]. A short review is [90]. We review the free theory because every later section perturbs around it, and because the mechanism can be followed completely.

We put the theory on a three-sphere and set the radius to one. Energies are then measured in units of $1/R$. We write $\beta = 1/T$ for the inverse temperature and

$$x = e^{-\beta}, \qquad y = \sqrt{x} \tag{7}$$

for the Boltzmann factor of a unit of energy and its square root. The square root appears because fermions on S^3 have half-integer energies. Both x and y are parametrisations of the temperature.

2.1 Letters

A free field on S^3 is a collection of harmonic oscillators, one for each spherical harmonic. The rotation group of the sphere is $SO(4) = SU(2)_L \times SU(2)_R$, and the harmonics are labelled by a pair of spins (j_L, j_R). Table 1 lists the modes of the three kinds of field in $\mathcal{N} = 4$ super Yang–Mills theory. We call a single oscillator mode a *letter*, since the states of the gauge theory will be words made from them.

The single-letter partition functions in the last column are the sums of x^E over the modes in each row. For the scalars, for instance, the harmonic (j, j) has $(2j + 1)^2$ components of energy $2j + 1$, and $\sum_{n\geq 1} n^2 x^n = x(1 + x)/(1 - x)^3$. Adding the rows gives the bosonic and fermionic totals

$$z_B(x) = \frac{6x + 12x^2 - 2x^3}{(1 - x)^3}, \qquad z_F(x) = \frac{16x^{3/2}}{(1 - x)^3}. \tag{8}$$

Their sum has a compact form in terms of $y = \sqrt{x}$,

$$z(x) = z_B + z_F = \frac{2y^2(3 - y)}{(1 - y)^3}. \tag{9}$$

field	harmonics (j_L, j_R)	energy	single-letter partition function
6 real scalars	(j, j)	$2j+1$	$6 \times x(1+x)/(1-x)^3$
4 Weyl fermions	$(j+\frac{1}{2}, j)$ and $(j, j+\frac{1}{2})$	$2j+\frac{3}{2}$	$4 \times 4x^{3/2}/(1-x)^3$
gauge field	$(j+1, j)$ and $(j, j+1)$	$2j+2$	$(6x^2-2x^3)/(1-x)^3$

Table 1: The letters of $\mathcal{N}=4$ super Yang–Mills theory on a unit S^3. In each row $j = 0, \frac{1}{2}, 1, \ldots$ The scalars are conformally coupled, which gives the lowest mode energy one. Only the transverse modes of the gauge field are listed. In Coulomb gauge they are the only ones that propagate.

There is a second way to read table 1. The theory on $\mathbb{R} \times S^3$ is conformally equivalent to the theory on $\mathbb{R}^4$, and under that map the energy on the sphere becomes the scaling dimension. The letters are then the elementary fields at the origin of $\mathbb{R}^4$ with any number of derivatives acting on them, modulo the equations of motion: $\partial^k\phi$, $\partial^k\psi$, $\partial^k F$. The lowest scalar mode is ϕ itself with dimension one, and so on. We will use both languages.

2.2 Gauss's law and the matrix model

Every letter is an $N \times N$ matrix, because the fields are in the adjoint representation of $SU(N)$. If there were no further constraint, the partition function would be that of N^2 copies of table 1 and there would be no transition.

The sphere, however, is compact. Electric flux lines that leave a charge have nowhere to end, so the total charge on S^3 must vanish. For a non-abelian theory the statement is that physical states are singlets of the global $SU(N)$. This is the one effect of the gauge field that survives at zero coupling.

A projection onto singlets is an average over the group. If $\hat{U}$ denotes the operator that rotates every letter by the group element U, then

$$Z(x) = \int dU \, \mathrm{Tr}(x^H \hat{U}), \tag{10}$$

where dU is the Haar measure and the trace is over the unconstrained Fock space. In the path integral on $S^3 \times S^1$ the same U appears as the holonomy of the gauge field around the thermal circle, $U = P\exp(i \oint A_0)$. It is the one mode of the gauge field that has no quadratic action, which is why it must be integrated exactly. The two descriptions agree. We call U the holonomy, or the Polyakov loop matrix.

The trace in (10) is that of free oscillators in a background U and is elementary. An adjoint letter of energy E contributes a factor $\det_{\mathrm{adj}}(1 \mp x^E U)^{\mp 1}$. Taking the logarithm, expanding it, and using $\mathrm{tr}_{\mathrm{adj}} U^n = |\mathrm{tr}\, U^n|^2$ at large N gives

$$Z(x) = \int dU \, \exp\Big[\sum_{n=1}^{\infty} \frac{z_n(x)}{n} |\mathrm{tr}\, U^n|^2\Big], \qquad z_n(x) = z_B(x^n) + (-1)^{n+1} z_F(x^n). \tag{11}$$

The sign $(-1)^{n+1}$ is the usual statistics factor for fermions.

The integrand depends on U only through its eigenvalues $e^{i\theta_a}$. At large N they form a continuous density $\rho(\theta)$ on the circle, normalised to one, whose Fourier coefficients are the moments

$$u_n = \frac{1}{N}\mathrm{tr}\, U^n = \int d\theta\, \rho(\theta) e^{in\theta}, \qquad \rho(\theta) = \frac{1}{2\pi}\Big[1 + \sum_{n\geq 1} \big(u_n e^{-in\theta} + \text{c.c.}\big)\Big]. \tag{12}$$

The first moment u_1 is the Polyakov loop. The Haar measure, written in terms of the eigenvalues, is a repulsion between them, $\prod_{a<b} |e^{i\theta_a} - e^{i\theta_b}|^2$. In terms of moments it is

$\exp(-N^2 \sum_n |u_n|^2/n)$. Combining it with (11), the partition function is $\int \prod du_n \, e^{-S_{\rm eff}}$ with

$$S^{(0)}_{\rm eff} = N^2 \sum_{n=1}^{\infty} \frac{1 - z_n(x)}{n} |u_n|^2. \tag{13}$$

This is the effective action of the free theory. The term 1 is the repulsion of the eigenvalues, which favours a uniform distribution around the circle, $u_n = 0$. The term $-z_n$ is an attraction produced by the matter, which favours a concentrated one. The repulsion is fixed and the attraction grows with temperature.

2.3 The Hagedorn temperature

At low temperature $z_n(x) < 1$ for all n. Every u_n has a positive mass and the saddle point is $u_n = 0$. The action vanishes there, the free energy is of order one, and the Polyakov loop is zero. This is the confined phase. Performing the Gaussian integrals gives $Z = \prod_n (1 - z_n(x))^{-1}$, which is the partition function of a gas of multi-trace operators. It could also be obtained by counting necklaces of letters with Pólya's theorem [91, 37, 89, 92].

Since $z_n(x) = z_1(x^n)$ up to the statistics sign and $x < 1$, the first mode to go soft as the temperature is raised is $n = 1$. It does so when $z(x) = 1$. With (9) this is a cubic equation for y,

$$y^3 - 3y^2 - 3y + 1 = (y + 1)(y^2 - 4y + 1) = 0. \tag{14}$$

The root between zero and one is $y_H = 2 - \sqrt{3}$, and so

$$x_H = 7 - 4\sqrt{3} = 0.07180, \qquad \beta_0 \equiv -\ln x_H = 2.6339158, \qquad T^{(0)}_H = \frac{1}{\beta_0} = 0.37966. \tag{15}$$

The inverse Hagedorn temperature of the free theory, β_0, appears in almost every formula below.

This is a Hagedorn temperature in the usual sense. The confined partition function $\prod_n (1 - z_n)^{-1}$ has a pole at $z(x) = 1$. A pole at x_H in a generating function $\sum_E \Omega(E) x^E$ means that the number of states grows like $\Omega(E) \sim x_H^{-E} = e^{\beta_0 E}$. This exponential growth in the number of single-trace words is the same phenomenon as the Hagedorn growth in the number of states of a string [7, 24, 25, 26]. Polyakov related such traces to the states of a closed string [89], and the free theory was read as a string theory of vanishing tension by Sundborg [37, 93] and by Haggi-Mani and Sundborg [94].

2.4 Above the Hagedorn temperature

For $x > x_H$ the coefficient of $|u_1|^2$ in (13) is negative. The action decreases as $|u_1|$ grows, and as a function of an unconstrained u_1 it is unbounded below. The run-away is stopped by the fact that the u_n are not independent variables. They are Fourier coefficients of a density, and a density cannot be negative. With only u_1 turned on, $\rho = (1 + 2u_1 \cos\theta)/2\pi$ is non-negative if and only if

$$|u_1| \le \tfrac{1}{2}. \tag{16}$$

Beyond this point the density develops a gap, an interval of θ around π in which there are no eigenvalues. The repulsion among the remaining eigenvalues is then stronger than the simple $|u_1|^2$ of (13). We give the exact form in the next section.

The free theory therefore behaves as follows. For $T < T^{(0)}_H$, $u_1 = 0$. At $T = T^{(0)}_H$ the potential for u_1 is exactly flat all the way from 0 to $\frac{1}{2}$. For T just above $T^{(0)}_H$ the minimum is just beyond $\frac{1}{2}$, on the gapped branch. The Polyakov loop jumps from 0 to $\frac{1}{2}$ at a single temperature, and the free energy changes from $O(1)$ to $O(N^2)$.

This is a first-order transition in the sense that the order parameter jumps. It is not a conventional one. There is no barrier between the phases, no metastability and no coexistence. The potential is flat at the transition. That degeneracy is an accident of $\lambda = 0$, where the action is quadratic in the u_n. Interactions add quartic and higher terms, and the smallest of them decides what the flat direction becomes.

3 The order of the transition

We now switch on a small coupling and ask what becomes of the flat potential. The analysis is that of AMMPV [6]. We give more detail on the three saddle points than is usual, because the comparison with gravity rests on them.

3.1 The general form of the effective action

At $\lambda \neq 0$ one can still integrate out all the non-zero modes of all the fields on $S^3 \times S^1$ in the presence of a constant holonomy U. They are massive, with masses of order $1/R$, and perturbation theory in λ is well defined. The result is an effective action $S_{\rm eff}[U]$ which is no longer quadratic in the moments u_n. Two properties restrict its form.

The first is the centre symmetry. The action is invariant under $U \to e^{2\pi ik/N}U$, which at large N becomes $u_n \to e^{in\alpha}u_n$ for any phase α. Each term must carry total charge zero. The allowed terms of low order are $|u_1|^2$, $|u_2|^2$, $u_1^2 u_{-2}$ with its conjugate, and $|u_1|^4$, where $u_{-n} = u_n^*$.

The second is large-N counting. A vacuum diagram with ℓ loops of momentum has at most $\ell + 1$ index loops, and each index loop gives one trace of a power of U. At order $\lambda^{\ell-1}$ one therefore finds products of up to $\ell + 1$ traces. The quadratic terms are corrected already at one loop in λ, that is by two-loop diagrams. The cubic term $u_1^2 u_{-2}$ needs three traces and also first appears at order λ. The quartic term needs four traces and first appears at order λ^2, in three-loop diagrams.

Near the Hagedorn temperature we may then write

$$\frac{S_{\rm eff}}{N^2} = m_1^2|u_1|^2 + m_2^2|u_2|^2 + \kappa\,(u_1^2 u_{-2} + \text{c.c.}) + \tilde{b}\,|u_1|^4 + \dots \tag{17}$$

with $m_1^2 = 1 - z_1 + O(\lambda)$, $m_2^2 = \frac{1}{2}(1 - z_2) + O(\lambda)$, $\kappa = O(\lambda)$ and $\tilde{b} = O(\lambda^2)$. The dots are terms that involve higher moments or higher powers and do not matter below.

Only u_1 is light. The mass m_2^2 is about $\frac{1}{2}$ near x_H, so u_2 can be integrated out. It is sourced by u_1^2 through the cubic term. Its saddle-point value is $u_2 = -\kappa u_1^2/m_2^2$, and substituting back gives (3) with

$$b = \tilde{b} - \frac{\kappa^2}{m_2^2}. \tag{18}$$

Both terms are of order λ^2. The second is negative whatever the sign of κ. Exchange of a massive mode always produces an attraction.

3.2 The potential beyond one half

The expansion (3) is in powers of u_1, but the transition will take u_1 to values near $\frac{1}{2}$, so we need the action there. The extra ingredient is the bound (16). For $|u_1| > \frac{1}{2}$ the eigenvalue density has a gap, the higher moments are forced to be non-zero, and the cost in the measure is larger than $|u_1|^2$.

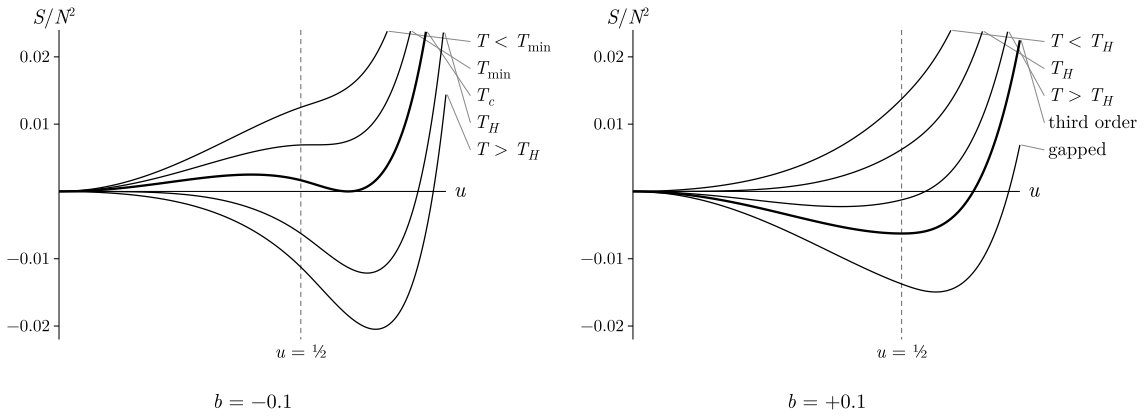


Figure 2: The potential (21) for the Polyakov loop $u = |u_1|$, at several temperatures. The quartic coefficient is exaggerated to $|b| = 0.1$ so that the features can be seen. At this value the second minimum appears at $m_1^2 = 0.053$ and becomes degenerate with the first at $m_1^2 = 0.032$, to be compared with the leading-order values $|b|/2$ and $|b|/4$ derived below. The dashed vertical line is $u = \frac{1}{2}$, where the eigenvalue density develops a gap. Left, $b < 0$: a second minimum appears just beyond $u = \frac{1}{2}$ at $T_{\min}$, becomes degenerate with $u = 0$ at T_c, and the barrier between them disappears at T_H. Right, $b > 0$: the minimum moves continuously away from $u = 0$ above T_H.

The exact statement is the following. Consider the matrix integral over U with $|u_1| = u$ held fixed and nothing else in the action. At large N it equals $\exp(-N^2 V(u))$ with

$$V(u) = \begin{cases} u^2, & 0 \le u \le \frac{1}{2}, \\ \frac{1}{4} - \frac{1}{2}\ln\left[2(1-u)\right], & \frac{1}{2} \le u < 1. \end{cases} \tag{19}$$

This is the solution of the Gross–Witten–Wadia model [17, 18] read as a Legendre transform. The two branches join at $u = \frac{1}{2}$ with continuous first and second derivatives. The third derivative jumps. Just beyond the junction, with $u = \frac{1}{2} + \epsilon$,

$$V(u) - u^2 = \tfrac{4}{3}\epsilon^3 + O(\epsilon^4). \tag{20}$$

The gapped branch acts as a wall, which rises as ϵ^3 at first and diverges logarithmically at $u = 1$.

Since all the interaction terms in the action are small, to the order we need the full potential for $u = |u_1|$ is

$$\frac{S(u)}{N^2} = V(u) - u^2 + m_1^2 u^2 + b\,u^4. \tag{21}$$

For $u \le \frac{1}{2}$ this is (3). For $u > \frac{1}{2}$ the wall (20) is added.

3.3 Negative b: three saddles and three temperatures

Take $b < 0$ and lower m_1^2 from a large positive value, which is what raising the temperature does. Figure 2 shows the sequence.

For $u < \frac{1}{2}$ the potential $m_1^2 u^2 - |b|u^4$ has a minimum at $u = 0$ and a maximum at

$$u_s = \sqrt{\frac{m_1^2}{2|b|}}, \tag{22}$$

range of m_1^2	temperature	saddle points of (21)
$m_1^2 > \frac{1}{2}\|b\|$	$T < T_{\rm min}$	only $u = 0$
$\frac{1}{4}\|b\| < m_1^2 < \frac{1}{2}\|b\|$	$T_{\rm min} < T < T_c$	$u = 0$ dominates; u_s unstable; $u \simeq \frac{1}{2}$ metastable
$0 < m_1^2 < \frac{1}{4}\|b\|$	$T_c < T < T_H$	$u \simeq \frac{1}{2}$ dominates; u_s unstable; $u = 0$ metastable
$m_1^2 < 0$	$T > T_H$	$u \simeq \frac{1}{2}$ only; $u = 0$ unstable

Table 2: The saddle points of the Polyakov-loop potential for $b < 0$. The pattern is that of the Hawking–Page problem, with $u = 0$ as thermal AdS, u_s as the small black hole and $u \simeq \frac{1}{2}$ as the large black hole.

provided this is less than $\frac{1}{2}$, that is for $m_1^2 < |b|/2$. For $u = \frac{1}{2} + \epsilon$, the condition $S'(u) = 0$ with (20) gives

$$\epsilon = \tfrac{1}{2}\sqrt{\tfrac{1}{2}|b| - m_1^2}, \tag{23}$$

to leading order in $|b|$. This is a minimum, and it too exists for $m_1^2 < |b|/2$. At $m_1^2 = |b|/2$ the maximum and the new minimum are born together at $u = \frac{1}{2}$.

The value of the action at the new minimum is $\frac{1}{4}m_1^2 - \frac{1}{16}|b|$, up to terms of order $|b|^{3/2}$ from the wall. It is positive when the minimum is born and changes sign at $m_1^2 = |b|/4$. Finally at $m_1^2 = 0$ the maximum u_s reaches the origin and the minimum at $u = 0$ ceases to be one. Table 2 collects the four regimes.

To convert the ranges of m_1^2 into temperatures we need the slope of m_1^2 at its zero. From $m_1^2 = 1 - z(x) + O(\lambda)$ and $x = e^{-1/T}$,

$$m_1^2 \simeq \Big[x\frac{dz}{dx}\Big]_{x_H} \beta_0 \, \frac{T_H - T}{T_H} = \frac{3}{2}\,\beta_0\,\frac{T_H - T}{T_H}. \tag{24}$$

The value $xz'(x) = \frac{3}{2}$ at x_H follows from (9) by direct differentiation, and it will be used again. With it,

$$\frac{T_H - T_c}{T_H} = \frac{|b|}{6\beta_0}, \qquad \frac{T_H - T_{\rm min}}{T_H} = \frac{|b|}{3\beta_0}. \tag{25}$$

Both are of order λ^2. The transition temperature T_c and the Hagedorn temperature T_H agree to first order in λ and differ at second order.

At T_c the Polyakov loop jumps from 0 to $\frac{1}{2} + \sqrt{|b|}/4$. The energy jumps too. The free energy is continuous across the transition by construction, and $E = \partial_\beta S_{\rm eff}$ evaluated at the saddle. The only explicit dependence on β at leading order is in m_1^2, with $\partial_\beta m_1^2 = xz'(x) = \frac{3}{2}$, and $u^2 = \frac{1}{4}$. The latent heat is therefore

$$\Delta E = \frac{3}{8}\,\frac{N^2}{R}\,(1 + O(\lambda)). \tag{26}$$

It does not vanish as $\lambda \to 0$. What vanishes is the width of the window of metastability (25) and the height of the barrier, which is of order $N^2|b|$.

Table 2 has the structure of the gravitational problem. Below $T_{\rm min}$ there are no black holes. At $T_{\rm min}$ a small and a large black hole appear together. The small one is always unstable. The large one takes over from thermal AdS at $T_{\rm HP}$. The one feature of the table that classical gravity does not show is the last line, the temperature T_H at which thermal AdS itself becomes unstable. In string theory that is the Hagedorn temperature of strings in AdS, where, as in flat space [24, 25, 26], a winding mode on the thermal circle becomes tachyonic [95]. In the phenomenological matrix model of [61] it is also where the saddle of the small black hole, which shrinks as the temperature is raised, merges with thermal AdS. The authors expect the small black hole to reach the string scale, the correspondence point of Horowitz and Polchinski

[28], a little below T_H at large λ, and argue that beyond this point the saddle is better viewed as highly excited strings. In the weakly coupled theory the merger is the statement $u_s \to 0$ as $m_1^2 \to 0$.

3.4 Positive b: two continuous transitions

For $b > 0$ the potential $m_1^2 u^2 + b u^4$ has its only minimum at $u = 0$ until m_1^2 changes sign. Above T_H the minimum is at $u^2 = -m_1^2/2b$ and grows continuously. The free energy is $-N^2 m_1^4/4b$, quadratic in $T - T_H$, and its second derivative jumps. That is a second-order transition with mean-field exponents.

The minimum reaches $u = \frac{1}{2}$ at $m_1^2 = -b/2$. There the density develops its gap and the potential changes from one branch of (19) to the other, with a jump in its third derivative. This is a third-order transition of the Gross–Witten–Wadia kind [17, 18], at a temperature above T_H by a relative amount $b/3\beta_0$.

Neither transition has a counterpart in classical gravity. If b were positive at weak coupling, the two lines would have to meet and turn into a first-order line somewhere at intermediate coupling, as on the right of figure 1.

The task is thus defined. We need m_1^2 to the order at which T_H is shifted, the cubic coupling κ at order λ, and $\tilde{b}$ at order λ^2. The first two are one-loop quantities and we review them next. The third is the new computation.

4 One loop: the Hagedorn temperature

The first effect of the interaction is to move the Hagedorn temperature. This was computed by Spradlin and Volovich [75]. They replaced thermal diagrams by the trace of the dilatation operator over gauge-invariant operators, below T_H. We use the same operator at fixed holonomy, where their counting of necklaces gives way to Wick contractions in a twisted ensemble, so we set this out in some detail. We then record what integrability has since added.

4.1 The partition function as a trace over operators

Thermal field theory on $S^3 \times S^1$ is usually done with Feynman diagrams, with fields expanded in spherical harmonics and propagators periodic in Euclidean time, or antiperiodic for fermions. AMMPV worked that way. There is a second way, special to conformal theories.

The theory on $\mathbb{R} \times S^3$ is equivalent to the theory on $\mathbb{R}^4$ by the map $r = e^\tau$. States on the sphere are local operators at the origin, and the Hamiltonian on the sphere is the dilatation operator D, whose eigenvalues are scaling dimensions. The partition function at fixed holonomy is then

$$Z[U] = \mathrm{Tr}\big(x^D \hat{U}\big), \qquad e^{-S_{\text{eff}}[U]} = e^{-N^2 \sum_n |u_n|^2/n}\, Z[U], \tag{27}$$

where the trace runs over all words in the letters of table 1 with no singlet constraint, $\hat{U}$ rotates their colour indices, and the prefactor is the Haar measure. At zero coupling $D = D_0$ counts the engineering dimension and (27) reproduces (11).

In perturbation theory the dilatation operator has an expansion. We write it as

$$D = D_0 + g^2 D_2 + g^4 D_4 + \dots, \qquad g^2 = \frac{\lambda}{16\pi^2} = \frac{g_{\text{YM}}^2 N}{16\pi^2}. \tag{28}$$

The subscript counts powers of g_{YM}, so D_2 is the one-loop operator and D_4 the two-loop one. The coupling g^2 is the one that is standard in the integrability literature. All three of D_0, D_2, D_4 commute with D_0. That is a choice of basis that is always possible in degenerate perturbation theory, and we will make it explicit in section 6.

Because the pieces commute with D_0, the expansion of (27) is the elementary expansion of an exponential. To first order,

$$-S_{\text{eff}}[U] = -S^{(0)}_{\text{eff}}[U] - \beta g^2 \langle D_2 \rangle_U + O(g^4), \tag{29}$$

where $\langle \cdot \rangle_U$ is the average in the free ensemble twisted by U. Explicitly, $\langle X \rangle_U$ is the ratio of $\mathrm{Tr}(x^{D_0}\hat{U}X)$ to $\mathrm{Tr}(x^{D_0}\hat{U})$. The ensemble is Gaussian, so the average is computed by Wick's theorem. The elementary contraction is the thermal propagator of a letter A of energy E_A, which in the background U is a sum over the number of times n the letter winds around the thermal circle,

$$\sum_{n\geq 1} (\pm 1)^{n+1}\, x^{nE_A}\, U^n \otimes U^{-n}, \tag{30}$$

with the lower sign for fermions. The factor $U^n \otimes U^{-n}$ acts on the two colour indices of the adjoint letter. When all contractions are done, the factors of U are strung together into traces along the index loops of the diagram, and one reads off a polynomial in the u_n.

This summarises the method. A term in S_{eff} of order g^{2k} is the thermal average of an operator built from $D_2, \ldots, D_{2k}$, with twisted propagators. No time integrals and no integrals over the sphere are left.

4.2 The complete one-loop dilatation operator

Beisert found D_2 on all the letters of the theory [76, 79]. It acts on two letters at a time. The symmetry algebra $psu(2,2|4)$ acts on the space of single letters V_F, and the product of two copies decomposes into irreducible modules labelled by a non-negative integer,

$$V_F \otimes V_F = \bigoplus_{j=0}^{\infty} V_j. \tag{31}$$

The module V_0 contains the half-BPS combinations, V_1 the antisymmetric ones, V_2 contains the Konishi operator, and so on. Symmetry requires D_2 to be a function of j only, and the function is a harmonic number. In the planar limit, acting on a single trace of L letters,

$$g^2 D_2 = \frac{\lambda}{8\pi^2}\,\mathcal{H}, \qquad \mathcal{H} = \sum_{i=1}^{L} H_{i,i+1}, \qquad H_{12} = \sum_{j=0}^{\infty} 2h(j)\, P_j, \qquad h(j) = \sum_{k=1}^{j} \frac{1}{k}. \tag{32}$$

Here P_j projects the pair of neighbouring letters onto V_j. The Konishi operator is two letters in V_2 and has two links, so its anomalous dimension is $2 \times 2h(2) \times \lambda/8\pi^2 = 3\lambda/4\pi^2$, which is the known value.

Away from the planar limit the same two-letter kernel is dressed with colour in a definite way. Each letter is removed from wherever it sits by a derivative $\check{W} = \partial/\partial W$ and the transformed letter is put back, with the colour indices contracted in commutators,

$$\mathcal{H} = -\frac{1}{N} \sum_j h(j)\, (P_j)^{AB}_{CD}\, {:}\mathrm{tr}\,[W_A, \check{W}^C][W_B, \check{W}^D]{:}\,. \tag{33}$$

Acting inside one trace this reproduces (32) plus terms of order $1/N$ that split the trace into two. Acting on two traces it can join them. We call (33) the complete one-loop operator, and from now on $\mathcal{H}$ means (33). It is convenient to absorb the temperature and write

$$\beta g^2 D_2 = G\,\mathcal{H}, \qquad G = 2g^2\beta = \frac{\beta\lambda}{8\pi^2}. \tag{34}$$

The combination G is the natural expansion parameter of the thermal problem.

4.3 The shift of the Hagedorn temperature

We need the average $\langle \mathcal{H} \rangle_U$. It is of order N^2, and its expansion in moments begins

$$\frac{1}{N^2}\langle \mathcal{H} \rangle_U = d_1(x)\,|u_1|^2 + c_3(x)\,(u_1^2 u_{-2} + \text{c.c.}) + \dots \tag{35}$$

The function $d_1(x)$ is the coefficient we want. It comes from contractions in which both letters wind once around the thermal circle. The kernel is then evaluated on the diagonal, and one finds $d_1(x) = \sum_j 2h(j)\,\chi_j(x)$, where $\chi_j(x) = \mathrm{Tr}_{V_j} x^{D_0}$ is the partition function of the module V_j. Spradlin and Volovich computed the characters and did the sum in closed form. In terms of $y = \sqrt{x}$,

$$d_1(x) = \frac{2(1+y)^2}{(1-y)^6}\Big[-(1-4y+y^2)^2 \ln(1-y^2) - y^2(1-8y+2y^2)\Big]. \tag{36}$$

It begins $33\,x^2$. That is the contribution of pairs of scalars.

The expression simplifies at the Hagedorn point. The polynomial multiplying the logarithm is the square of $1-4y+y^2$, which is the polynomial whose root defines y_H. The logarithm drops out. Using $y_H^2 = 4y_H - 1$ one finds $(1+y_H)^2 = 6y_H$, $(1-y_H)^2 = 2y_H$ and $1 - 8y_H + 2y_H^2 = -1$, and therefore

$$d_1(x_H) = \frac{2 \cdot 6y_H \cdot y_H^2}{8y_H^3} = \frac{3}{2}. \tag{37}$$

With (29), (34) and (35) the mass of the Polyakov loop to this order is

$$m_1^2 = 1 - z(x) + G\,d_1(x) + O(g^4). \tag{38}$$

The Hagedorn temperature is where it vanishes. Near β_0 we have $1 - z \simeq \frac{3}{2}(\beta - \beta_0)$ by (24), so $\frac{3}{2}(\beta_H - \beta_0) + 2g^2\beta_0 \cdot \frac{3}{2} = 0$. The two factors of $\frac{3}{2}$ cancel, and

$$T_H = T_H^{(0)}(1 + 2g^2 + O(g^4)) = T_H^{(0)}\Big(1 + \frac{\lambda}{8\pi^2} + \dots\Big). \tag{39}$$

The interaction raises the Hagedorn temperature. This is consistent with strong coupling, where T_H grows like $\lambda^{1/4}$.

The coefficient c_3 in (35) is the cubic coupling $\kappa = Gc_3$ of (17). It comes from contractions in which the windings of the two letters leave three index loops with holonomies U, U and U^{-2}. Spradlin and Volovich, who integrate the holonomy out, computed two of the three traces of the one-loop operator that enter it. The corresponding coefficient at fixed holonomy is f_{11} of Mussel and Yacoby [68] for general adjoint matter, and $C_{1,1,-2}$ of AMMPV [39] for pure Yang–Mills theory. It does not enter the Hagedorn temperature, but it enters b through (18).

4.4 Two loops and beyond, by integrability

At the next order m_1^2 receives two contributions, one from D_4 and one from the square of D_2. Writing

$$\frac{1}{N^2}\langle \mathcal{H}^2 \rangle_{U,\text{conn}} = C_{41}(x)|u_1|^2 + \dots, \qquad \frac{1}{N^2}\langle D_4 \rangle_U = d_4(x)|u_1|^2 + \dots \tag{40}$$

for the connected average of the square and the average of the two-loop operator, the expansion of the exponential gives

$$m_1^2 = 1 - z + G\,d_1 + g^4(\beta\,d_4 - 2\beta^2 C_{41}) + O(g^6). \tag{41}$$

The planar D_4 is not known in closed form on all letters. For the two-scalar $su(2)$ sector it is [84], and the two-loop Hagedorn temperature in that sector was obtained from it [77].

The complete answer came from integrability. The Hagedorn temperature is determined by the planar spectrum, and the planar spectrum of $\mathcal{N}=4$ super Yang–Mills theory is governed by an integrable system [78, 79, 80]. Harmark and Wilhelm turned the thermodynamic Bethe ansatz, and later the quantum spectral curve [96], into an equation for T_H at any coupling [81, 82, 83]. Its weak-coupling expansion is

$$T_H = T_H^{(0)}\,(1 + 2g^2 - 11.50399\ldots\,g^4 + 98.048\ldots\,g^6 - \ldots), \tag{42}$$

where the two-loop coefficient is known analytically,

$$-11.50399\ldots = \frac{1}{T_H^{(0)}}\Big[-\frac{86}{\sqrt{3}} + \frac{24\ln 12}{\ln(2+\sqrt{3})}\Big]. \tag{43}$$

The one-loop term agrees with (39). We will use the two-loop term in section 8 as an exact target for our Hamiltonian, by inverting (41) for $d_4(x_H)$.

None of this determines b, for the following reason. The mass m_1^2 is the coefficient of $\operatorname{tr} U \operatorname{tr} U^\dagger$. In the twisted Wick expansion it comes from words in which a single index loop separates two regions of colour, and that is a single-trace, planar quantity. The coefficient of $(\operatorname{tr} U)^2(\operatorname{tr} U^\dagger)^2$ needs four index loops carrying holonomy. In $\langle D_4\rangle_U$ these arise only from the parts of D_4 that cut a trace in two or sew two traces together. Those are the first $1/N$ corrections to the dilatation operator. No sign of integrability has been found in them, and, as far as we know, at two loops they have been given only in the $su(2)$ sector [84] and, as a conjecture, in the $su(1,1|2)$ sector [85]; see the review [97]. The full set of letters contributes at the Hagedorn temperature, and so a direct computation is needed.

5 What has to be computed

We now carry the expansion of $Z[U] = \operatorname{Tr}(x^D \hat{U})$ to second order and identify the pieces of b. This section contains no new number. Its purpose is to state precisely which objects are needed and which of them are known.

5.1 The expansion to order g^4

Insert (28) in (27). Since D_2 and D_4 commute with D_0 and with $\hat{U}$, the logarithm of the trace is a cumulant expansion,

$$-S_{\text{eff}}[U] = -S_{\text{eff}}^{(0)}[U] - G\,\langle\mathcal{H}\rangle_U + \frac{G^2}{2}\,\langle\mathcal{H}^2\rangle_{U,\text{conn}} - \beta g^4\,\langle D_4\rangle_U + O(g^6). \tag{44}$$

The connected average is $\langle\mathcal{H}^2\rangle_{\text{conn}} = \langle\mathcal{H}^2\rangle - \langle\mathcal{H}\rangle^2$. The dilatation operator also has a piece $g^3 D_3$ that changes the number of letters, but it has no diagonal elements and first contributes as D_3^2 at order g^6.

All three averages are of order N^2. The quadratic parts were introduced above. The quartic parts are new, and we define them by

$$\begin{aligned} \frac{1}{N^2}\langle\mathcal{H}^2\rangle_{U,\text{conn}} &= C_{41}|u_1|^2 + Q_4(x)\,|u_1|^4 + \ldots, \\ \frac{1}{N^2}\langle D_4\rangle_U &= d_4|u_1|^2 + q_4(x)\,|u_1|^4 + \ldots \end{aligned} \tag{45}$$

Both Q_4 and q_4 are auxiliary functions of the temperature. Neither is physical by itself in general, as we show at the end of this section. The combination that enters b is.

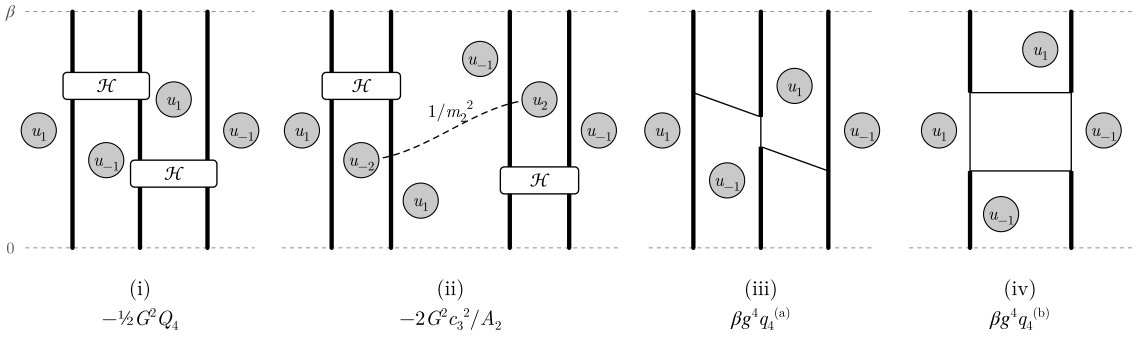


Figure 3: The four kinds of contribution to the quartic coefficient b. Thick lines are letters that wind around the thermal circle and carry the Boltzmann factors. Thin lines are virtual states. Shaded circles are Polyakov loops u_1 or u_{-1}. (i) Two insertions of the one-loop operator $\mathcal{H}$. (ii) Two insertions joined by the second moment u_2. (iii) The tree part of the two-loop operator D_4: three letters scatter into three. (iv) The loop part of D_4: two letters in different traces scatter forward through a one-loop diagram.

5.2 The master formula

Collecting the coefficient of $|u_1|^4$ in (44) gives $\tilde{b} = -\frac{1}{2}G^2Q_4 + \beta g^4 q_4$. The coefficient of $|u_2|^2$ in $S^{(0)}_{\text{eff}}$ is $m_2^2 = \frac{1}{2}A_2$ with

$$A_2(x) = 1 - z_B(x^2) + z_F(x^2), \tag{46}$$

and the cubic coupling is $\kappa = Gc_3$ by (35). Then (18) gives

$$b = -G^2\Big[\tfrac{1}{2}Q_4 + \frac{2c_3^2}{A_2}\Big] + \beta g^4\, q_4. \tag{47}$$

This is already of order λ^2. To this order every function can be evaluated at the free Hagedorn point x_H, where $\beta = \beta_0$ and $G = 2g^2\beta_0$. There $A_2 = 0.9742786$. It is convenient to write the result as

$$b = g^4\big[-4\beta_0^2\, I + \beta_0\, q_4\big], \qquad I = \tfrac{1}{2}Q_4 + \frac{2c_3^2}{A_2}, \tag{48}$$

with everything at x_H. We need three numbers: Q_4, c_3 and q_4.

5.3 Four kinds of contribution

Figure 3 shows what the terms are. In each, four index loops carry the holonomies U, U, U^{-1} and U^{-1}, and the question is what sits between them.

The square of the one-loop operator. The term Q_4 is the connected average of two copies of $\mathcal{H}$. Each copy acts on two letters. For the average to be connected and to produce four index loops, the two copies must share at least one letter, and the colour structures of (33) must be contracted in a non-planar way. It can be computed from the one-loop operator alone, and it needs no regularisation.

Exchange of u_2. The cubic coupling c_3 is a one-loop quantity and the exchange is a tree diagram of the matrix model. It is the analogue, in this problem, of a contribution that Atick and Witten identified for strings near their Hagedorn temperature [26]. There the winding mode that becomes massless couples to the dilaton, and integrating out the dilaton gives the winding mode a negative quartic self-coupling. That is why they argued the string Hagedorn

transition is first order. Here u_1 is the winding mode and u_2 plays the part of the dilaton. It turns out to be a small part of the answer.

The two-loop operator, tree part. The operator D_4 contains a piece that acts on three letters at once and turns them into three others. It comes from tree-level scattering at order g^4, for instance two cubic vertices and a quartic one. When it acts across two traces it contributes to q_4. We call this part $q_4^{(a)}$. It has no loop and is finite.

The two-loop operator, loop part. The operator D_4 also contains a piece that acts on two letters and returns them to themselves, through a one-loop diagram. The planar part of it renormalises m_1^2. The part that contributes to q_4 is of the double-trace form $:\mathrm{tr}(W_A \check{W}^A)\,\mathrm{tr}(W_B \check{W}^B):$, in which each letter is returned to its own trace while the loop connects the two. We call this part $q_4^{(b)}$. Each diagram in it is logarithmically divergent.

There is a third part of D_4, which acts on a single letter through a two-loop self-energy. It produces only two index loops and contributes to m_1^2, not to b. It will appear only in section 8.

5.4 What is known and what is not

Two of the three traces of the one-loop operator that enter c_3 are in the work of Spradlin and Volovich, and the corresponding coefficient for general adjoint matter is given as a sum over angular momenta in [68]. The function Q_4 has not appeared before, but it is a finite computation with a known operator.

The function q_4 requires the two-loop dilatation operator at the first non-planar order on all letters. It is known for the two holomorphic scalars of the $su(2)$ sector [84]. The planar part is known on the larger $su(2|3)$ sector [98], for the pure scalar piece of the $so(6)$ sector, which is not closed at this order [99], and for twist-two operators through the anomalous dimensions of [100, 101]. For the non-compact $su(1,1|2)$ sector Zwiebel found the two-loop generator and conjectured that its lift to finite N holds for any gauge group [85]. None of this covers what we need. At the Hagedorn temperature all letters contribute. The scalars without derivatives, which make up the well-studied sectors, carry less than half of the weight in $z(x_H) = 1$. We therefore construct the relevant parts of D_4 from the Hamiltonian.

5.5 A freedom of scheme

One subtlety must be addressed before numbers are quoted.

The effective action $S_{\text{eff}}[U]$ is not unique. Only its integral over U is physical. Consider adding to the dilatation operator a term proportional to the generator of gauge transformations, $\mathcal{G} = \sum_A [W_A, \check{W}^A]$. Such a term vanishes on every gauge-invariant state and does not change the spectrum. The ensemble $\langle\,\cdot\,\rangle_U$ at fixed U contains non-singlet states, however, and there the term does not vanish. One finds that it changes $Z[U]$ by a total derivative on the group manifold. In terms of the moments it is a change of variables, of the form $u_2 \to u_2 + g^2\gamma\, u_1^2$ and $u_1 \to u_1 + g^2\gamma' u_2 u_{-1}$, with γ and γ' functions of the temperature.

This matters because two natural forms of the one-loop operator differ by exactly such a term. Beisert's form (33) has all of its content in a two-letter kernel. The operator that one obtains literally from second-order perturbation theory of the Hamiltonian has a different two-letter kernel, with no diagonal part, together with a one-letter self-energy. On singlets the two agree. At fixed U they give different functions $c_3(x)$ and $Q_4(x)$. We call the two choices the commutator scheme and the literal scheme.

A change of variables cannot change the order of a phase transition. Indeed the redefinitions above shift $\tilde{b}$ and κ^2/m_2^2 in (18) by equal and opposite amounts at the critical point, and shift $q_4(x)$ by an amount proportional to $1 - z(x)$, which vanishes there. Hence I and $q_4(x_H)$ are

separately invariant. We have computed I in both schemes as a check,

	$c_3(x_H)$	$Q_4(x_H)$	I
literal scheme	$+0.16821$	2.1222	$1.11918(15)$
commutator scheme	-0.4523	1.400	$1.1200(16)$

(49)

The individual entries differ, even in sign. The combination does not. The practical consequence is that c_3, Q_4 and q_4 must all be computed in one scheme. We use the literal scheme throughout, since that is what the Hamiltonian gives.

6 The computation

We need the parts of the two-loop dilatation operator that connect two traces. We obtain them from the Hamiltonian of the theory on $\mathbb{R} \times S^3$, by ordinary quantum-mechanical perturbation theory. This section describes the Hamiltonian, the perturbation theory, the two pieces of q_4 and how each was evaluated.

6.1 The Hamiltonian in Coulomb gauge

We expand every field in spherical harmonics on S^3 [102]. The coefficients are matrices in colour, and the theory becomes a quantum mechanics of infinitely many matrices. The free part H_0 is a sum of oscillators with the frequencies of table 1. We use Coulomb gauge, $\nabla \cdot A = 0$. It has two advantages here. Only physical polarisations propagate, so the letters of table 1 are the complete set. There are also no ghosts in the Hamiltonian formulation: A_0 is a Lagrange multiplier that imposes Gauss's law, and solving Gauss's law produces a determinant that cancels the Faddeev–Popov determinant exactly.

The price is the instantaneous Coulomb interaction. With ρ the colour charge density of all the fields together,

$$H = H_0 + g_{\mathrm{YM}} V_3 + g_{\mathrm{YM}}^2 V_4 + H_C, \qquad H_C = \frac{g_{\mathrm{YM}}^2}{2} \iint \rho^a \, K^{ab}[A] \, \rho^b. \tag{50}$$

Here V_3 contains the cubic gauge vertex, the couplings of the gauge field to scalars and fermions, and the Yukawa couplings. V_4 contains the quartic gauge vertex, the seagull and the scalar potential. The kernel K is the Coulomb Green's function in the presence of the transverse gauge field. If $M = -\nabla \cdot D$ is the Faddeev–Popov operator, then $K = M^{-1}(-\nabla^2)M^{-1}$. Writing $M = \Delta + g_{\mathrm{YM}}\, a$, where $\Delta = -\nabla^2$ and a is linear in A, so that Δ^{-1} is the free Coulomb propagator,

$$K = \Delta^{-1} - 2g_{\mathrm{YM}}\, \Delta^{-1} a\, \Delta^{-1} + 3g_{\mathrm{YM}}^2\, \Delta^{-1} a\, \Delta^{-1} a\, \Delta^{-1} - \ldots \tag{51}$$

The Coulomb interaction therefore contributes vertices with four, five and six fields,

$$C_2 = \tfrac{1}{2}\rho\, \Delta^{-1} \rho, \qquad C_3 = -\rho\, \Delta^{-1} a\, \Delta^{-1} \rho, \qquad C_4 = \tfrac{3}{2}\rho\, \Delta^{-1} a\, \Delta^{-1} a\, \Delta^{-1} \rho, \tag{52}$$

at orders g_{YM}^2, g_{YM}^3 and g_{YM}^4. All three are needed.

There is a question of operator ordering, since $K[A]$ multiplies charge densities that contain the momentum conjugate to A. Christ and Lee showed that the correct quantum Hamiltonian is the Weyl-ordered classical one plus terms of order $\hbar^2$ [103]. At order g_{YM}^4 those extra terms are quadratic in the fields. They correct the energy of a single gluon and cannot contribute to b. The rule is therefore to Weyl-order H_C and then to normal-order it. The second step leaves remainders, in which two of the six fields of C_4 or of the five of C_3 are contracted with each other. They do matter, and they are part of the loop piece below.

6.2 Fourth-order degenerate perturbation theory

The spectrum of H_0 is highly degenerate. All words with the same total engineering dimension have the same energy. The dilatation operator of section 4 is the effective Hamiltonian that acts within one degenerate level and reproduces the exact spectrum order by order. Let P project onto a level of energy E_0, let $Q = 1 - P$, and let $R = Q/(E_0 - H_0)$ be the resolvent. Collect the interaction by powers of the coupling, $\mathcal{V}_1 = V_3$, $\mathcal{V}_2 = V_4 + C_2$, $\mathcal{V}_3 = C_3$, $\mathcal{V}_4 = C_4$. Since $\mathcal{V}_1$ changes the number of letters by one, $P\mathcal{V}_1 P = 0$. The effective Hamiltonian at second order is

$$h_2 = P\mathcal{V}_2 P + P\mathcal{V}_1 R \mathcal{V}_1 P. \tag{53}$$

This is the literal one-loop operator of section 5, up to the factor g_{YM}^2. At fourth order, in the hermitian form of Bloch and des Cloizeaux [104, 105],

$$\begin{aligned} h_4 = {} & P\mathcal{V}_4 P + P\mathcal{V}_1 R \mathcal{V}_3 P + P\mathcal{V}_3 R \mathcal{V}_1 P + P\mathcal{V}_2 R \mathcal{V}_2 P \\ & + P\mathcal{V}_1 R \mathcal{V}_1 R \mathcal{V}_2 P + P\mathcal{V}_1 R \mathcal{V}_2 R \mathcal{V}_1 P + P\mathcal{V}_2 R \mathcal{V}_1 R \mathcal{V}_1 P \\ & + P\mathcal{V}_1 R \mathcal{V}_1 R \mathcal{V}_1 R \mathcal{V}_1 P - \tfrac{1}{2}\{P\mathcal{V}_1 R^2 \mathcal{V}_1 P,\ h_2\}. \end{aligned} \tag{54}$$

The last term is the familiar wave-function renormalisation of fourth-order perturbation theory. Up to normalisation, h_2 is D_2 and h_4 is D_4.

We do not need h_4 as an operator. We need its thermal average with four holonomies. It is efficient to obtain it together with the $\mathcal{H}^2$ term. One expands $\mathrm{Tr}(x^H \hat{U})$ directly to order g_{YM}^4 in old-fashioned, time-ordered perturbation theory. The integrals over the Euclidean times of the vertices turn the Boltzmann factors into divided differences of $e^{-\beta E}$ over the energies of the successive intermediate states. When two intermediate states are degenerate the divided difference becomes a derivative, and a power of β appears. The term linear in β is $-\beta\langle h_4\rangle$ and the term quadratic in β is $\frac{1}{2}\beta^2\langle h_2^2\rangle_{\mathrm{conn}}$. We checked this rule, including the fermion signs and the degenerate cases, against exact diagonalisation of small matrix models with gauge groups $U(2)$ and $U(3)$, to ten digits.

The fact that the same diagrams give both terms is a strong check. The quadratic term must agree with Q_4 computed from the one-loop operator alone, which involves no energy denominators. It does, order by order in y, to nine digits.

6.3 Which diagrams feed $|u_1|^4$

A term in h_4 is a product of letters W and derivatives $\check{W}$ under traces. Its thermal average closes each $\check{W}$ onto a W with a twisted propagator (30). We need four index loops with holonomy. Terms that act on a single letter give two. The planar terms that act on two neighbouring letters give three. Two classes give four.

(a) Three letters to three letters. Connected tree diagrams with three incoming and three outgoing letters. With the vertices of (50) and (52) the possible contents are: four cubic vertices; two cubic vertices and one quartic or C_2; two quartic or C_2; one cubic and one C_3; one C_4. Every colour ordering of the six external legs is needed, since the planar orderings give three index loops and only the others give four.

(b) Two letters to two letters at one loop. The same contents with one more contraction: boxes, triangles, bubbles, a loop through C_3, the self-contraction of C_4, and the ordering remainders. The colour factor of a loop of adjoint fields with four external legs is

$$\begin{aligned} \mathrm{tr}_{\mathrm{adj}}(T^a T^b T^c T^d) = {} & N\big[\mathrm{tr}(abcd) + \mathrm{tr}(dcba)\big] \\ & + 2\big[\mathrm{tr}(ab)\mathrm{tr}(cd) + \mathrm{tr}(ac)\mathrm{tr}(bd) + \mathrm{tr}(ad)\mathrm{tr}(bc)\big] + \ldots, \end{aligned} \tag{55}$$

where the dots are terms with a single generator under a trace, which vanish for $SU(N)$. The single-trace part is planar. The double-trace part is what we want. After the thermal average

only the forward structure $:\mathrm{tr}(W_A\check{W}^A)\mathrm{tr}(W_B\check{W}^B):$ survives with four holonomies. The double-trace part is totally symmetric in the four legs. It multiplies one kinematic function, which is the sum over the three inequivalent orderings of the legs around the loop.

6.4 Piece (a): the tree kernel

Every diagram is a product of vertex coefficients, which are integrals of three or four harmonics over S^3, times energy denominators, summed over the magnetic quantum numbers and species of all internal lines. For fixed external letters the internal sums are finite, because angular momentum is conserved at each vertex. The result is a polynomial in y for each set of external letters, and the thermal average is a power series in y with rational coefficients. We find

$$q_4^{(a)}(y) = -450\,y^6 - 2184\,y^7 - 6246\,y^8 - 13632\,y^9 - \tfrac{231931}{9}\,y^{10} - \tfrac{132776}{3}\,y^{11} - \dots \tag{56}$$

The series is known to y^{16} and is given in appendix B. The leading term comes from three scalars. All coefficients are negative. The coefficients grow like a power of n, as they must for a function whose nearest singularity is at $y = 1$, and at $y_H = 0.268$ the series converges geometrically. The sum is

$$q_4^{(a)}(x_H) = -0.7340(1). \tag{57}$$

6.5 Piece (b): the loop kernel and its divergences

Here one angular momentum runs freely around the loop, and each diagram diverges logarithmically. We cut the sum off at a maximum angular momentum J on one line of the loop. The divergences must cancel in the sum of diagrams, since there is no counterterm in the theory of the form $(\mathrm{tr}\,\Phi^2)^2$. They do. For every pair of external multiplets the coefficients of $\ln J$ contributed by scalars, gauge bosons and fermions in the loop stand in the ratio

$$6 : 2 : -8. \tag{58}$$

These are the numbers of bosonic and fermionic degrees of freedom of the theory, and their sum is zero.

A finite remainder is more delicate, and the pure Yang–Mills calculation of AMMPV shows why. When logarithmic divergences cancel only between diagrams, a sharp cut-off on modes can leave a finite, regulator-dependent term. AMMPV found that a finite double-trace counterterm was needed to restore gauge invariance, a five per cent effect in their answer. We determined this counterterm for a general matter content. The double-trace part of (55) is totally symmetric, so it can be computed in a constant commuting background, where the one-loop energy is $\frac{1}{2}(n_B - n_F)\sum\omega$. A sharp cut-off leaves a term from the surface of the cut-off sphere. It is proportional to

$$n_B - n_F, \tag{59}$$

the number of bosonic minus fermionic modes at each momentum. For pure glue $n_B - n_F = 2$ and we recover AMMPV's counterterm exactly. For $\mathcal{N} = 4$ it is $8 - 8 = 0$. No counterterm is needed, provided the cut-off is applied to the same line in the same way in every diagram, time ordering and species. We return to this in section 9.

With this understood the loop kernel is again a power series in y with rational coefficients, each obtained by extrapolating $J \to \infty$,

$$\begin{aligned} q_4^{(b)}(y) = &-42\,y^4 - 384\,y^5 - \tfrac{2181}{2}\,y^6 - 2100\,y^7 \\ &- \tfrac{118841}{36}\,y^8 - \tfrac{128452}{27}\,y^9 - \tfrac{306863}{48}\,y^{10} - \dots \end{aligned} \tag{60}$$

It starts two orders earlier than piece (a) because two scalars are enough. The direct sum with an estimate of the tail, and five Padé approximants, give values between -1.4987 and -1.5044. We quote

$$q_4^{(b)}(x_H) = -1.500(3). \tag{61}$$

6.6 Independent evaluations

An error in one vertex coefficient among several hundred would be invisible in the final number. The computation was therefore organised so that, with the one exception recorded at the end of this subsection, no number is used until two independent routes agree on it.

There are two constructions of the vertices. One follows the harmonic expansion of [102] and expresses the integrals over S^3 through $9j$ symbols. The other realises the harmonics as homogeneous harmonic polynomials on $\mathbb{R}^4$ and integrates them directly. They share no code. They agree on every cubic, quartic and Coulomb coefficient, and they give the same one-loop series c_3, d_1 and Q_4 to y^{14}.

There are three contraction engines for piece (a) and two for piece (b). One works with reduced matrix elements and recoupling coefficients, one with explicit magnetic quantum numbers, and one at the level of words of matrices with mechanical normal ordering. The three agree on piece (a) coefficient by coefficient from y^6 to y^{12}, and topology by topology to y^{10}.

There is a separate route that does not use the effective Hamiltonian at all. It evaluates three-loop vacuum diagrams on $S^3 \times S^1$ in the manner of AMMPV, with the time integrals done by divided differences and the contributions classified by the number of lines that wind. It shares the vertex coefficients with the first construction and nothing else. It reproduces piece (a) exactly to y^{10}, separately for each vertex content and each power of β, and it reproduces the first two coefficients of piece (b).

Finally there is an analytic test. If the thermal lines are restricted to the two scalars of the $su(2)$ sector, with fugacities x_Z and x_ϕ and unrestricted virtual states, the known two-loop operator of [84] predicts both pieces. Piece (a) must be the polynomial $-(x_Z - x_\phi)^2(x_Z^2 + x_\phi^2 - 3x_Z - 3x_\phi)$, and on the critical line $x_Z + x_\phi = 1$ piece (b) must be $-2(x_Z^2 + x_Z x_\phi + x_\phi^2)$. Three engines reproduce the first exactly. For the coefficient -2 in the second we find -2.0000000 with one engine and $-2.00(1)$ with the other.

One caveat must be recorded. The coefficients of piece (b) from y^7 onwards were produced by one engine only. The second engine confirms y^4, y^5 and the two largest entries of y^6. The unconfirmed terms contribute -0.34 of the -1.50. The margin for the sign of b is fourteen in these units.

7 The result

7.1 The quartic coefficient

The one-loop quantities at the Hagedorn point, in the literal scheme, are $c_3 = 0.16821(1)$ and $Q_4 = 2.1222(3)$. With $A_2 = 0.9742786$ they give $I = 1.11918(15)$ in (48). The two-loop quantity is the sum of (57) and (61),

$$q_4(x_H) = -0.7340(1) - 1.500(3) = -2.234(3). \tag{62}$$

With $\beta_0 = 2.6339158$ and $\beta_0^2 = 6.93751$ the master formula gives

$$b = g^4\big[-4\beta_0^2\, I + \beta_0\, q_4\big] = g^4\big[-31.057(5) - 5.884(8)\big] = -36.94(1)\, g^4. \tag{63}$$

In terms of the 't Hooft coupling, $g^4 = \lambda^2/256\pi^4$ and

$$b = -1.481 \times 10^{-3}\, \lambda^2. \tag{64}$$

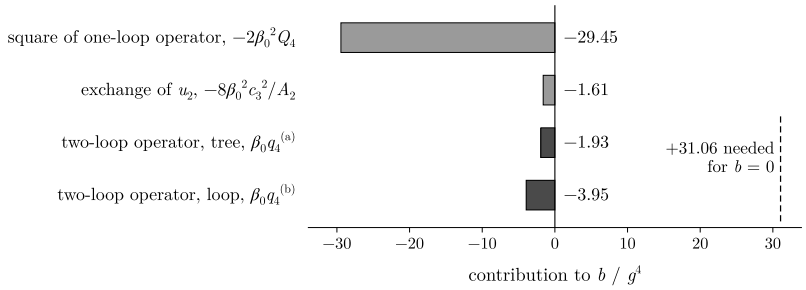


Figure 4: The four contributions to b in units of g^4, in the literal scheme. The division between the first two bars depends on the scheme. Their sum, and each of the other two, does not. The dashed line marks the value that the sum of the last two bars would need to reach for b to vanish.

The quartic coefficient is negative. The deconfinement transition of weakly coupled $\mathcal{N} = 4$ super Yang–Mills theory on S^3 is first order.

Figure 4 shows the composition of the result. The square of the one-loop operator gives -29.45, the exchange of u_2 gives -1.61, the tree part of the two-loop operator gives -1.93 and its loop part gives -3.95. All four are negative. The terms that come from the one-loop operator make up 84 per cent of the total.

The sign is not marginal. For b to be positive the two-loop term would have to satisfy

$$q_4(x_H) > \frac{4\beta_0^2 I}{\beta_0} = 11.79, \tag{65}$$

and we find -2.23. An error in q_4 of order one, which is already far larger than any discrepancy we have met, would not matter. The sign of b could have been guessed from I alone if one had a reason to believe that the two-loop operator contributes a number of order one. We know of no such reason in advance. In pure Yang–Mills theory the corresponding term is positive in our evaluation, and cancels about thirty per cent of the rest.

For comparison, the pure Yang–Mills value of AMMPV is $b = -5.7 \times 10^{-4}\lambda_A^2$ with their coupling $\lambda_A = \lambda/2$, that is $-1.4 \times 10^{-4}\lambda^2$. At the same 't Hooft coupling the $\mathcal{N} = 4$ theory has a quartic coefficient ten times as large. The matter fields make the transition more strongly first order.

7.2 The transition temperature and the three saddles

Combine (63) with the Landau analysis of section 3. From (25),

$$\frac{T_H - T_c}{T_H} = \frac{|b|}{6\beta_0} = 2.337\, g^4 = 9.37 \times 10^{-5}\lambda^2, \qquad \frac{T_H - T_{\min}}{T_H} = 4.67\, g^4. \tag{66}$$

Together with the two-loop Hagedorn temperature (42) this gives all three characteristic temperatures to order λ^2,

$$\begin{aligned} T_H &= T_H^{(0)}(1 + 2g^2 - 11.50\, g^4), \\ T_c &= T_H^{(0)}(1 + 2g^2 - 13.84\, g^4), \\ T_{\min} &= T_H^{(0)}(1 + 2g^2 - 16.18\, g^4). \end{aligned} \tag{67}$$

Below $T_{\min}$ the only saddle point is the confined one, $u_1 = 0$. Between $T_{\min}$ and T_H there are three: the confined one, an unstable one at $|u_1| = u_s$ given by (22), and a deconfined one at

$$|u_1| \simeq \tfrac{1}{2} + \frac{\sqrt{|b|}}{4} = \tfrac{1}{2} + 1.52\, g^2. \tag{68}$$

sector	$\tilde{x}_H$	A_2	c_3	Q_4	$b/\tilde{G}^2$
$su(2)$	$1/2$	0.5	0.25	1	-0.75
$su(1\|1)$	0.569840	0.86032	-0.12495	0.69701	-0.38480
$su(1\|2)$	0.381966	0.76393	0.11146	1.41020	-0.73762
$su(2\|3)$	$1/4$	0.84375	0.10547	1.74023	-0.89648
$su(1,1)$ bosonic	$1/2$	$2/3$	-0.23105	1.80509	-1.06270
$su(1,1)$ fermionic	0.569840	1.27402	-2.00053	-12.2707	-0.1473
$su(1,1\|1)$	0.381966	0.89443	-0.50591	0.31743	-0.73103
$su(1,1\|2)$	$1/4$	0.9	-0.27467	1.41794	-0.87662
$su(1,2\|3)$	0.145898	0.94900	-0.40721	1.20645	-0.95268

Table 3: The quartic coefficient in nine of the twelve non-trivial decoupling limits of [87], in the commutator scheme. $\tilde{x}_H$ is the Hagedorn value of $e^{-1/\tilde{T}}$ in the free decoupled theory. The last column is negative in every sector.

The confined and deconfined saddles exchange dominance at T_c. At T_H the unstable saddle merges with the confined one, which disappears as a minimum. The latent heat at T_c is $\frac{3}{8}N^2/R$ to leading order.

The window is narrow. At $\lambda = 1$ the three temperatures differ by one part in ten thousand. This is expected. The first-order character of the transition is a second-order effect in λ on top of a degenerate zeroth-order problem. What is robust is the ordering $T_{\min} < T_c < T_H$ and the list of saddles, and those are the ordering and the list of the gravitational problem.

7.3 Near-BPS limits

There is a family of cases in which b can be obtained from the one-loop operator alone. Harmark and Orselli considered the theory with chemical potentials for the R-charges [86, 106], and with Kristjánsson they added those for the spins [87]. The potentials are set in fixed ratios to one parameter Ω, and the limit is

$$T \to 0, \qquad \Omega \to 1, \qquad \lambda \to 0, \qquad \tilde{T} = \frac{T}{1-\Omega} \text{ and } \tilde{\lambda} = \frac{\lambda}{1-\Omega} \text{ fixed.} \tag{69}$$

In this limit only the letters that saturate a BPS bound survive, and the Hamiltonian of what remains is $D_0 + \tilde{g}^2 D_2$ exactly, at any N, with $\tilde{g}^2 = \tilde{\lambda}/16\pi^2$. Depending on those ratios, the surviving letters form a representation of a subalgebra of $psu(2,2|4)$. There are fourteen such limits, twelve of them non-trivial [87], and we treat nine of the twelve. Each non-trivial decoupled theory has its own Hagedorn transition in $\tilde{T}$; those with scalar letters are described as Spin Matrix theories in [107]. The one-loop Hagedorn temperatures were found in [86] for $su(2)$ and $su(2|3)$ and in [87] for the rest. The order of the transitions was left open [106, 87]; for $su(2)$ a first-order transition was called likely in [107], with a second-order one left as an alternative.

Since D_4 is absent, the master formula reduces to $b = -\tilde{G}^2 I$ with $\tilde{G} = \tilde{\beta}\tilde{\lambda}/8\pi^2$, and I is computed with the letters of the sector. Table 3 gives the results. For the compact sectors the functions are polynomials and the entries are exact. For the non-compact ones they are series, which we summed to between y^{26} and y^{60}.

The coefficient is negative in all nine. The Hagedorn transitions of these nine decoupled theories are first order at small $\tilde{\lambda}$. The fermionic $su(1,1)$ sector is instructive. There Q_4 is large and negative, so that the first term of I alone would make b positive. The exchange of u_2 overturns it. This illustrates again that the individual terms have no separate meaning, and that the sign of b is not fixed by any simple positivity argument.

check	outcome
$\lvert u_1\rvert^2$ coefficient of $\langle\mathcal{H}\rangle_U$ against Spradlin and Volovich [75]	series identical; $d_1(x_H) = \frac{3}{2}$
confined phase at orders g^2 and g^4: Gaussian integral over the u_n against direct traces over cyclic spin chains, including multi-traces	identical through y^8
$su(2)$ sector: $Q_4 = 4x^3 + 8x^4$, $c_3 = 2x^3$; Hagedorn temperature of [106] to second order in $\tilde{G}$	exact
$su(2\lvert3)$ sector at one loop: $\tilde{T}_H = (1 + \frac{3}{8}\tilde{\lambda}_{\text{HO}})/\ln 4$ [86]	exact
non-planar two-loop $su(2)$ operator of [84]: $d_4 = -8x^2 - 8x^3$, hence the two-loop $su(2)$ Hagedorn temperature of [77]	exact
trace of the two-loop $su(2\lvert3)$ Hamiltonian of [98] over three-letter states at $x = \frac{1}{4}$: $-351/64$	-5.4843765
effective-Hamiltonian rules against exact diagonalisation of $U(2)$ and $U(3)$ matrix models	10^{-10}
part of order β^2 of the three-loop diagrams against $\langle\mathcal{H}^2\rangle$ from the harmonic action [76]	3.5×10^{-10}, every order
two-loop energies of non-BPS operators of lengths 3, 4 and 5 from the Bethe ansatz [108]: -24, -48, -42, -6, $-34 \pm 10\sqrt{5}$ (in units of g^4)	see section 9

Table 4: Comparisons with exact results.

8 Checks

The internal checks of section 6 show that the computation is consistent with itself. This section compares it with the literature. There are three kinds of comparison: exact results in closed sectors, the pure Yang–Mills calculation of AMMPV, and the two-loop Hagedorn temperature of Harmark and Wilhelm. The last two were the most instructive.

8.1 Exact results in closed sectors

Table 4 lists the comparisons with exact results. All of them are passed exactly or to the numerical precision available.

8.2 Pure Yang–Mills theory

If all lines are restricted to gauge bosons, our codes compute the quantities that AMMPV computed in [39]. The dictionary is $\lambda_A = \lambda/2$ for their coupling, $x_c = 2 - \sqrt{3}$ for the Hagedorn point of pure glue, and $C_{1,1,-2} = c_3/4\pi^2$, $C_{1,1,-1,-1} = (q_4 - 2\beta_c Q_4)/64\pi^4$ for their cubic and quartic coefficients, where $\beta_c = -\ln x_c$ and for pure glue q_4 includes the finite counterterm.

At two loops AMMPV give the three contributions to $C_{1,1,-2}$ from the quartic vertex, from two cubic vertices and from the Coulomb interaction. In units of 10^{-4} we find 6.53537, -22.87089 and 9.16397. They give 6.53536, -22.87088 and 9.16396. We also find the closed form $c_3(x) = -\frac{3}{4} z_V(x^2)$ for pure glue, where z_V is the last entry of table 1. This fixes the normalisation of every type of vertex to six digits.

At three loops AMMPV list fourteen diagrams, which they label 3a to 3n, with a finite part for each after subtraction of the logarithmic divergence. The diagrams can be grouped by vertex content into seven classes that are separately meaningful in both calculations. Both calculations use a sharp cut-off on angular momentum, so the finite parts can be compared

class	AMMPV diagrams	this work	AMMPV
four cubic vertices	3i, 3l	-7.84	$-7.6(5)$
two cubic, one quartic	3g, 3j	3.574	3.564
two cubic, one Coulomb	3h, 3k	3.326	3.33
two quartic	3a, 3d	0.217	0.217
quartic and Coulomb	3b, 3e	-1.065	-1.066
cubic and quintic	3m	0.462	0.46
two Coulomb, and sextic	3c, 3f, 3n	-2.095	-3.388
sum		-3.42	$-4.5(3)$

Table 5: Finite parts of the three-loop contributions to $C_{1,1,-1,-1}$ in pure Yang–Mills theory, in units of 10^{-4}, grouped by vertex content. The AMMPV column gives the sums of their printed entries. The error on the first row is ours, from the single digit of their entry 3l; the error on the sum is theirs.

without a translation constant. The logarithmic coefficients agree exactly, diagram by diagram. Table 5 compares the finite parts.

Five classes agree with AMMPV within the rounding of their entries, and the class of 3g and 3j, whose entries sum to 3.564, agrees to within one unit in the last digit of 3g. The single diagrams 3d and 3e, which can be isolated, agree to three digits, and 3m to the two that AMMPV quote. We also reproduce their finite counterterm exactly, as described in section 6.

The seventh class does not agree. It contains two Coulomb interactions C_2, together with the sextic vertex C_4 whose self-contraction is of the same form. We find -2.095, and the entries of AMMPV sum to -3.388. This class accounts for the difference between our pure-glue result $b = -4.3 \times 10^{-4}\lambda_A^2$ and their $-5.7 \times 10^{-4}\lambda_A^2$. In the units of table 5 it differs by $+1.29$ and the sums by about $+1.1$. The first row, where their entry 3l has a single digit, gives back -0.24.

We have not resolved this. The following can be said. On our side the part of this class proportional to β^2 is obtained from three codes. The logarithmic coefficient is exact. The first two finite coefficients of exactly this class, at x^4 and x^5, were computed by two engines with independently written ordering remainders, with results 36.9553(5) against 36.957(6) and 65.93(5) against 65.87(6). The sextic vertex is the one in (52), from the Weyl-ordered Hamiltonian. On the side of AMMPV, in the Lagrangian formalism this class involves contact terms $\delta(t)$. They recomputed 3c and 3n, though not 3f, with a second regulating function, and the sum of each diagram and its counterterms did not change. They print the expression for every diagram and point to a Mathematica file for the integrals, so the comparison can be carried further, diagram by diagram, than we have taken it here. One of the two calculations has an error in this class.

For the purpose of this paper the important point is its size. In units of q_4 the disagreement is 0.8. It is in the direction of a more negative b if AMMPV are right. The margin for the sign of b in $\mathcal{N} = 4$ is fourteen. The disagreement therefore does not affect our conclusion. It should be resolved in the future, and section 10 says what would be needed.

8.3 The two-loop Hagedorn temperature

The second external check is of a different nature. It does not test b. It tests the Hamiltonian, the perturbation theory and the engines on a quantity that is known exactly, through the coefficient of $|u_1|^2$ at order g^4.

The target. The Hagedorn temperature is the zero of (41). Write $w(\beta) = 1 - z(e^{-\beta})$ and

$\beta_H = \beta_0 + g^2\beta_1 + g^4\beta_2$. At order g^2 one finds $\beta_1 = -2\beta_0$, as in section 4. At order g^4,

$$\beta_0\, d_4 = 2\beta_0^2\, C_{41} - \Big[w'\beta_2 + \tfrac{1}{2}w''\beta_1^2 + 2\beta_1 d_1 + 2\beta_0\beta_1\, \partial_\beta d_1\Big], \tag{70}$$

with everything evaluated at β_0. The ingredients are $w' = \frac{3}{2}$ and $w'' = -\frac{3}{2}\sqrt{3}$ from (9); $d_1 = \frac{3}{2}$ and $\partial_\beta d_1 = -(8\sqrt{3} - 9)$ from the closed form (36); $\beta_2 = \beta_0(4 + 11.50399)$ from the result (42) of Harmark and Wilhelm; and $C_{41} = 8.353829$, which we computed from the one-loop operator as $\langle H_{12}^2\rangle$ on two letters plus $\langle H_{12}H_{23} + H_{23}H_{12}\rangle$ on three. The four terms in the bracket are 61.25, -36.05, -15.80 and $+134.77$, and the first term on the right is 115.91. The result is

$$d_4(x_H) = -10.7287. \tag{71}$$

This is the number that our two-loop operator must reproduce. We validated the conversion formula (70) by brute force on $su(2)$ spin chains, where everything is known.

The direct computation. The coefficient d_4 receives contributions from all three parts of h_4: the tree part acting on three letters, the planar loop part acting on two, and the two-loop self-energy acting on one. The first is finite and gives -0.156. The second is logarithmically divergent diagram by diagram and finite in the sum, like piece (b) above, and gives $-5.65(2)(6)$, where the second error is an estimate of the extrapolation in the cut-off. The third is problematic. The two-loop self-energy of a letter, computed with a cut-off J on the angular momenta of the virtual states, does not converge. It grows like J^2. We explain why in the next section. The remedy is to fix the one-body terms by symmetry instead. The anomalous dimensions of half-BPS operators must vanish, and those of their descendants are determined. Requiring this of the full h_4, acting on states with one impurity in a background of Z letters, determines the one-body energies c_4 in terms of two-body kernels that do converge. In units of g^4 per letter we find

$$c_4(Z) = 2\zeta_3 - 1, \qquad c_4(\psi) = 2\zeta_3 - 9, \qquad c_4(DZ) = 2\zeta_3 - \tfrac{105}{8}, \tag{72}$$

and numerical values for the next three letters. The six lightest letters carry 98 per cent of the thermal weight at x_H, and their one-body terms sum to -4.476. For the remaining letters we extrapolate the measured trend, which gives $-0.41(2)$.

There is one more ingredient. The exact two-loop energies in the last line of table 4 revealed that the cut-off leaves a finite renormalisation of the Coulomb interaction, which we describe in the next section. It shifts the two-body term by -0.017 and enters the one-body terms through the bootstrap. The value of $c_4(DZ)$ in (72) includes it.

Adding the pieces,

$$d_4(x_H) = -0.156 - 5.65 - 0.017 - 4.476 - 0.41 = -10.71(2)(6), \tag{73}$$

against the target -10.7287. The agreement is at the level of half a per cent, within the errors.

The value of this check should be stated precisely. It is not a blind test. The first version of our number was -9.7, short by ten per cent. The discrepancy led to the discovery of the Coulomb counterterm, whose coefficient was then fixed by other data and not by the target. After that the number agreed. The check therefore shows that the regulated Hamiltonian, supplemented by finite counterterms that are fixed independently, reproduces a non-trivial two-loop result of integrability. It does not show that the correct value would have been obtained had the target not been known.

9 The mode cut-off and its counterterms

The only regulator that is natural for a Hamiltonian on S^3 is a cut-off on the angular momentum of the modes. It is not a good regulator in the usual sense. This section describes

what it breaks, the three finite counterterms that repair it, and why the quartic coefficient b is not affected by any of them. The first counterterm was found by AMMPV. The second is a two-loop relative of theirs. The third has precedents as an operator: a renormalisation of the A_0 propagator, with a finite part, is among the quadratic counterterms of AMMPV [39], and the term is listed for $\mathcal{N} = 4$ in [102]. We have not seen its finite coefficient in $\mathcal{N} = 4$, or its effect on the spectrum, elsewhere.

9.1 What the cut-off preserves

The theory on $\mathbb{R} \times S^3$ is invariant under the superconformal group. A cut-off J on the angular momentum of every mode preserves the rotations $SO(4)$ of the sphere, the R-symmetry $SU(4)$ and time translations. It preserves nothing else. The conformal boosts mix harmonics of neighbouring angular momentum and do not commute with the projection onto modes below the cut-off. Neither do the supercharges, once the interaction is switched on. If the cut-off is placed on the left spin j_L only, as is convenient, parity is lost too.

The general principle is then that every local operator of dimension four or less that is allowed by the surviving symmetries will be induced, with a coefficient that is a power of J fixed by the dimension of the operator, and a finite part that no surviving symmetry fixes. In a Lorentz-invariant regularisation most of these operators are forbidden. Here they must be found and removed by hand, by imposing the broken symmetries as renormalisation conditions. AMMPV met this at one loop [39], with a quadratically divergent gluon mass and different wave-function renormalisations for the time and space components. Aharony, Marsano and Van Raamsdonk added a curvature-dependent gluon mass counterterm [40], and Mussel and Yacoby, who follow them with matter included [68], a scalar mass whose finite part is fixed by conformal invariance.

9.2 The double-trace quartic term

The first counterterm is the one of section 6. It is a quartic, double-trace, dimension-four operator without derivatives, such as $(\mathrm{tr} A_i A_j)^2$ or $\mathrm{tr}(A_i A_i)\mathrm{tr}(X_a X_a)$, where X_a are the scalars. Its divergent part cancels between diagrams and its finite part is proportional to $n_B - n_F$. For pure glue we find the coefficients $\frac{1}{60}$ and $\frac{1}{60}$ of AMMPV. For $\mathcal{N} = 4$ it vanishes, mode by mode.

This is the only one of the three counterterms that has the colour structure to contribute to b. It is absent. The argument for its absence assumes, however, that the cut-off is applied uniformly. If one cuts off different diagrams on different lines, or cuts off the total energy of the intermediate state, the diagrams see effectively different values of J and the cancellation of logarithms leaves a finite piece. We apply the cut-off to the angular momentum of one specified line of the loop, the same in every diagram.

9.3 The mass term

The second counterterm appeared when we tried to compute the two-loop self-energy of a single letter directly. Figure 5 shows the result for the lowest scalar mode Z. In units of $(\lambda/8\pi^2)^2$ the values for $J = 0, 1, \ldots, 6$ are

$$-1.594,\ -29.477,\ -84.509,\ -170.044,\ -281.395,\ -422.012,\ -588.717. \tag{74}$$

They are fitted by $-13.9(3)J^2 - 15J$. The correct answer, fixed by the vanishing anomalous dimension of $\mathrm{tr}\, Z^L$, is $(2\zeta_3 - 1)/4 = 0.351$.

An error in the code is excluded by a second code, which builds the Fock space explicitly for gauge group $SU(2)$ and normal-orders mechanically with no diagrammatic input. It reproduces every class of diagrams at $J = 0$ and $J = 1$ as exact rational numbers.

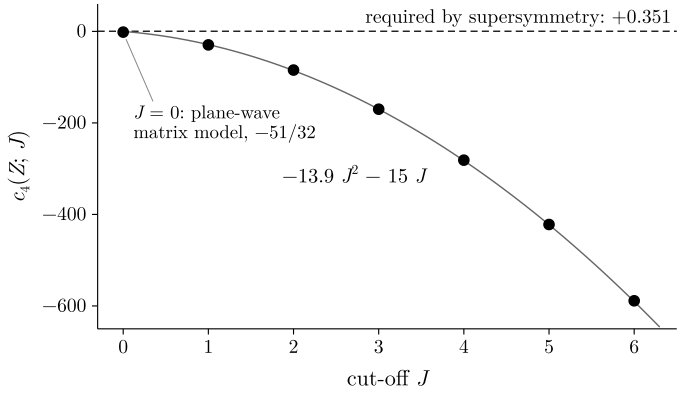


Figure 5: The two-loop self-energy $c_4(Z;J)$ of the lowest scalar mode on S^3, in units of $(\lambda/8\pi^2)^2$, as a function of the cut-off J on the doubled left spin of all virtual modes. The curve is $-13.9J^2 - 15J$. The value required by supersymmetry is $+0.351$. The point at $J = 0$ is the plane-wave matrix model.

The point $J = 0$ offers a test that needs no regulator. If only the lowest mode of each field is kept, the theory on S^3 reduces to the plane-wave matrix model [109, 110]. This is a consistent truncation with an exact $SU(2|4)$ symmetry of its own. Inside it our Hamiltonian, with no counterterm, gives exactly vanishing two-loop energies for the protected states, through cancellations between classes of diagrams of size several hundred. It gives $-90g^4$ for the state $\mathrm{tr}[Z,\phi]^2$, in agreement with [111], and it reproduces the one-body coefficient $-\frac{51}{32}$ and the singlet energy -114 of [110]. The value -1.594 is $-\frac{51}{32}$. The Hamiltonian is therefore correct, and it is the cut-off theory at $J > 0$ that is not supersymmetric.

The divergence is a mass term. For the scalar modes Z, DZ and D^2Z with energies $E = 1, 2, 3$ the coefficient of J^2 in the self-energy, multiplied by E, is -13.9, -16.2 and -14.8. That is the pattern $\delta E = \delta m^2/2E$ with $\delta m^2 \simeq -28J^2$. The J^2 comes from the region where all virtual lines are hard. For fermions the growth is linear in J, as befits an operator of dimension three. We also checked that more elaborate cut-offs, with different limits for inner and outer loops, do not help: the result then depends logarithmically on the ratio.

The remedy is not to extrapolate but to renormalise. The mass counterterm is fixed by requiring that half-BPS operators and their descendants have the dimensions that the superconformal algebra dictates. Those conditions are the bootstrap equations used in section 8, and the values (72) are the renormalised self-energies.

9.4 The Coulomb term

The bootstrap assumes that the two-body kernels need no finite correction. For letters without spin this can be tested in many ways and it holds. With letters that carry spin it fails, and that is the third counterterm.

It was found as follows. After the bootstrap the two-loop Hagedorn coefficient (73) came out as -9.7, short of the target by ten per cent. We then tested the two-loop Hamiltonian on the exact energies of short non-BPS operators, which are known from the Bethe ansatz [108]. It reproduced them exactly in every sector built from scalars, fermions and field strengths. It failed in every sector that contains the letter DZ, a scalar with one derivative, by rational amounts such as $\frac{16}{3}$ and $\frac{80}{9}$. A dispersion test located the problem. For a single DZ impurity moving in a background of Z letters, the amplitude to hop by one site came out as 7 where the algebra requires 9. An independently written engine, with 5811 planar templates and explicit magnetic quantum numbers, gave 7.00 as well, for every way of labelling the loop momentum.

The discrepancy is therefore a property of the regulated theory and not of the code.

What is missing is a finite renormalisation of the instantaneous Coulomb interaction,

$$\Delta^{-1} \;\to\; (1 - \tfrac{4}{3}g^2)\,\Delta^{-1}, \qquad \text{that is} \qquad \delta h_4 = -\tfrac{4}{3}\,h_2^{\text{Coul}}, \tag{75}$$

where $h_2^{\text{Coul}} = PC_2P$ is the Coulomb part of the one-loop Hamiltonian, in units where h_2 is of order g^2. The tree-level Coulomb exchange between two letters vanishes identically when either letter has $j_L = 0$ or $j_R = 0$, since such a letter has no charge density in the relevant harmonic. This is why every earlier test, all of which involved letters of that kind, was blind to it.

The coefficient is heavily over-determined. We fitted three independent coefficients, for the Coulomb kernel in its two lowest multipoles and for a possible companion contact term, to fourteen exact two-loop energies in sectors of lengths three, four and five. The fit gives -1.3332, -1.3296 and -0.0002, with residuals below 10^{-3}. With the values $-\frac{4}{3}$, $-\frac{4}{3}$ and 0 imposed there is no free parameter and the residuals stay below 1.1×10^{-3}, which is the noise of the extrapolation in J. With the hop amplitude this makes fifteen exact conditions for one number.

We have not derived the coefficient $\frac{4}{3}$. It is not an artefact of labelling: cut-offs on j_L, on j_R, on their maximum, minimum or mean, and smooth cut-offs on the energy, all give the same hop amplitude 7. It does have a relative. The same factor $\frac{4}{3}$ multiplies a finite kinetic counterterm for the fermions that we had found earlier, $\delta H = \frac{4}{3}g^2 H_0^{\text{ferm}} + \ldots$ Both are what one would expect if the cut-off induced a finite relative renormalisation, by $\frac{4}{3}g^2$, between the terms in the action with time derivatives and those with space derivatives. In a theory without boosts nothing forbids that. It is the two-loop analogue of the unequal wave-function renormalisations of [39, 68]. A derivation along these lines should be possible, and would be valuable. A regulator that preserves sixteen supercharges does exist, in the form of the plane-wave matrix model expanded around fuzzy spheres [112], and in it none of these counterterms should arise.

9.5 Why b is not affected

None of this affects the quartic coefficient, for two reasons.

The first is topological. The mass term and the Coulomb term are single-trace operators with two and four fields, and they are of order g^4. At the order we work they can only be inserted once, at tree level. The resulting diagrams have the topology of a one-loop or two-loop vacuum diagram, with at most three index loops. The coefficient of $|u_1|^4$ needs four. This is the argument of AMMPV [39]. These counterterms contribute to m_1^2, and to the cubic coupling at the next order, but they cannot contribute to b at order λ^2.

The second is that the quantities that do enter b are insensitive to how the cut-off is labelled, which is the practical symptom of a missing counterterm. Piece (a) has no loop. In piece (b) the double-trace kernel converges absolutely once the species are summed. As an illustration, the entry of the kernel between the lowest scalar and the first excited scalar multiplet comes out as -606.0000, -605.9998 and -606.0002 for three different choices of the line that carries the cut-off. The exact value is -606. The planar kernels that enter d_4 are different. Some of them converge only conditionally, and there the choice of line matters at the level of $\frac{4}{9}$ to $\frac{4}{3}$ in individual entries. The exact two-loop energies select one choice unambiguously.

The resulting picture is coherent. The quantity we set out to compute is the part of the three-loop free energy that is cleanest: double-trace, protected from counterterms by $n_B = n_F$, and absolutely convergent. The quantity we used to test the machinery, the two-loop Hagedorn temperature, is the part that is most sensitive to this regularisation. That it nevertheless comes out right, once the broken symmetries are restored, is the stronger test.

10 Discussion

10.1 What has been shown

The quartic coefficient of the Polyakov-loop effective action of $\mathcal{N} = 4$ super Yang–Mills theory on S^3 is negative at order λ^2. It follows that at small λ and large N the theory has a single first-order deconfinement transition, at a temperature T_c below the Hagedorn temperature by a relative amount $9.4 \times 10^{-5}\lambda^2$. In a window of temperatures around T_c there are three saddle points: a confined one with free energy of order one, a deconfined one with free energy of order N^2 and a gapped eigenvalue distribution, and an unstable one between them.

This is the structure of the gravitational problem. There the three saddles are thermal anti-de Sitter space, the large black hole and the small black hole, and they exist together above a temperature $T_{\min} = \sqrt{2}/\pi R$, with the first two exchanging dominance at $T_{\rm HP} = 3/2\pi R$. The identification of the saddles across the two regimes was proposed in [6] and sharpened in [61, 62, 63], and the present result adds only that it is consistent at weak coupling. The simplest phase diagram in the plane of λ and T, a single line of first-order transitions from $\lambda = 0$ to $\lambda = \infty$, is allowed. The alternative, in which the line splits into two at some finite coupling, was the only possibility had b been positive. It is now the less economical of the two.

We cannot say more than allowed. Whether the line in fact continues unbroken through intermediate coupling is not something that a weak-coupling calculation can test.

10.2 The unstable saddle and the Hagedorn temperature

The unstable saddle merits a comment. At weak coupling it sits at $|u_1| = u_s \propto \sqrt{T_H - T}$, it merges with the confined saddle at T_H, and it carries the information that the confined phase, although locally stable all the way to T_H, is only metastable above T_c. This is the scenario that Atick and Witten proposed for string theory in flat space [26]: the Hagedorn temperature is never reached in equilibrium, because a first-order transition driven by the winding mode intervenes. They argued for it from the sign of a quartic coupling of the winding mode, induced by its coupling to the dilaton and the graviton. The argument here has the same structure. The winding mode is u_1, and the exchange of u_2, which makes a negative contribution to b whatever its coupling, plays the part of the massless exchange.

On the gravity side, a small black hole in anti-de Sitter space becomes as small as the string length as its temperature approaches the Hagedorn temperature of the string, and it is expected to turn into a highly excited string [28, 63, 29, 113]. At weak coupling the corresponding statement is that the unstable saddle merges with the confined phase at T_H. The three temperatures (67) thus have direct counterparts. The interpolation of $T_H(\lambda)$ is known from integrability [81, 82, 83]: it rises from 0.380 at $\lambda = 0$ and grows like $\lambda^{1/4}/(2\sqrt{2}\,\pi)$ at large λ, where it is the Hagedorn temperature of the string in a nearly flat region. The first correction to this behaviour has been derived on the string side by Urbach, who records that Maldacena found it independently (unpublished) [113], and it agrees with the numerical integrability result. Formulas for the next orders have been conjectured or proposed, partly with that numerical input, and they agree with it as well [114, 115, 116]. The transition temperature stays of order one, reaching $3/2\pi = 0.477$. At weak coupling the two are separated by a relative $10^{-4}\lambda^2$, and at strong coupling by a factor that grows like $\lambda^{1/4}$. It would be interesting to follow $T_c(\lambda)$, but no analytic method is known. A Monte Carlo route through the plane-wave matrix model has been proposed [117]. The free energy of the deconfined phase is not a spectral problem of the planar dilatation operator.

10.3 Open problems

Several extensions are within reach of the same methods.

Derive the $\frac{4}{3}$. The finite renormalisation (75) should follow from a one-loop computation of the Coulomb propagator and the fermion kinetic term with a mode cut-off. We expect it to be the statement that the cut-off renormalises the speed of light.

Resolve the pure Yang–Mills class. This needs a comparison with the expressions and integrals that [39] give for each diagram, or a third calculation. A Lagrangian calculation of diagrams 3c, 3f and 3n alone would do.

Chemical potentials. With chemical potentials for the R-charges and the spins, b becomes a function on a five-dimensional space, which interpolates between (63) and the entries of table 3. The codes take the chemical potentials as input. The phase diagram with R-symmetry chemical potentials was mapped at zero coupling, and at weak coupling and high temperature, in [118], and near the critical chemical potentials in [119]. The Hagedorn temperature with chemical potentials has been studied with integrability [83, 120]. The gravitational side has charged and rotating black holes with a phase structure of their own, and a comparison at the level of the order of the transition should be possible.

Other theories. For a gauge theory on S^3 with adjoint matter, the first term in (48) is a function of the letter content and the one-loop operator only, and the second is not. The one example known to us of a weakly coupled large-N gauge theory with a single-trace Lagrangian on a sphere of two or more dimensions that was reported to have $b > 0$ is pure Yang–Mills theory on a small S^2 [47]. When scalar fields with arbitrary couplings are added, b can be given either sign, in more than two space-time dimensions by a double-trace term [39]. It would be useful to know whether a single-trace example exists on S^3, and what decides the sign. The Yang–Mills coupling to matter seems to favour $b < 0$: the plane-wave matrix model in perturbation theory [44], the massive matrix quantum mechanics of [46], pure glue on S^3 and now $\mathcal{N} = 4$ all have it.

The next order. The λ^3 term of b needs the three-loop dilatation operator off shell, and four-loop vacuum diagrams. No qualitative question that we know of needs it.

10.4 A closing remark

Witten's identification of the Hawking–Page transition with deconfinement is one of the oldest entries in the AdS/CFT dictionary. It has been tested at strong coupling and at zero coupling. At zero coupling it holds in a weak sense only, since the free transition is of a degenerate kind that fits no gravitational picture. The computation reported here removes the degeneracy. The first effect of the interaction is to make the transition into what it is at strong coupling: first order, with a small unstable black hole in between. This outcome was not guaranteed. The one-loop operator alone makes it plausible, and the two-loop operator, which might have opposed it, as it does in pure Yang–Mills theory, turns out to help.

A Conventions and dictionary

The radius of the sphere is one. The gauge group is $SU(N)$, and we work at leading order in $1/N$. The Yang–Mills coupling g_{YM} enters through the 't Hooft coupling $\lambda = g_{\mathrm{YM}}^2 N$. Table 6 collects the couplings that appear in the text and in the papers we compare with.

The dilatation operator is $D = D_0 + g^2 D_2 + g^4 D_4 + \ldots$ On two adjacent letters of a single-trace operator the planar part of $g^2 D_2$ acts as $2g^2 \sum_j h(j) P_j$, where P_j projects onto total spin j of $psu(2,2|4)$ and $h(j) = \sum_{k=1}^{j} 1/k$. We write $\mathcal{H}$ for the complete one-loop operator in the normalisation $g^2 D_2 = (\lambda/8\pi^2)\mathcal{H}$. On $\mathbb{R} \times S^3$ the dilatation operator is the Hamiltonian,

symbol	definition	used by
λ	$g_{\rm YM}^2 N$	this paper, [75]
g^2	$\lambda/16\pi^2$	this paper, [81, 82]
G	$2g^2\beta = \beta\lambda/8\pi^2$	this paper; the combination in (47)
λ_A	$\lambda/2$	[6, 39]
$\lambda_{\rm HO}$	$\lambda/4\pi^2 = 4g^2$	[86, 106]

Table 6: Couplings.

and h_2, h_4 are the terms of order g^2 and g^4 of the effective Hamiltonian in the degenerate subspaces of D_0.

The Polyakov loops are $u_n = \mathrm{tr}\, U^n/N$, with U the holonomy of the gauge field around the thermal circle and $u_{-n} = u_n^*$. The effective action is normalised as $Z = \int dU\, e^{-S_{\rm eff}(U)}$, and $\langle \ldots \rangle_U$ is the average over free thermal states twisted by U, defined in section 4. Table 7 lists the functions of temperature that enter it. All of them are evaluated at the free Hagedorn point $x_H = 7 - 4\sqrt{3}$ unless an argument is shown.

symbol	meaning	value at x_H
$z(x)$	single-letter partition function, (9)	1
β_0	$-\ln x_H$	2.6339158
A_2	$1 - z_2(x_H)$, twice the mass squared of u_2	0.9742786
d_1	coefficient of $\lvert u_1\rvert^2$ in $\langle \mathcal{H}\rangle_U/N^2$, (35)	$\frac{3}{2}$
c_3	coefficient of $u_1^2 u_{-2}$ + c.c. in $\langle \mathcal{H}\rangle_U/N^2$	0.16821
Q_4	coefficient of $\lvert u_1\rvert^4$ in $\langle \mathcal{H}^2\rangle_{U,\rm conn}/N^2$, (45)	2.1222
I	$\frac{1}{2}Q_4 + 2c_3^2/A_2$	1.11918
C_{41}	coefficient of $\lvert u_1\rvert^2$ in $\langle \mathcal{H}^2\rangle_{U,\rm conn}/N^2$	8.353829
d_4	coefficient of $\lvert u_1\rvert^2$ in $\langle D_4\rangle_U/N^2$	-10.71
q_4	coefficient of $\lvert u_1\rvert^4$ in $\langle D_4\rangle_U/N^2$	-2.234
m_1^2	coefficient of $\lvert u_1\rvert^2$ in $S_{\rm eff}/N^2$	0 at T_H
b	coefficient of $\lvert u_1\rvert^4$ in $S_{\rm eff}/N^2$ after integrating out u_2	$-36.94\, g^4$

Table 7: Functions of temperature. Values of c_3, Q_4 are in the literal scheme.

We use short names for the lightest letters. Z and ϕ are two of the three complex scalars in their lowest harmonic, with energy one. ψ is a fermion in its lowest harmonic, with energy $\frac{3}{2}$. F is the lowest mode of the gauge field, with energy two. DZ, $D\psi$ and D^2Z are the first and second excited harmonics, which in the language of local operators are letters with one or two covariant derivatives. The letter DZ has spins $(\frac{1}{2}, \frac{1}{2})$, and is the lightest letter with both spins non-zero.

The cut-off J is an upper limit on $2j_L$ for every virtual mode.

B The series for q_4

We write $q_4^{(a)}(y) = \sum_n a_n y^n$ and $q_4^{(b)}(y) = \sum_n b_n y^n$ with $y = \sqrt{x}$. Tables 8 and 9 give the coefficients, the size of each term at $y_H = 2 - \sqrt{3}$ and the partial sums.

The leading powers have a simple origin. In piece (a) the first term needs three letters, and the lightest are three scalars of energy one, which gives $x^3 = y^6$. In piece (b) two letters are enough, and two scalars give $x^2 = y^4$.

The one-loop functions $c_3(x)$ and $Q_4(x)$ were obtained as power series in y in the same

n	a_n	$a_n y_H^n$	partial sum
6	-450	-0.16654	-0.1665
7	-2184	-0.21658	-0.3831
8	-6246	-0.16597	-0.5491
9	-13632	-0.09706	-0.6461
10	$-231931/9$	-0.04916	-0.6953
11	$-132776/3$	-0.02262	-0.7179
12	$-5104045/72$	-0.00971	-0.7276
13	-107405.298	-0.00394	-0.7316
14	-155890.649	-0.00153	-0.7331
15	-218506.809	-0.00058	-0.7337
16	-297723.117	-0.00021	-0.7339

Table 8: Piece (a), the tree kernel. The coefficients through y^{12} are exact rational numbers. The rest were obtained in floating-point arithmetic and are rational too. Successive terms fall by a factor that tends to 0.37, and the remainder after y^{16} is -0.0001.

n	b_n	$b_n y_H^n$	partial sum
4	-42	-0.21650	-0.2165
5	-384	-0.53039	-0.7469
6	$-2181/2$	-0.40359	-1.1505
7	-2100	-0.20825	-1.3587
8	$-118841/36$	-0.08772	-1.4464
9	$-128452/27$	-0.03387	-1.4803
10	$-306863/48$	-0.01220	-1.4925

Table 9: Piece (b), the loop kernel. Each coefficient is the limit $J \to \infty$ of a sequence computed at finite cut-off, identified as a rational number. The coefficients at $n = 4, 5, 6$ were obtained by two independent codes. A geometric estimate of the remainder gives -0.007, and Padé approximants give totals between -1.4987 and -1.5044.

way, to high enough order that the truncation error is below the precision quoted in (49). In the $su(2)$ sector they reduce to $c_3 = 2x^3$ and $Q_4 = 4x^3 + 8x^4$, which can be checked by hand.

C How the computation was done

This appendix records how the work was organised, since this bears on how the result should be judged.

Organisation

The work was divided among many instances of the same AI system, several at a time, each with a narrow brief and no memory of the others except through files. One instance coordinated. It wrote the briefs, kept a design document with the conventions and the current state of each quantity, and decided what to believe.

Three rules were imposed from the start.

The first was that no number enters the result unless two independently written programs agree on it, or it has been checked against an exact result. It was kept with one exception, recorded in section 6.6: the coefficients of piece (b) from y^7 onwards come from a single

engine. The independence extended to the method. For the vertex coefficients, for instance, one construction used the $9j$ symbols of [102], and another used explicit harmonic polynomials in $\mathbb{R}^4$ restricted to the sphere. Three contraction engines were written on top of them.

The second was that every program must pass a gate before it is used in production. A gate is a case with a known answer, run by the same code with no change but the input. The gates were the $su(2)$ sector, the matrix models with $N = 2$ and 3, the two-loop results of AMMPV, the supertrace identities and, later, the exact two-loop energies.

The third was that a disagreement is never averaged or argued away. It is pursued until one side is shown to be wrong. The Coulomb counterterm of section 9 was found this way. Two engines agreed with each other and disagreed with the Bethe ansatz, and it took the dispersion test to show that both were faithfully computing the wrong theory.

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