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Free energy of rectangular domains at criticality

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Abstract. We calculate the universal part F of the free energy of rectangular domains at critical points by use of conformal field theory. F includes a term logarithmic in the size (or area), due to the corners. In addition, there is a term F_0 depending on the aspect ratio, which we determine by integrating the stress tensor $\langle T \rangle$ over the rectangle. This term involves complete elliptic integrals, but may be more simply expressed in terms of the Dedekind η-function. For central charge $c>0$, we find that F_0 is maximal for squares, providing a thermodynamic driving force for the elongation of small domains, and argue that this should be a general tendency.

1. Introduction

The free energy of a finite two-dimensional region or domain may generally be written in the form

$$F_{\text{tot}} = f_0 A + f_1 E + F \tag{1}$$

where A is the area of the domain, E the edge length, f_0 the free energy per unit area, and f_1 the free energy per unit edge length, with all free energies in units of $k_B T$ (in equation (1) and below). In the thermodynamic limit the term f_0 dominates, while for smaller domains f_1 becomes important. In most circumstances, the term F is a geometry-independent constant. However, at criticality, it may depend on the size and shape of the domain. Indeed, Cardy and Peschel [1] have shown that corners on the boundary induce a trace anomaly in the stress tensor. This gives rise to a term in F proportional to $\ln L$, where L measures the size of the domain. (There are similar effects arising from curved boundaries or metrics, but we are not concerned with them here.) Such geometry dependence is possible at criticality since the correlation length is infinite, allowing one side of the domain to influence the other.

In this work we calculate the universal (geometry-dependent) part of F for an L by L' rectangle at conformally invariant critical points as

$$F = -c/8 \ln A + c/4 \ln[\eta(q)\eta(q')] \tag{2}$$

where c is the central charge, $q = \exp(-2\pi x)$ and $q' = \exp(-2\pi/x)$ with x the aspect ratio L'/L, and η the Dedekind function. Equation (2) applies for any conformally invariant (uniform) boundary condition around the edge of the rectangle. It is known [2] that in a given theory the number of such boundary conditions is the same as the number of conformal blocks. More generally, equation (2) is an example of the Casimir effect [3], first encountered in quantum electrodynamics.

The terms f_0 and f_1 in equation (1) are non-universal, and cannot be calculated by model-independent methods. However, Cardy [4] has shown that $f_1 > 0$ for the minimal models with free boundary conditions. This sign coincides with physical expectations, since it prefers domains of compact shape.

We proceed by computing the derivative of F with respect to L'. Aside from the trace anomaly term [1], this is given by a line integral of the stress tensor $\langle T\rangle$ in the rectangular geometry. $\langle T\rangle$, in turn, is determined by the Schwarz derivative of the Schwarz–Christoffel transformation from the half plane to the rectangle. We give expressions for the indefinite integral of $\langle T\rangle$ in the rectangle, which may be useful in other calculations. Next we include the trace anomaly ($\ln L$) term, which is easily determined. Our initial form for F includes a combination of complete elliptic integrals. However, these can be more simply expressed in terms of the Dedekind η-function, as quoted above. This observation allows for a simple approximation to the x-dependent term. This quantity is proportional to the central charge c. When $c > 0$, it is minimal for large (or small) aspect ratio x. Thus it provides a thermodynamic driving force for elongation, acting in competition with the edge term. We also argue that the decrease of free energy with elongation should be a general effect. Such behaviour may in fact be manifest in very small domains on real surfaces [5].

If operators with negative dimensions are present, the free energy may include extra terms, as has already been pointed out for the case of an infinite strip with periodic boundaries [6] and actually occurs for the Lee–Yang edge singularity [7]. We argue below that equation (2) remains valid even in this case because the boundary conditions of the rectangle allow coupling only to the conformal block of the unit operator [8].

Related results for specific heats and correlation functions in finite domains at the Ising critical point have been obtained via conformal techniques [9]. It is interesting that the correction to the leading ($x \to 0$ or $x \to \infty$) shape dependence in equation (2) resembles the shape dependence of the free energy of the simple Ising model on a torus [10], which involves elliptic θ functions, and may be understood in terms of a one-dimensional array of domain walls [11].

2. Calculation of the free energy

The change in F induced by a general coordinate transformation $z \to z + \alpha(z)$, where $z = x + \mathrm{i}y$, is [12]

$$\delta F = (1/2\pi) \int \mathrm{d}^2 r \langle T_{ij}\rangle \, \mathrm{d}\alpha^j/\mathrm{d}r_i \tag{3}$$

where $\langle T_{ij}\rangle$ is the expectation value of the stress tensor and the integral extends over the domain in question. Now we consider a rectangle in the $w = u + \mathrm{i}v$ plane, of length L in the u (horizontal) and L' in the v (vertical) directions, respectively. The transformation

$$u \to u \qquad v \to v + \delta v \, \Theta(v - v_0) \tag{4}$$

where Θ is a unit step function and $0 < v_0 < L'$ stretches the rectangle in the v direction, so that $L' \to L' + \delta v$. Thus, equation (3) becomes [12]

$$\delta F_0 = (1/2\pi)\delta v \int \mathrm{d}u \langle T(v_0) + \bar{T}(v_0)\rangle. \tag{5}$$

We denote the free energy F_0 in anticipation of an additional term not included in equation (5) which will be discussed below. To evaluate equation (5), we take advantage of the behaviour of the stress tensor under a (finite) conformal transformation [13],

$$T(z) = (\mathrm{d}w/\mathrm{d}z)^2 T(w) + (x/12)\{w, z\} \tag{6}$$

where the curly brackets denote the Schwarz derivative

$$\{w, z\} = [w'''w' - \tfrac{3}{2}(w'')^2]/(w')^2 \tag{7}$$

and $\bar{T}$ obeys a similar equation.

If z is the coordinate in the half plane, $\langle T(z)\rangle = 0$. The Schwarz-Christoffel transformation,

$$\mathrm{d}w/\mathrm{d}z = 1/[(1-z^2)(1-k^2z^2)]^{1/2} \qquad w(0) = 0 \tag{8}$$

maps the upper half plane on to a rectangle. The points $z = \pm 1$, $\pm 1/k$ on the real axis are transformed into the corners at $w = \pm K(k)$, $\pm K(k) + \mathrm{i}K'(k)$, respectively. Here K and K' are complete elliptic integrals of the first kind with module k, $0 < k < 1$. Thus $L = 2K$, $L' = K'$ and the aspect ratio becomes

$$x = K'/2K. \tag{9}$$

Making use of equations (6) and (8), one finds after some algebra that

$$\begin{aligned}\langle T(w)\rangle = -(c/12)[&(1-3k^2z^2) + k^2 + \tfrac{3}{2}z^2(1-k^2z^2)/(1-z^2) \\ &+ (3k^4/2)z^2(1-z^2)/(1-k^2z^2)].\end{aligned} \tag{10}$$

Using equations (8) and (10) it is easy to show that as $w \to w_0$, where w_0 is the coordinate of a corner of the rectangle, $\langle T(w)\rangle \to -(c/8)/(w-w_0)^2$, the correct form for a right angle corner [1].

Transforming the expression for δF_0, equation (5), into the z plane, and making use of equations (8) and (10), one can calculate the RHS by contour integration. The contributing singularities are taken as two poles connected by a branch cut on the real axis. The contribution of the $\bar{T}$ term is used to close the contour. The result is

$$\delta F_0/\delta v = (c/6\pi)[\tfrac{5}{2}K(k) - \tfrac{1}{2}k^2K(k) - 3E(k)] \tag{11}$$

where E is a complete elliptic integral of the second kind. The derivative of F_0 with respect to L' then follows by scale invariance,

$$\mathrm{d}F_0/\mathrm{d}L' = (2K/L)\delta F_0/\delta v. \tag{12}$$

By considering the behaviour of the elliptic integrals as $k \to 0$, one can verify that equation (11) reproduces the known [14] limiting behaviour for large aspect ratio (i.e. for an infinite strip), namely

$$\mathrm{d}F/\mathrm{d}L' = -c\pi/24L. \tag{13}$$

The corresponding expression for an infinite strip in the perpendicular direction is similarly obtained by taking the limit $x \to 0$ ($k \to 1$). These conclusions are not altered by the inclusion of the logarithmic term in F discussed below.

One may also determine δF_0 by performing the integration in equation (5) in the w plane. The details of this calculation are described in the appendix.

Now the free energy must be invariant under the modular transformation S, i.e. interchange of L and L'. It follows that F, if it were a function of x only, must necessarily be symmetric in $x \leftrightarrow 1/x$, so that $\mathrm{d}F/\mathrm{d}L' = 0$ for a square ($L = L'$). Equation (12), however, does not vanish for $x = 1$ ($k = 0.171\,573\ldots$). This is because the transformation we have employed, equation (4), changes the area A of the rectangle and there is a term in F proportional to $\ln A$ due to the corners. The formula given in equation (5) and hence our result (equation (12)) miss this effect because they assume that the stress tensor has trace $\langle\Theta\rangle = 0$, while the singularity of the Schwarz–Christoffel transformation at the corners of the rectangle mentioned above implies a non-zero value for $\langle\Theta\rangle$ [1]. This situation may be remedied by simply adding a term $-(c/4)\ln L$ to F_0, consistent with the prescription in [1]. With this additional term $(\mathrm{d}F/\mathrm{d}L')_A$ vanishes for $x = 1$, as it must.

It is possible to express F in a more compact form, explicitly displaying its x dependence, by use of the Dedekind η-function [15]

$$\eta(q) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n). \tag{14}$$

We set $q = \exp(-2\pi x)$, and make use of the relations [15, 16]

$$\eta = 2^{1/3} k^{1/12} k'^{1/3} K^{1/2} / \pi^{1/2} \qquad \mathrm{d}K/\mathrm{d}k = E/kk'^2 - K/k \tag{15}$$

where $k'^2 = 1 - k^2$, along with equation (9), and the Legendre relation

$$EK' + E'K - KK' = \pi/2. \tag{16}$$

It follows that

$$F_0 = c/2 \ln \eta(q) \tag{17}$$

satisfies equation (12), and that

$$F = -c/4 \ln L + c/2 \ln \eta(q). \tag{18}$$

In writing equation (18) we have ignored a possible geometry-independent additive constant. Using equation (18) and the modular properties of F or η leads directly to the symmetric form of equation (2).

3. Further remarks

The definition of η (equation (14)) suggests a first approximation to equation (2)

$$F = -c/8 \ln A - c\pi/24(x + 1/x) \tag{19}$$

which has the proper area dependence and preserves the correct limiting behaviour as $x \to 0$ or ∞. The shape-dependent term in equation (19) is 1.98... times the exact result at $x = 1$; this ratio decreases slowly with x (1.29... and 1.11... at $x = 10$ and 50, respectively) and is symmetric in $x \leftrightarrow 1/x$.

Now for $c > 0$, *if the area is fixed and the shape varied*, the approximate F is maximal for a square ($x = 1$) as is the exact result. So there is a thermodynamic driving force for *elongation* of the domain. This may be regarded as due to an attraction of the walls of the rectangle, with a force per unit length inversely proportional to the square of their separation. Thus the tendency to elongation should be a general effect, not limited to domains of rectangular shape. Hence the shape dependence in equation

(19) may be more widely useful [5]. In fact, it follows from equations (5) and (6) that $\delta F = 0$ for a circle, since this figure can be mapped to the half plane via a projective transformation, for which the Schwarz derivative vanishes. Thus F is extremal for any set of figures interpolating between infinite strips and including a circle, e.g. ellipses with x replaced by the ratio of the axes.

In addition, one expects a similar tendency to elongation to extend into the critical region. The attraction of the walls arises since the correlation length ξ is infinite at criticality, allowing one wall to influence the other. On the other hand, the free energy of a finite domain must be continuous, so there should be similar behaviour whenever the system is close enough to criticality that $\xi > L, L'$.

Equation (18) has been derived for the Ising model with fixed boundary conditions by an argument based on operator content and modular invariance [17]. Essentially, this result follows from knowledge of the corner term $-c/4 \ln L$ and the fact that F involves an analytic function of q. In these circumstances, use may be made of the known classification of modular invariant functions [18]. Note that analyticity in q implies invariance under the other modular operation, $T: x \to x - \mathrm{i}$. An argument directly demonstrating the T invariance or analyticity in the general case would be interesting.

It is also interesting to interpret our result in terms of transfer matrices in the infinite strip (see [12], for instance). Then the partition function may be expressed in terms of a sum over eigenstates of the primary operators. It follows immediately from equation (18) that only the conformal tower of the unit operator contributes. In the present case the partition function is the expectation value (and not the trace) of a power of the transfer matrix between boundary states. Since these states do not couple to operators with fractional dimensions $h > 0$ for theories where all dimensions h_i are positive, one expects the same to hold true when there are operators with dimension $h < 0$ [8]. Thus equation (18) or (2) will be valid in this case as well, and the Casimir energy of a long strip will not be corrected by $h_{\min}$, as occurs for an infinite strip with periodic boundaries [6].

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Appendix

The inverse Schwarz-Christoffel transformation is given by the Jacobian elliptic function

$$z = \operatorname{sn} w. \tag{A1}$$

Substituting this into equation (10) and making use of the relations

$$1 - z^2 = \operatorname{cn}^2 w \qquad 1 - k^2 z^2 = \operatorname{dn}^2 w \tag{A2}$$

one finds

$$\langle T(w) \rangle = -\tfrac{1}{2}(1 + k^2) + \tfrac{3}{2}(k^2 \operatorname{cn}^2 w / \operatorname{dn}^2 w + \operatorname{dn}^2 w / \operatorname{cn}^2 w). \tag{A3}$$

The indefinite integral in equation (5) is then

$$\int \langle T \rangle \, \mathrm{d}w = \tfrac{1}{2}(5-k^2)w + \tfrac{3}{2}(k^2 \operatorname{sn} w \operatorname{cn} w/\operatorname{dn} w + \operatorname{sn} w \operatorname{dn} w/\operatorname{cn} w) - 3E(\operatorname{am} w, k) \qquad \text{(A4)}$$

where am w is the amplitude. Evaluating the definite integral leads once again to the result obtained by integration in the z plane, equation (11).

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