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# Domain boundary energies in finite regions at 2D criticality via conformal field theory

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Abstract. By use of conformal field theory, we calculate universal results for the energies of curved domain boundaries at two-dimensional critical points in circular and rectangular regions. This work extends the theory of finite-size effects at criticality, complementing previous exact results for the energies of domain boundaries in infinite strips.

## 1. Introduction

The theory of finite-size effects near critical points has been extensively studied via scaling arguments, numerical methods, exact model results and conformal invariance—for reviews see [1] and references therein. In this paper, we consider the effects of finite size on domain boundary free energies (also called the interfacial or domain wall free energies) in two-dimensional systems at criticality.

Previous work [2] demonstrates that the (extra) free energy of an excitation in a two-dimensional system at criticality is simply related to the correlation function of the scaling operators that create it. In particular, boundary operators in the upper half plane may be employed to create a domain boundary. The basic statement of conformal invariance of correlation functions then allows computation of the corresponding energy in a new geometry. Another fundamental tenet of the theory, the operator product expansion, may be used to determine the interaction energy of two or more such domain boundaries. The consequences of these statements were worked out for a particular geometry, namely an infinite strip (with edges).

Domain boundaries created in this fashion are often referred to as 'pinned' or 'anchored', since their ends are fixed. Realizations are possible by appropriately changing the microscopic degrees of freedom at the edge of the region. For example, in an Ising model, constraining the spins to be up over part of the edge and down over the rest will induce a domain boundary running between the points where the spin direction changes. Other realizations include stepped surface systems with phase transitions involving surface reconstruction, and boundaries arising from kinks in the terrace edge.

In this paper, we calculate the energies of domain boundaries in two fully finite geometries, the circle and the rectangle (with arbitrary aspect ratio). This extends our previous results for the strip.

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In section 2 we review the basic equations used to find the energy. In section 3 we employ them to find the energy of a single boundary and the interaction energy of two boundaries in a circle. Section 4 treats the rectangular geometry. Section 5 summarizes our results. To our knowledge, the results in this paper are new, with the single exception noted in section 4.

#### 2. Domain boundary energies

In this section we recall the method by which domain boundary energies may be obtained [2]. Consider first the upper half plane, with conformally invariant (uniform) boundary condition and boundary operators  $\psi(x_i)$  at positions  $x_i$  on the real axis. These operators mediate a change in the boundary conditions at  $x_i$  [3, 4]. Then the (extra) free energy (in units of  $k_BT$ ) of the corresponding excitation is simply

$$\Delta F = -\ln\langle \psi(x_1)\psi(x_2)\dots\rangle. \tag{1}$$

The energy in any geometry obtainable by conformal mapping of the upper half plane may be determined by use of equation (1) and the basic statement of conformal invariance [5],

$$\langle \psi(x_1) \dots \rangle = | w'(x_1) |^{\Delta} \dots \langle \psi(w_1) \dots \rangle.$$
<sup>(2)</sup>

In equation (2), w(z) is any analytic function, and  $\Delta$  the scaling dimension of  $\psi$ . Since there is only a single Virasoro algebra operative in the half plane [6], only a single scaling dimension and one independent coordinate enter equation (2) [7]. It should be noted that, for certain operators and certain (finite) transformations, there is the possibility of a sign change in equation (2), e.g. under inversions [7]. This does not apply to the cases we treat below. In making use of equation (2), it is often convenient to express z = z(w) and compute the derivative via w'(z) = 1/z'(w).

A single boundary (figure 1) is created by a pair of operators at  $x_1$  and  $x_2$ , so that, for properly normalized operators,

$$\langle \psi(x_1)\psi(x_2)\rangle = 1/x_{12}^{\Delta} \tag{3}$$

where  $x_{12} \equiv |x_1 - x_2|$ . In calculating the energy from equations (1) and (3), one must be aware that creating domain boundaries in a specific model generally involves non-normalized operators, so the RHs of equation (3) is multiplied by a non-universal constant. Our formulae for single domain energies correspondingly ignore a nonuniversal but geometry-independent additive constant. However, this constant does not affect the interaction energies.



Figure 1. Domain boundary in the upper half plane created by boundary operators at  $x_1$  and  $x_2$ . A and B refer to the two domains, or, on the real axis, the two types of boundary conditions. Although our energy formulae apply to any pair of boundary operators and any conformally invariant boundary condition, the geometry of the boundary may differ from that illustrated here or in the other figures [2].

A pair of domain walls may be created by four boundary operators at points  $x_1 < x_2 < x_3 < x_4$ . The total energy then depends on a four-point correlation function. If at least one pair of points is near each other, the situation simplifies, since the (boundary) operator product expansion may be used. For  $x_{12} \ll x_{13}$ , one finds [2] that the leading term in the interaction energy of the two domains is always attractive, and given as

$$E_2 = -C^2 \left(\frac{x_{12} x_{34}}{x_{a3} x_{a4}}\right)^{\Delta_1} \tag{4}$$

where  $\Delta_1$  is the dimension of the most relevant operator  $\psi_1$  appearing in the expansion of  $\psi$  with itself,  $x_a$  a point in the neighbourhood of  $x_1$  and C the appropriate (boundary) operator product expansion coefficient. The form of  $E_2$  in the w-coordinates follows on simply substituting x = x(w) in equation (4), since the scale factors in equation (2) subtract out of any interaction energy.

The energy of one or more domain boundaries in an infinite strip of width L (with edges) was determined [2] by employing equations (1)-(4) with the transformation  $w = L/\pi \ln(z)$ , which maps the upper half plane into the strip. In what follows, we calculate corresponding results for a circle of radius R and rectangles of arbitrary aspect ratio by use of the appropriate conformal maps.

Domain boundary energies may also be computed by integrating their derivatives with respect to the positions of the boundary operators. These derivatives are in turn given by contour integrals of the (expectation value of) the stress tensor with boundary operators present. This general method was used to compute the universal part of the free energy of a rectangular region [8]. For domain boundaries, the appropriate stress tensor in the half plane may be computed from the conformal Ward identity [9], or directly by consideration of the effects of the boundary conditions [10]. This programme has been explicitly carried out for one or two boundaries in the strip geometry [11] and gives (as expected) the same results as the simpler method described here.

### 3. Circular geometry

The upper half plane may be mapped into a circle of radius R (figure 2) by means of a projective map, for instance



Figure 2. Domain boundary in a circle.

Since the form of the correlation function is invariant under projective transformations, it follows immediately from equations (1) and (3) that the energy of a domain boundary in the circle is

$$E_{\rm cir} = E_{1/2} = 2\Delta \ln(d) \tag{6}$$

where d is the distance between the boundary end-points on the circle and  $E_{1/2}$  is the energy in the half plane.

Alternatively, equation (6) may be expressed as

$$E_{\rm cir} = 2\Delta \ln\left[2R\,\sin\!\left(\frac{|\theta_2 - \theta_1|}{2}\right)\right] \tag{7}$$

where  $\theta_1$ ,  $\theta_2$  are the angles of the end-points (the images of  $x_1$  and  $x_2$ ). Note that (assuming  $\Delta > 0$ )  $E_{cir}$  increases with angular separation, being maximal for  $|\theta_2 - \theta_2| = \pi$ , when the points are on a radius. In many cases the boundary in the half plane will be a half circle [2]. Since equation (5) is projective, the boundary in the circle will also follow the arc of a circle. Thus, for a given circle, the energy grows with the boundary length. One must distinguish this length dependence from the dependence on length scale, here the radius *R*. Normally, conformally invariant energies are scale-independent. The logarithmic dependence on *R* is an effect of the trace anomaly (see below).

Now for a given d,  $E_{cir}$  is independent of the radius R (however, the condition  $d \leq 2R$  must be satisfied). This independence is consistent with the heuristic idea that, other factors being the same, correlations increase with the possible number of paths connecting the points. According to equation (1), the corresponding energy will decrease, which may be regarded as an effect of the increase of entropy. For the circle, as R increases, the number of paths crossing to one side of the line connecting the two end-points goes up, while the number involving the other side decreases, with the two tendencies exactly compensating.

It is also interesting to contrast  $E_{cir}$  with the energy of a 'bubble'—a boundary defined by two points separated by distance d on the same side of an infinite strip of width L [2]:

$$E_{\rm b} = 2\Delta \ln\left[\frac{2L}{\pi}\sinh\left(\frac{\pi d}{2L}\right)\right].$$
(8)

Since  $\sinh(x) \ge x$  for  $x \ge 0$ ,  $E_{cir} = E_{1/2} \le E_b$  for any L. This is consistent with the path picture since the strip limits the paths available in the half plane. In fact, in two dimensions one can show quite generally that limiting the geometry always leads to an increase of the boundary energy [12].

Using equation (4), we find

$$E_2 = -C^2 \left( \frac{\sin[(\theta_2 - \theta_1)/2] \sin[(\theta_4 - \theta_3)/2]}{\sin[(\theta_4 - \theta_a)/2] \sin[(\theta_3 - \theta_a)/2]} \right)^{\Delta_1}$$
(9)

for the interaction energy  $E_2$  of two similar boundaries, where we have chosen  $\theta_a = (\theta_1 + \theta_2)/2$ , and ignored correction terms  $O[(\theta_2 - \theta_1)^2]$ , since  $E_2$  is small, and equation (4) valid, only in the case that at least one boundary is small, e.g.  $|\theta_2 - \theta_1| \ll 1$ . This latter condition clearly arises from the steric constraints of the fully finite geometry—one boundary can only avoid the other by being much smaller than R. Thus in fact the interaction can only vanish as a power of the domain *size*,  $E_2 \propto d^{\Delta_1}$ , and the exponential decrease of the interaction with domain *separation* found in the strip [2] does not occur. Clearly this will be true in any other finite geometry as well,

unless there is a long dimension allowing large separation, as for the rectangles with large aspect ratio discussed below.

### 4. Rectangular geometries

## 4.1. Preliminaries

The upper half plane may be mapped into a rectangle via the Schwarz-Christoffel transformation

$$w = \int_{0}^{z} \frac{\mathrm{d}z}{\sqrt{(1-z^{2})(1-k^{2}z^{2})}}.$$
 (10)

The points  $z = \pm 1, \pm 1/k$  on the real axis are transformed into the corners at  $w = \pm K(k)$ ,  $\pm K(k) + iK'(k)$ , respectively, K and K' being complete elliptic integrals of the first kind with modulus k, 0 < k < 1. The aspect ratio x is then x = K'/2K, which takes on all values  $0 < x < \infty$  as k varies over the allowed range. The inverse Schwarz-Christoffel transformation is given by the Jacobian elliptic function

$$z = \operatorname{sn}(w). \tag{11}$$

For simplicity, the results quoted below apply to the rectangle defined by equation (10). Corresponding formulae for rectangles of arbitrary size with the same aspect ratio x may be obtained via a scale transformation, as illustrated in equation (13).

The universal term in the energy of the rectangle itself is also known [8]. The domain boundary in the rectangle (figure 3) follows a path that may be obtained by mapping the boundary in the half plane with equation (10).



Figure 3. Domain boundary in a rectangle.

Applying equations (1)-(3), one finds the energy of a single domain boundary in the rectangle to be

$$E_{\text{rect}} = \Delta \ln \left| \frac{[\operatorname{sn}(w_1) - \operatorname{sn}(w_2)]^2}{\operatorname{cn}(w_1) \operatorname{cn}(w_2) \operatorname{dn}(w_1) \operatorname{dn}(w_2)} \right|$$
(12)

where cn and dn are Jacobian elliptic functions, and the points  $w_1$  lie anywhere on the boundary of the rectangle, except for the corners (see below). One can transcribe this result into an expression for the energy in a rectangle with the same aspect ratio x but differing in size by a scale factor b = L/K' = L'/2K by use of the scale transformation t = bw. The result is

$$E_{\text{rect}} = 2\Delta \ln(b) + \Delta \ln \left| \frac{[\sin(t_1/b) - \sin(t_2/b)]^2}{\cos(t_1/b) \cos(t_2/b) \sin(t_1/b) \sin(t_2/b)} \right|.$$
 (13)

Note that the first term on the RHS of equation (13) includes a part proportional to ln(L). Logarithmic terms of this type also occur in the free energy of finite systems.

They are ascribable to a trace anomaly term in the stress tensor at a corner of angle  $\theta$ , whereby if we put the corner at z = 0,  $\langle T \rangle \rightarrow (c/24z^2)[1 - (\pi/\theta)^2]$ , with c the central charge [8, 13]. Such logarithmic terms may be understood via a 'dimensional resonance' argument [14]. Changing boundary conditions, or equivalently inserting boundary operators, also give rise to trace anomaly terms with coefficient  $2\Delta$  [10], and therefore terms logarithmic in the size occur for boundary energies as well [2]. It follows that the first term on the RHS of equation (13) is equivalent to the effects of a trace anomaly at a corner of an effective angle  $\theta_{\text{eff}}$  that can be computed in terms of  $\Delta$  by equating free energies.

# 4.2. Semi-infinite rectangle

In what follows, we evaluate equation (12) for various special cases. First we consider a semi-infinite rectangle. This allows us to determine the effects of a single end on our previous results for the strip [2]. On taking the limit  $k \rightarrow 1$ ,  $K' \rightarrow \pi/2$ , and  $K \rightarrow \infty$ , so the rectangle approaches an infinite horizontal strip of width  $\pi/2$ . We replace w by w - K, so that the coordinate is given relative to the lower left corner of the rectangle. This emphasizes the effects of the end relative to the infinite strip. Making use of the formulae for  $\operatorname{sn}(w - K)$ , etc., and the expansions of the Jacobian functions for  $k \rightarrow 1$ gives

$$E_{\rm end} = 2\Delta \ln |\sinh(w_2 - w_1)| - \Delta \ln \left| 1 - \left( \frac{\sinh^2(w_2 - w_1)}{\sinh^2(w_2 + w_1)} \right) \right|.$$
 (14)

Equation (14) is directly comparable to an infinite strip in two cases. First, take  $w_1 = u_1$ ,  $w_2 = u_2$  with  $u_1$ ,  $u_2$  real, so both points are on the same long side of the rectangle. Then the first term on the RHS of equation (14) is exactly the energy of a single boundary ('bubble') in an infinite strip of width  $\pi/2$  [2]. The second term in equation (14) is a correction term due to the effects of the end of the rectangle. Since  $u_1, u_2 > 0$  (and assuming  $\Delta > 0$ ) the correction is always positive. The confining effects of the end of the rectangle act to *increase* the boundary energy. The corresponding reduction of the correlation function is consistent with the reduction in the number of paths, and an example of a much more general theorem [12] as in the circular case mentioned. For a boundary of fixed width  $u_2 - u_1$ , the correction decreases exponentially as the boundary moves away from the end of the rectangle, over a distance set by the width of the rectangle. If we take both points on the opposite side of the rectangle, the result is the same. If we take one point on each long side, e.g.  $w_1 = u_1$ ,  $w_2 = u_2 + i\pi/2$ , the sinh functions in equation (14) are replaced by cosh. The first term on the RHS is then the energy of a 'wall' in the infinite strip of width  $\pi/2$ . The correction is again positive, for the same reasons, and decreases exponentially as before.

A third possibility involves one point on each of two adjacent sides of the rectangle, e.g.  $w_1 = u_1$ ,  $w_2 = iv_2$ ,  $0 < v_2 < \pi/2$ . Here the energy may be expressed as

$$E_{\rm end} = \Delta \ln \left| \frac{[\sinh^2(u_1) + \sin^2(v_2)]^2}{\sinh(2u_1)\sin(2v_2)} \right|.$$
 (15)

A fourth case occurs when both points are on the short side of the rectangle, i.e.  $w_1 = iv_1$ ,  $w_2 = iv_2$ ,  $0 < v_1$ ,  $v_2 < \pi/2$ . Here

$$E_{\rm end} = 2\Delta \ln |\sin(v_2 - v_1)| + \Delta \ln \left| \frac{\sin^2(v_2 + v_1)}{\sin^2(v_2 + v_1) - \sin^2(v_2 - v_1)} \right|.$$
 (16)

By the general result, this energy must be larger than  $E_{1/2}$  for  $d = v_2 - v_1$ .

Next we consider the semi-infinite rectangle with one point in a corner. We again define the coordinate w with respect to -K, as in equations (14)-(16). As the point approaches the corner, the boundary operator  $\omega$  is replaced by a corner operator  $\phi$  [6], e.g.

$$\psi(w) \to a w^{-\Delta + \Delta_c} \phi(0) \tag{17}$$

where  $\Delta_c$  is the dimension of the corner operator. This depends on the corner angle  $\theta$  via  $\Delta_c(\theta) = (\pi/\theta)\Delta$ , so that  $\Delta_c = 2\Delta$  here, and  $\psi$  vanishes as  $w^{\Delta}$ . Our correlation functions satisfy this prescription, in all cases. Equation (17) also involves the boundary-corner expansion coefficient *a*, a constant which is suppressed in what follows.

The vanishing of the correlation as one point *approaches* a corner implies a logarithmic divergence of the boundary energy. With one point actually *in* a corner, the boundary is created by the corner operator  $\phi$ . Then the energy will depend, via equation (1), on a  $\langle \phi \psi \rangle$  correlation function. This we determine, using equation (17), as the coefficient of  $w^{\Delta}$ . For the semi-infinite strip, letting  $w_1 \rightarrow 0$ , we find

$$E_{\rm cor} = \Delta \ln \left| \frac{\sinh^3(w)}{4\cosh(w)} \right| \tag{18}$$

where  $w_2$  has been relabelled w. Equation (18) is easily evaluated for w on a long or short side of the rectangle. When the rectangle is scaled by a factor b, as above, the energy is given by the analogue of equation (13), except that the first term becomes  $(\Delta + \Delta_c) \ln(b) = 3\Delta \ln(b)$ . For  $w = i\pi/2$ , the other point is in a corner and equation (17) must be employed again; the energy depends on a  $\langle \phi \phi \rangle$  correlation function. Using the same prescription gives  $-2\Delta \ln(2)$ . Scaling here gives rise to the term  $2\Delta_c \ln(b)$ .

### 4.3. General case

Next we consider the general case of the rectangle. In the following, the origin is again in the centre of the lower side of the rectangle, as in equation (10). The boundary energy has already been quoted in equation (12). There are various ways to re-express this result. One suggestive form is

$$E_{\text{rect}} = -\Delta \ln \left| \frac{1}{\mathrm{sn}_{-}^{2}} - \frac{1}{\mathrm{sn}_{+}^{2}} \right| + \Delta \ln \left| 1 - \left( \frac{\mathrm{cs}_{+} + \mathrm{ds}_{+}}{\mathrm{cs}_{-} + \mathrm{ds}_{-}} \right)^{2} \right|$$
(19)

where cs and ds are the Jacobian elliptic functions cn/sn and dn/sn, respectively, and + or - denotes the argument  $w_1 + w_2$  or  $w_1 - w_2$ , respectively. For the same separation  $w_1 - w_2$ , the energy given in equation (19) must exceed that of equation (14), scaled to a semi-infinite strip of the same width as the rectangle, as long as neither point in the rectangle is closer to an end than either point in the strip.

If both points are on the horizontal side ('bubble'),  $E_{\text{rect}}$  may simply be taken as equation (12) or (19) with  $w_i = u_i$ . For  $w_1 = u_1$ ,  $w_2 = u_2 + iK'$  ('wall'), it becomes

$$E_{\rm rect} = -\Delta \ln |k^2 ({\rm sn}_-^2 - {\rm sn}_+^2)| + \Delta \ln \left| 1 - \left( \frac{{\rm dn}_+ + k \, {\rm cn}_+}{{\rm dn}_- + k \, {\rm cn}_-} \right)^2 \right|.$$
(20)

This result may be compared to the energy of a 'wall' in a strip of the same width, i.e. L = K', which is given by equation (8) with sinh replaced by  $\cosh and d = |u_1 - u_2|$  [2]. According to the general result mentioned, the energy in the rectangle is always larger than in the strip.

With  $w_1 = u_1$ ,  $w_2 = -K + iv_2$ , i.e. a boundary across a corner, we have not found a simple expression for  $E_{rect}$ . Jacobian elliptic functions of  $w_2$  and modulus <u>k</u> are expressed as Jacobian elliptic functions of  $v_2$  with complementary modulus  $k' = \sqrt{1 - k^2}$ , but this leads to a rather involved formula. However, for a 'wall' in the horizontal direction, i.e.  $w_1 = -K + iv_1$ ,  $w_2 = K + iv_2$ , one finds

$$E_{\text{rect}} = -\Delta \ln \left| \frac{\mathrm{cn}_{+}^{2}}{\mathrm{sn}_{+}^{2}} - \frac{\mathrm{cn}_{-}^{2}}{\mathrm{sn}_{-}^{2}} \right| + \Delta \ln \left| \frac{4 \,\mathrm{dn}(v_{1}) \,\mathrm{dn}(v_{2})}{(\mathrm{dn}(v_{1}) - \mathrm{dn}(v_{2}))^{2}} \right|$$
(21)

where + and - refer to  $v_1 + v_2$  and  $v_1 - v_2$ , respectively, and all elliptic functions are evaluated at modulus k'. This result describes the same physical situation as equation (20), except for the change in dimensions of the rectangle. Thus the two functions must be equal for appropriate choices of arguments, moduli and scaling factors.

Finally, we consider the case of one or both points in a corner. For  $w_1 = -K$ , proceeding as above, we find

$$E_{\rm cor} = \Delta \ln \left| \frac{{\rm cn}^3(w)}{k'^2 \,{\rm dn}(w) [{\rm sn}(w) - 1]^2} \right|.$$
(22)

It is easy to evaluate equation (22) explicitly with w on any of the sides of the rectangle. If we put w in the corner K, proceeding as above, we find

$$E_{\rm cor} = \Delta \ln \left| \frac{4}{(1-k^2)^2} \right| \qquad E_{\rm cor} = \Delta \ln \left| \frac{4}{[1-(\vartheta_2/\vartheta_3)^4]^2} \right|$$
(23)

where the  $\vartheta_i = \vartheta_i(0, \tau)$  are elliptic theta functions, and we have made use of the relation  $k = (\vartheta_2/\vartheta_3)^2$ . If we let  $w \to K + iK'$ , the result is

$$E_{\rm cor} = -\Delta \ln \left| k (1-k)^2 \right|$$
  

$$E_{\rm cor} = -\Delta \ln \left| \left( \frac{\vartheta_2}{\vartheta_3} \right)^2 \left[ 1 - \left( \frac{\vartheta_2}{\vartheta_3} \right)^2 \right]^2 \right|.$$
(24)

By means of the behaviour of the theta functions under the modular transformation  $\tau \rightarrow \tau/2$  [15], we may express equations (23) and (24) as

$$E_{\rm cor} = -\ln\left|\frac{\pi^2\vartheta_3^2\vartheta_4^2}{8K^2}\right| \qquad E_{\rm cor} = -\ln\left|\frac{\pi^2\vartheta_2^2\vartheta_4^2}{8K^2}\right| \tag{25}$$

respectively, where we have set  $\Delta = \frac{1}{2}$ , and all the  $\vartheta$ -functions are now evaluated at  $\tau/2$ . Equations (25) agree exactly (up to an additive constant) with results for the Ising class in rectangles with fixed boundary conditions obtained via an argument based on operator content and symmetry [16].

Finally, it is interesting to contrast these last results with the energy of a domain boundary in the Ising model on a torus defined by insertion of an 'antiferromagnetic seam' [17, 18]. For a boundary in the diagonal direction, for instance, one finds

$$E_{xy} = \ln \left| \frac{\sqrt{k} + \sqrt{k'} + 1}{\sqrt{k} + \sqrt{k'} - 1} \right|$$
(26)

where  $k = (\vartheta_2/\vartheta_3)^2$  as before (with the  $\vartheta$ -functions evaluated at  $\tau = m/n$  = aspect ratio of the torus). In comparing equations (26) and (24) or the second member of equations (25) one must remember that the  $\tau$  appearing in equations (24) is *twice* the aspect ratio of the rectangle, and, since the domain boundary on a torus has no end, there is no logarithmic term in the size dependence of its energy.

# 5. Conclusions

By application of conformal field theory we have determined universal results for the free energies and interactions of curved domain boundaries at two-dimensional critical points in fully finite geometries. In particular, we have studied circular and rectangular regions. We have concentrated on the effects of finite size on the energy of a single domain boundary, including the influence of corners. Our results extend the theory of finite-size effects at criticality, complementing previous work on the energies of domain boundaries in infinite strips.

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