Domain Boundary Energies and Interactions at 2D Criticality via Conformal Field Theory

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By use of conformal field theory, we calculate the energies of one or more curved domain boundaries at two-dimensional critical points. We find the interaction of two separated boundaries of the same type to be weakly attractive, and proportional to the square of an operator-product expansion coefficient. In a strip of width L, the interaction vanishes exponentially with separation, over a distance set by L. It is also small for nearby domains when one of them is much smaller than L. Many-body interaction energies are weak as well.

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The principle of conformal invariance has led to an abundance of interesting and beautiful results for systems at criticality, especially in two dimensions. By application of fundamental developments in conformal field theory [1,2] new results for many theoretical (for recent reviews see [3–5]) and experimental systems [6–8] have been obtained. In this Letter we employ the basic principles of the theory to compute the energies and interactions of curved domain boundaries in two-dimensional systems at criticality. Our results are to our knowledge new, extending previous work on finite-size effects on interfacial properties [9], especially the energy (interfacial tension) of a single long straight boundary [10] and the role of domain boundaries in the critical region of the Ising model on a torus [11].

Consider an excitation or other perturbation created by a set of scaling operators $A=\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)\cdots$, in a critical system with fixed-point Hamiltonian $\mathcal{H}$. The partition function in the perturbed ensemble is then simply $Z'=\mathrm{Tr}A\,e^{-\mathcal{H}}$, and the change in (free) energy (in units of k_BT) just

$$\Delta F=-\ln\langle\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)\cdots\rangle\,. \tag{1}$$

The basic statement of conformal invariance is that any correlation function of scaling operators transforms according to [12]

$$\langle\varphi(\bar z_1,z_1)\cdots\rangle=w'(z_1)^{\Delta}\bar w'(\bar z_1)^{\bar\Delta}\cdots\langle\varphi(\bar w_1,w_1)\cdots\rangle\,, \tag{2}$$

where $w=w(z)$ is any analytic function, $|w'(z)|$ is the local scale factor introduced by the transformation, and $\Delta,\bar\Delta$ the scaling dimensions of φ. Equation (2) is a local generalization of global scale invariance at a critical point.

The other tool we make use of is the operator-product expansion (OPE) [13]. For identical (bulk) operators this may be written as

$$\varphi(\mathbf{r}_1)\varphi(\mathbf{r}_2)=\sum C_k r^{-2x+x_k}\varphi_k(\mathbf{R})\,, \tag{3}$$

where $r=|\mathbf{r}_1-\mathbf{r}_2|$, $\mathbf{R}$ is a vector in the vicinity of $\mathbf{r}_1$ and $\mathbf{r}_2$, $x=\Delta+\bar\Delta$, and $x_k=\Delta_k+\bar\Delta_k$ is the scaling dimension of φ_k. The OPE coefficients C_k are pure numbers and universal. By convention, the scaling operators are normalized so the leading ($k=0$) term on the right-hand side of Eq. (3) is r^{-2x}. Equation (3) may be used in correlation functions when r is much less than the distance from $\mathbf{r}_1$ or $\mathbf{r}_2$ to any other operator.

In the context of critical fluctuations, the OPE may be understood as follows [6]. In general, there will be some set $\{\varphi_i(\mathbf{r}_i)\}$ of most relevant scaling operators. Therefore, any product of two of these, in an expectation value with any $\varphi_j(\mathbf{r}_j)$, will have one or more terms that decay most slowly as $\mathbf{r}_j\to\infty$. But these must just be the expectations of the right-hand side of Eq. (3) times $\varphi_j(\mathbf{r}_j)$. (The $\mathbf{r}$ dependence on the right-hand side follows from scale invariance.)

For the purposes of this paper, we first consider a system in the upper half plane with a given conformally invariant [14,15] boundary condition. A simple example is a model in the Ising class with all spins held up on the real axis. The boundary condition may be changed by the introduction of an appropriate boundary operator [14,15] $\psi(x)$ on the real axis. In our Ising example, placing boundary operators at x_1 and x_2 will create a domain of (predominantly) down spins, as illustrated in Fig. 1. The domain boundary, defined by the locus along which the average of the order parameter is zero, is a half circle of radius $r=x_{12}/2$ (in what follows, $x_{ij}\equiv|x_i-x_j|$ and, similarly, $u_{ij}\equiv|u_i-u_j|$). This may be understood as follows. With one operator at the origin and the other

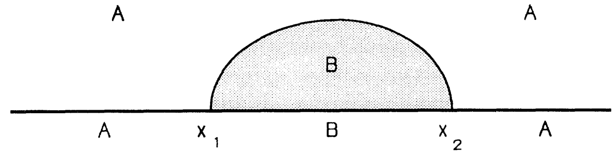

FIG. 1. Domain boundary in the upper half plane. For the Ising example mentioned in the text, A and B refer to "up" and "down" domains.

at ∞, the boundary runs along the imaginary axis. One can place the end points anywhere on the real axis via a projective transformation, which takes straight lines into circles. The new boundary must intersect the axis at 90°, since conformal transformations preserve angles. Note that this latter conclusion is consistent with the two phases being equivalent at criticality. The correlation function in this circumstance is [16]

$$\langle\psi(x_1)\psi(x_2)\rangle = x_{12}^{-2\Delta}, \tag{4}$$

where Δ is the boundary scaling dimension of ψ, so that $\Delta=\frac{1}{2}$ for our Ising-class example. (The notation x is used in Refs. [17,18].) The energy of this domain boundary follows immediately from Eq. (1).

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 strip. Examples include switching the spin configurations in the Ising example mentioned or, in a stepped-surface system with a phase transition involving surface reconstruction, introducing a kink in the terrace edge.

The transformation $w=u+iv=L/\pi\ln(z)$ maps the upper half plane into an infinite strip of width L, with edges. We refer to the resulting domain boundary in the strip as a "bubble," if x_1 and x_2 are on the same side of the origin, or a "wall" if not, as shown in Fig. 2. The associated energies, from Eqs. (1) and (2), are

$$E_b = 2\Delta\ln[2L/\pi\sinh(\pi u_{12}/2L)], \tag{5a}$$

$$E_w = 2\Delta\ln[2L/\pi\cosh(\pi u_{12}/2L)]. \tag{5b}$$

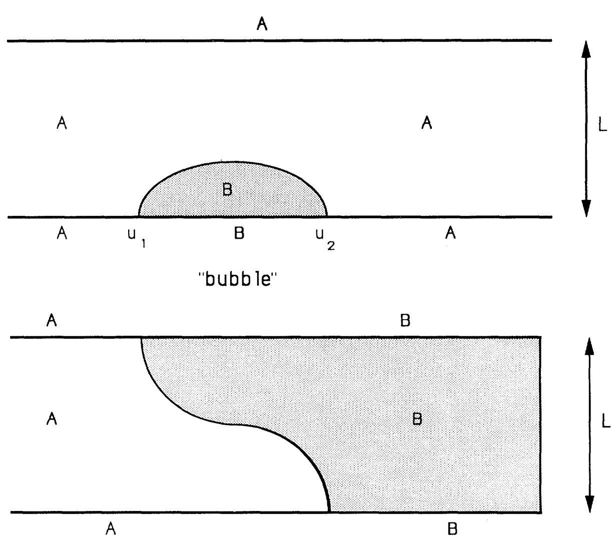

FIG. 2. "Bubble" and "wall" domains in the strip geometry. The boundaries are defined by mapping the boundary in Fig. 1 with $w=L/\pi\ln(z)$. The "bubble" never crosses the midpoint of the strip, and is not elliptical.

For domain width $u_{12}\to 0$ or $L\to\infty$, Eq. (5a) reproduces the upper half plane result, as it should. For $u_{12}\to\infty$ the boundary is straight and Eq. (5a) or (5b) gives a domain boundary energy $\pi\Delta/L$ per unit length, in agreement with previous results [17] obtained by analysis of the effects of boundary conditions on the transfer matrix. The expression for E_w has been verified for the Ising model by direct calculation [19]. Terms proportional to $\ln L$ also appear in finite-size corrections to the free energy [9], and may be understood via a "dimensional resonance" argument [20].

Next we consider the effects of introducing several domains. In what follows, we study the effects of various combinations of domain boundaries by placing boundary operators ψ at points $x_1<x_2<x_3<x_4$ on the real axis. 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. Suppose first that $x_{12}\ll x_{13}$. Then, by use of the OPE for boundary operators [15,21], the four-point correlation function may be reduced to a sum of three-point functions. These have the same x dependence as the z dependence for bulk operators [12,22], since the boundary implies that there is only a single Virasoro algebra [18]. The leading term is

$$\langle\psi(x_1)\cdots\psi(x_4)\rangle = (x_{12}x_{34})^{-2\Delta}[1+C^2(x_{12}x_{34}/x_{a3}x_{a4})^{\Delta_1}+\cdots], \tag{6}$$

where Δ_1 is the dimension of the most relevant boundary operator ψ_1 appearing in the expansion of ψ with itself and C is the appropriate boundary OPE coefficient. For later convenience, we choose $x_a=(x_1x_2)^{1/2}$. Applying Eq. (1) then gives a total energy which, in this limit, is close to the energy of two isolated boundaries [23]. Subtracting their energy from the total implied by Eq. (6) then gives

$$E_2 = -C^2(x_{12}x_{34}/x_{a3}x_{a4})^{\Delta_1} \tag{7}$$

for the pair interaction energy in the upper half plane. Thus, in the half plane, the pair interaction energy decays algebraically with the distance between domains and its magnitude depends on the ratio of domain size to domain separation. We may then regard these weakly interacting domains as distinct entities.

We now derive results for E_2 in the strip geometry by use of the logarithmic transformation mentioned and Eq. (2). Note that the scale factors give an additive contribution to the total energy that drops out of E_2 (and all other interaction energies as well). First consider the case $0<x_1$. Here the two boundaries in the half plane map into two bubbles on the same side of the strip. One finds

$$E_2 = -C^2\left[\frac{\sinh(\pi u_{12}/2L)\sinh(\pi u_{34}/2L)}{\sinh(\pi u_{3a}/2L)\sinh(\pi u_{4a}/2L)}\right]^{\Delta_1}, \tag{8}$$

where the domain location $u_a \equiv (u_1+u_2)/2$. Note that E_2 is always attractive, and proportional to the square of a (boundary) OPE coefficient. For domains of fixed size, it again vanishes with domain separation $u_{ab} \equiv |u_4+u_3-u_2-u_1|/2$, but exponentially as $e^{-\pi u_{ab}\Delta_1/L}$. Its magnitude again depends on the relation of domain size to separation, but in a more complicated way than in the half plane. It is interesting that the sinh factors in the numerator of Eq. (8) may be reexpressed in terms of the bubble energies by use of Eq. (5a), so that the magnitude of the interaction depends exponentially on the energy of the single-domain boundaries.

For the Ising example mentioned above, the OPE involves only the unit operator I. In such cases, the interaction is given by a higher-order term in the conformal tower of I. As a result, in Eqs. (6)–(8), $\Delta_1=2$ and C^2 is replaced by $2\Delta^2/c$, where c is the central charge.

We next consider some implications of the symmetries of the interaction energy. The scale invariance of E_2 in the half plane simply corresponds to translation invariance along the strip [24]. However, the half plane expression is also translation invariant, which leads to some interesting consequences in the strip. Translating the x_i along the real axis, the value of E_2 remains fixed, but the form of Eq. (8) changes and the type, width, and location of the boundaries in the strip is altered. For instance, given $x_{12} \ll x_{34}$, one goes from a narrow bubble to the left of a wide one ($u_{12} \ll u_{34}$) to the opposite case as the origin approaches x_1 and $u_1 \to \infty$. Now with $x_i x_j > 0$, the corresponding factor in Eq. (8) is as written. However, for $x_i x_j < 0$, the corresponding sinh is replaced by a cosh. Thus for $x_1 < 0 < x_2$ the factor $\sinh(\pi u_{12}/2L)$ in Eq. (8) is replaced by $\cosh(\pi u_{12}/2L)$ [25]. The altered formula describes a bubble-wall interaction, with the wall bending away from or toward the bubble, for $|x_1| < x_2$ or $|x_1| > x_2$, respectively. For $x_2 < 0 < x_3$ one has two bubbles on opposite sides of the strip with E_2 as given in Eq. (8), except that the sinh factors in the denominator are replaced by cosh. Note that this case includes the situation where $u_a = u_b$. For $x_3 < 0 < x_4$ one again has a bubble-wall arrangement.

Some new situations arise if we let x_2 approach x_3. The form of E_2 follows from Eq. (8) on the permutation of indices and redefinition of u_a. Proceeding as above, the translation invariance gives rise to bubble-bubble, bubble-wall, and also wall-wall interactions. The former case includes two bubbles inside each other (on the same side of the strip, with one small compared to L). The mixed situation includes $u_a = u_b$—here the bubble is small, so the wall avoids it. The latter case includes all four possible orientations of two walls, on changing the location of the origin and allowing $|x_1| < x_4$ or $|x_1| > x_4$. (Recall that a small interaction of domain walls in the perpendicular direction on a long torus was assumed in Ref. [11].) In all the above, the interaction energy is small either because the width of at least one domain boundary is small compared to the domain separation or because the width of a bubble domain is much less than L, so that its boundary does not approach the other.

Finally, one can compute many-domain interaction energies in a similar way. For instance, for six points with the 12, 34, and 56 separations all small compared to the separation of any two pairs, one has three domains in the upper half plane. Here, in an obvious notation, one finds

$$E_3 = -C_1 C^3 (x_{12}x_{34}x_{56}/x_{ab}x_{bc}x_{ac})^{\Delta_1}, \qquad (9)$$

where C_1 is the OPE coefficient of ψ_1 in the expansion of ψ_1 with itself. (If C_1 vanishes, E_3 will be determined by a higher-order OPE term.) Note that E_3 does not have a definite sign. In the strip, E_3 will decay with separation as $\exp[-\pi(u_{ab}+u_{bc}+u_{ac})\Delta_1/2L]$. This decrease is at least as rapid as that of any E_2 for the same set of domains, if all domain separations are multiplied by the same scale factor. In this sense the three-domain interaction is no stronger than the pair interaction. Higher-order many-domain terms should behave similarly.

In deriving the above results, we have restricted ourselves to the case of a single type of boundary operator. Several generalizations are possible. First, for a given boundary condition for $x_1 < 0$, one can introduce any allowed boundary operator (or a descendant) at x_1 (and x_2). The energies of one or more domain of this type are then given as above. However, the geometrical interpretations may differ. For instance, a boundary operator with dimension $\Delta = \frac{1}{16}$ mediates a change between fixed and free boundary conditions in the Ising class [15]. But in this case the "domain boundary," defined as above, is along the real axis [26]. Second, one may calculate interactions between different types of domains via four-point correlations of two pairs of boundary operators. Here E_2, for example, will be determined by the most relevant common operator in the OPEs of the two types of operators defining the two different domains. For this reason, the pair interaction may not be attractive. Third, analogous results may be computed in fully finite geometries (e.g., a circle or rectangle) by use of the appropriate conformal map. Finally, one may make similar use of Eqs. (1) and (2) in the bulk, and by transformation in a strip with periodic boundary conditions. One can easily compute, for instance, the interaction of "defect lines" introduced by disorder operators.

Consider the strip geometry treated above with a given boundary condition for $x_1 < 0$. Introducing all allowed boundary operators pairwise at x_1 and x_2 will give rise to "domain" energies involving the entire spectrum of conformal dimensions in the boundary theory, including those in the conformal tower of the unit operator [14,15,27]. Thus the domains may be regarded as weakly interacting excitations of all possible degrees of freedom of the theory. This picture suggests that one can reconstruct the entire free energy in terms of domain boundaries, or some appropriate generalization of that concept. General scaling arguments [28] are not inconsistent with this possibility.

In summary, we have presented a general method for computing the energy of curved domain boundaries in two-dimensional systems at second-order phase transitions. We also find that two or more domains are weakly interacting.

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[21] In the present context, this is the same as Eq. (3), except that all operators are located on the real axis and the scaling dimensions x_i are replaced by Δ.

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[23] In a real system there will be a lattice cutoff a, so it is natural to set the energy at zero via $E=2\Delta\ln(x_{12}/a)$. Then a boundary of width a has vanishing energy. Thus, when the second term in square brackets in Eq. (6) is small, the condition that $E_2 \ll E_{\rm tot}$ is just $x_{12}x_{34} \gg a^2$.

[24] By contrast, the single domain energies in Eq. (5) are not translation invariant. This is due to the effects of the scale factors, which are not invariant, and enter via Eq. (2).

[25] In this case the definition of u_a requires $|x_a| = (|x_1|x_2)^{1/2}$. Thus the factor in the denominator changes if we choose $x_a < 0$.

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