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LETTER TO THE EDITOR

Surface critical behaviour of the honeycomb O(n) loop model with mixed ordinary and special boundary conditions

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Abstract. The O(n) loop model on the honeycomb lattice with mixed ordinary and special boundary conditions is solved exactly by means of the Bethe ansatz. The calculation of the dominant finite-size corrections to the eigenspectrum yields the mixed boundary scaling index and the geometric scaling dimensions describing the universal surface critical behaviour. Exact results follow in the limit $n = 0$ for the polymer adsorption transition with a mixed adsorbing and free boundary. These include the new configurational exponent $\gamma_1 = \frac{85}{64}$.

The critical behaviour of semi-infinite d-dimensional systems with free surfaces can be very rich, with the possibility of 'special' or multicritical surface behaviour when the surface couplings are sufficiently enhanced [1,2]. One fundamental model of relevance in this context is the semi-infinite two-dimensional n-vector or O(n) model [3]. In the limit $n = 0$, which describes self-avoiding walks [4], the special transition corresponds to the polymer adsorption transition [5].

In this letter we derive the surface critical behaviour of the O(n) loop model on the honeycomb lattice with 'ordinary' (O) and 'special' (S) boundary conditions on either side of a finite strip, i.e. a strip finite in one direction and infinite in the other. Such mixed boundary conditions are of current interest for general d, being of relevance to the Casimir interaction between two spherical particles in a fluid at the critical point (see e.g. [6] and references therein). In $d = 2$, with boundary conditions a and b on opposite edges of a strip of width N, the free energy per site of a critical system scales as (see [7] and references therein)

$$f_N \simeq f_{\rm B} + f_a N^{-1} + f_b N^{-1} + \Delta_{ab} N^{-2} \tag{1}$$

for large N. Here $f_{\rm B}$ is the bulk free energy, f_a and f_b are surface free energies and Δ_{ab} is the universal Casimir amplitude. This Casimir contribution to the free energy has recently been calculated for the O(n) model with various mixed boundary conditions via conformal-invariance methods [7]. Here we derive this quantity exactly for mixed O–S boundary conditions, along with the surface scaling dimensions, from the Bethe ansatz solution of the corresponding O(n) loop model [8] on the honeycomb lattice.

The partition sum of our O(n) loop model is defined as

$$\mathcal{Z} = \sum x^L y_a^{L_a} y_b^{L_b} n^P \tag{2}$$

where the sum is over all configurations of closed and non-intersecting loops on the lattice depicted in figure 1. Here P is the total number of closed loops of fugacity n in a given configuration. We take boundary condition a (b) on the left (right) edge of the strip. At $n = 0$, x is the fugacity of a step in the bulk and y_a (y_b) is the fugacity of a step along the left (right) edge. Thus L is the number of steps in the bulk and L_a (L_b) is the number of steps along the left (right) edge.

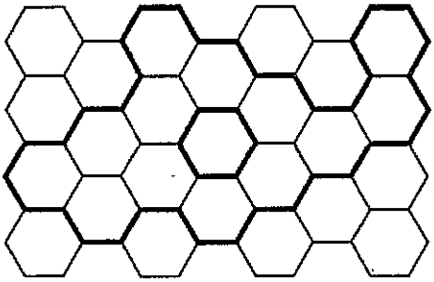

Figure 1. The open honeycomb lattice. The transfer matrix acts in the vertical direction.

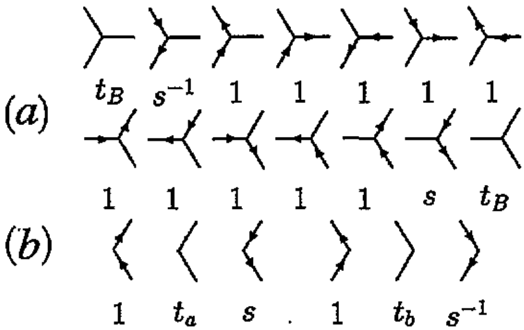

Figure 2. The allowed arrow configurations and corresponding Boltzmann weights for (a) bulk and (b) surface vertices.

We have found that the equivalent three-state vertex model can be solved for a number of boundary conditions. The possible arrow configurations and their corresponding Boltzmann weights are shown in figure 2. Here the phase factors are such that $n = s + s^{-1} = -2\cos 4\lambda$. The integrable bulk weights follow in a particular limit of the Izergin–Korepin R-matrix [9, 10], with $t_{\mathrm{B}} = 2\cos\lambda$, or equivalently, with critical bulk coupling [11]

$$1/x^* = \sqrt{2 \pm \sqrt{2-n}}. \tag{3}$$

On the other hand, the integrable boundary weights follow [12] from appropriate combinations of the three known reflection or K-matrices satisfying the boundary version of the Yang–Baxter equation [13].

Three inequivalent integrable sets of boundary weights are known to be compatible with O(n) symmetry. One set corresponds to O–O boundary conditions [14], with boundary weights and equivalent critical surface couplings given by

$$t_a = t_b = t_{\mathrm{B}} \Rightarrow y_a^* = y_b^* = x^*. \tag{4}$$

Another corresponds to S–S boundary conditions [15], with

$$t_a = t_b = \frac{\cos 2\lambda}{\cos\lambda} \Rightarrow y_a^* = y_b^* = y^* \tag{5}$$

where

$$1/y^* = \sqrt{\pm\sqrt{2-n}}. \tag{6}$$

The third set is a mixture of the above, and corresponds to O–S boundary conditions, with

$$t_a = t_{\rm B} \qquad t_b = \frac{\cos 2\lambda}{\cos\lambda} \Rightarrow y_a^* = x^* \qquad y_b^* = y^*. \tag{7}$$

The self-avoiding walk point at $n = 0$ occurs at $\lambda = \pi/8$, where $1/x^* = \sqrt{2+\sqrt{2}}$ and $1/y^* = 2^{1/4}$ [15]. In the lattice model of the polymer adsorption transition [5], the self-avoiding walk has energy

$$E = -\epsilon L_{\rm s} \tag{8}$$

where ϵ is a constant and $L_{\rm s}$ is the number of steps along the adsorbing boundary, in this case the right-hand side of the strip. For the O–S boundary conditions, we thus obtain the same critical adsorption temperature

$$\exp\left(\frac{\epsilon}{kT_a}\right) = y^*/x^* = \sqrt{1+\sqrt{2}} = 1.553\ldots \tag{9}$$

as for the S–S boundary conditions [15], i.e. with adsorbing boundaries on both sides of the strip. Recent phenomenological renormalization transfer matrix calculations on the square lattice with one adsorbing and one free boundary are consistent with this finding [16].

We have previously solved the corresponding vertex model by means of the coordinate Bethe ansatz for the O–O and an analytic Bethe ansatz for S–S boundary conditions [14, 12, 15]. Proceeding in a similar manner to [12], we find that the eigenvalues of the transfer matrix for the O–S boundary conditions are given by

$$\Lambda = \prod_{j=1}^{m} \frac{\sinh(u_j + {\rm i}3\lambda/2)\sinh(u_j - {\rm i}3\lambda/2)}{\sinh(u_j + {\rm i}\lambda/2)\sinh(u_j - {\rm i}\lambda/2)} \tag{10}$$

where the u_j follow as roots of the Bethe ansatz equations

$$\left[\frac{\sinh(u_j - {\rm i}\lambda/2)\sinh(u_j - {\rm i}3\lambda/2)}{\sinh(u_j + {\rm i}\lambda/2)\sinh(u_j + {\rm i}3\lambda/2)}\right]^N = -\frac{\sinh(2u_j + {\rm i}\lambda)}{\sinh(2u_j - {\rm i}\lambda)}$$
$$\times \prod_{\substack{k=1\\ \neq j}}^{m} \frac{\sinh(u_j - u_k + {\rm i}\lambda)\sinh(u_j + u_k + {\rm i}\lambda)\sinh(u_j - u_k - {\rm i}2\lambda)\sinh(u_j + u_k - {\rm i}2\lambda)}{\sinh(u_j - u_k - {\rm i}\lambda)\sinh(u_j + u_k - {\rm i}\lambda)\sinh(u_j - u_k + {\rm i}2\lambda)\sinh(u_j + u_k + {\rm i}2\lambda)}. \tag{11}$$

Here N is the width of the strip (e.g. $N = 8$ in figure 1) and m labels the sectors of the transfer matrix, with $m = N$ for the largest eigenvalue Λ_0. A more convenient sector label is $\ell = N - m$.

The direct calculation of the finite-size corrections to the eigenvalue spectrum follows a well-trodden path (see e.g. [14] and references therein). In this case the largest eigenvalue in a given sector m is characterized by real positive roots with related integers $I_j = j$, $j = 1, \ldots, m$. Defining the free energy per site as $f_N = N^{-1}\log\Lambda_0$, we find

$$f_N \simeq f_{\rm B} + f_{\rm O\text{-}S} N^{-1} + \Delta_{\rm O\text{-}S} N^{-2}. \tag{12}$$

This result is to be compared with equation (1). Dealing with the non-universal terms first,

$$f_{\rm B} = \int_{-\infty}^{\infty} \frac{\sinh(\frac{1}{2}\pi - \lambda)x \sinh\lambda x}{x\sinh\frac{1}{2}\pi x(2\cosh\lambda x - 1)}\,{\rm d}x \tag{13}$$

is the bulk free energy [14, 17] and

$$f_{\text{O-S}} = \frac{1}{2}\log\left(\frac{1-\cos\lambda}{1-\cos 3\lambda}\right) + 2\int_{-\infty}^{\infty} \frac{\sinh\frac{1}{2}\lambda x \cosh\frac{1}{4}(\pi-2\lambda)x \sinh\frac{1}{4}(\pi-6\lambda)x}{x\sinh\frac{1}{2}\pi x(2\cosh\lambda x - 1)}\,\mathrm{d}x \tag{14}$$

is the surface free energy for the mixed O–S boundary conditions. We note, however, the *identity*

$$f_{\text{O-S}} = \tfrac{1}{2}(f_{\text{O-O}} + f_{\text{S-S}}) = f_{\text{O}} + f_{\text{S}} \tag{15}$$

where $f_{\text{O-O}}$ and $f_{\text{S-S}}$ have been derived previously [14, 15, 18]. The individual surface contributions are thus

$$f_{\text{O}} = \frac{1}{4}\log\left(\frac{1-\cos\lambda}{1-\cos 3\lambda}\right)$$
$$+2\int_{-\infty}^{\infty} \frac{\sinh\frac{1}{2}\lambda x \cosh\frac{1}{4}\lambda x \cosh\frac{1}{4}(\pi-2\lambda)x \sinh\frac{1}{4}(\pi-3\lambda)x(2\cosh\frac{1}{2}\lambda x - 1)}{x\sinh\frac{1}{2}\pi x(2\cosh\lambda x - 1)}\,\mathrm{d}x \tag{16}$$

and

$$f_{\text{S}} = \frac{1}{4}\log\left(\frac{1-\cos\lambda}{1-\cos 3\lambda}\right)$$
$$-2\int_{-\infty}^{\infty} \frac{\sinh\frac{1}{2}\lambda x \sinh\frac{3}{4}\lambda x \cosh\frac{1}{4}(\pi-2\lambda)x \cosh\frac{1}{4}(\pi-3\lambda)x}{x\sinh\frac{1}{2}\pi x(2\cosh\lambda x - 1)}\,\mathrm{d}x. \tag{17}$$

In particular, at $n = 0$ we have $\Lambda_0 = (2+\sqrt{2})^N/(1+\sqrt{2})$ with $f_{\text{B}} = \log(2+\sqrt{2})$, $f_{\text{O}} = 0$ and $f_{\text{S}} = -\log(1+\sqrt{2})$. Here the sign change in f_{S} represents an attraction towards the adsorbing boundary.

The Casimir amplitude appearing in (1) and (12) is given by

$$\Delta_{\text{O-S}} = \frac{\pi\zeta\hat{c}}{24} \tag{18}$$

where $\zeta = 2/\sqrt{3}$ is a lattice-dependent scale factor. The effective central charge is

$$\hat{c} = 1 - \frac{12\lambda^2}{\pi(\pi-2\lambda)} \tag{19}$$

with $\hat{c} = 0$ at $n = 0$. The mixed boundary scaling index [19, 20] follows as

$$t_{\text{O-S}} = \tfrac{1}{24}(c-\hat{c}) = \frac{-\pi+8\lambda}{8(\pi-2\lambda)} \tag{20}$$

in agreement with the conformal invariance prediction [7].

The geometric scaling dimensions defining the surface critical behaviour follow from the inverse correlation lengths via [21]

$$\xi_\ell^{-1} = \log\frac{\Lambda_0}{\Lambda_\ell} \simeq \frac{\pi\zeta X_\ell}{N}. \tag{21}$$

These dimensions govern the geometric correlation

$$G_\ell(x-y) \sim |x-y|^{-2X_\ell} \tag{22}$$

between ℓ non-intersecting self-avoiding walks tied together at their extremities x and y, which for surface critical phenomena are near the boundary of the half-plane [22]. For mixed boundary conditions there is a discontinuity at the origin between boundary conditions a and b corresponding to the insertion of a boundary operator [19].

Here the scaling dimensions X_ℓ are associated with the largest eigenvalue in each sector of the transfer matrix. We find

$$X_\ell = \tfrac{1}{4}g\ell^2 + \tfrac{1}{2}(g-2)\ell \qquad \ell = 1, 2, \ldots \tag{23}$$

where $\pi g = 2\pi - 4\lambda$. These dimensions are to be compared with the other Bethe ansatz results. For the ordinary (O–O) transition [14]

$$X_\ell = \tfrac{1}{4}g\ell^2 + \tfrac{1}{2}(g-1)\ell \tag{24}$$

or $X_\ell = h_{\ell+1,1}$ in terms of the Kac formula [22, 23]. On the other hand, for the special (S–S) transition [15]

$$X_\ell = \tfrac{1}{4}g(\ell+1)^2 - \tfrac{3}{2}(\ell+1) + \frac{9-(g-1)^2}{4g} \tag{25}$$

or $X_\ell = h_{\ell+1,3}$ [24–26]. For the mixed O–S boundary conditions we have $X_\ell = h_{\ell+1,1} - \frac{1}{2}\ell$.

At $n = 0$ ($g = \frac{3}{2}$), corresponding to mixed adsorbing and free boundaries in the polymer problem, (23) gives

$$X_\ell = \tfrac{3}{8}\ell^2 - \tfrac{1}{4}\ell. \tag{26}$$

The first two values are $X_1 = \frac{1}{8}$ and $X_2 = X_\epsilon = 1$. These dimensions define critical exponents for polymers in the upper half-plane, with one boundary condition on the positive and the other on the negative x-axis, the two geometries (the strip and the half-plane) being related via a conformal map (see e.g. [19]). In particular, the number of self-avoiding walks which begin near the origin (where the boundary conditions meet in the half-plane) scales as $L^{\gamma_1 - 1}\mu^L$ where $\mu = 1/x^*$ and the universal value $\gamma_1 = \frac{85}{64}$ follows from the usual scaling relation [1, 2]

$$\gamma_1 = (2 - X_1 - X_1^{\text{bulk}})\nu \tag{27}$$

where $\nu = \frac{3}{4}$ and $X_1^{\text{bulk}} = \frac{5}{48}$ [11]. The exponent $\gamma_1 = \frac{85}{64}$ is to be compared with the exact values for the non-mixed cases, where $\gamma_1 = \frac{61}{64}$ for a non-adsorbing boundary (ordinary transition) and $\gamma_1 = \frac{93}{64}$ for an adsorbing boundary (special transition).

A detailed account of our results is currently in preparation [18].

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