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LETTER TO THE EDITOR

Solid on solid model for an interface crossing a grain boundary

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Abstract
Recent work has demonstrated a new structural transition occurring at an internal defect in a two-dimensional Ising model. The new behaviour is induced by boundary conditions that constrain the interface to lie at an angle across the defect line. This gives rise to the energy–entropy competition familiar from other examples of pinning–depinning transitions. We demonstrate how a horizontal solid-on-solid (SOS) model can be used to obtain comparable results to this exact calculation. This simpler model can then be easily extended to encompass a situation where the interface has a differing stiffness on either side of the grain boundary.

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1. Introduction

Recent exact Ising calculations have revealed the presence of a structural interfacial phase transition taking place in a system with an interior defect [1]. While it is well established that an interface will be pinned to an interior defect for all temperatures $T < T_c$, this new work has demonstrated a transition between this pinned state and an angular state induced by the boundary conditions [2]. In a certain sense this calculation can be thought of as being complementary to problems in classical optics that lead to Snell's law, but for interfaces rather than ray paths. Although related interfacial problems have been considered previously in the literature, these works have either not included an explicit defect between two differing regions [3] or have not considered the implications of imposing asymmetric boundary conditions [4, 5].

In this letter we shall show how a horizontal solid-on-solid (SOS) model can be used to recover results from the Ising study in a particular scaling limit, which we shall justify. This approach is strongly suggested by the results emerging from the exact calculation. In that

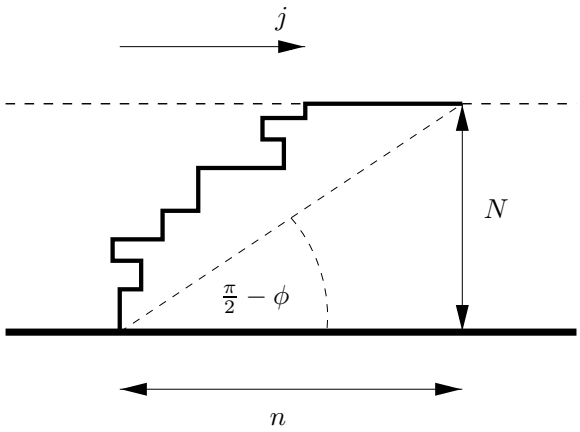

Figure 1. The simple half system. The change from plus to minus boundary conditions induces the interface emerging from the bottom wall. We have suppressed the similar interface emerging from the top half of the system, instead pinning the interface to the defect line a horizontal distance n across the system. The full system can be seen in figure 2.

calculation, it was found that the phase boundary for the new transition was independent of the horizontal Ising coupling K_2—a result also verified numerically over several orders of magnitude. The implication of this surprising result is that the equilibrium configurations in this system are dominated by structures which have a constant vertical length (N); those having no overhangs in the x-direction. This would thus correspond to a SOS approximation, but horizontally, rather than the vertical approximation typically used in wetting. This is in contrast to the approach used by previous authors [3], but it is not without precedent [6]. After developing the model we shall then extend the results to a similar model but with differing bond strengths on either side of the defect—a result not immediately accessible in the Ising case. The calculation also includes previously unreported intermediate results.

2. Half system

A simplified system is shown in figure 1. For calculational reasons, which will become apparent, we shall first consider a half system. The full system consists of two parallel walls with fixed spins but no wetting boundary conditions. There is a change in the orientation of the fixed spins at the origin on the bottom wall which is mirrored by a similar change in the top wall. The change in the top wall is however offset from the one in the bottom wall by a distance $2n$. The walls are a distance $2N$ apart (on the dual lattice) imposing an angular boundary condition with $\tan\phi = n/N$ shown in figure 1. The interface induced by such boundary conditions has a stiffness K. We assume that the inverse temperature β is absorbed into this constant ($K \equiv \beta J$) for convenience. The two walls are bisected by a line of weakened bonds (on the lattice) which correspond to a weakened stiffness (bK, $0 < b < 1$) for horizontal steps on the central line for the SOS model. We can thus write a partition function for this model as

$$Z = \sum_j \langle 0|\mathcal{T}^N|j\rangle \, \mathrm{e}^{-bK|j-n|} \tag{1}$$

where $\langle x|\mathcal{T}|y\rangle = \mathrm{e}^{-K|x-y|}$ is the one step transfer matrix for an interface starting at x and finishing at y. The computation of the spectrum of the iterated transfer matrix in (1) uses

standard methods. We find

$$\langle 0|\mathcal{T}^N|j\rangle = \sum_k \psi_0^{(k)}\bar{\psi}_j^{(k)}(\lambda^{(k)})^N$$
$$= \frac{(2K)^N}{L}\int_0^\infty \frac{\cos kj}{(K^2+k^2)^N}\,\mathrm{d}k \tag{2}$$

where L is a large constant box width emerging through normalization and k has become a continuous variable between the steps above as it becomes an index for the continuum of scattering states in the absence of any bound states [7][3]. It turns out that (2) is in fact an exact integral representation of a spherical Bessel function [8] and thus we derive an elegant intermediate result for the horizontal SOS model

$$\langle 0|\mathcal{T}^N|j\rangle = \frac{j^{N-\frac{1}{2}}\Gamma\left(\frac{1}{2}\right)(2K)^{\frac{1}{2}}}{\Gamma(N)L}\mathcal{K}_{N-\frac{1}{2}}(jK). \tag{3}$$

If we now allow the length j to be continuous, parametrizing all lengths as multiples of the vertical distance N we can substitute (3) into the expression for the partition function to yield the integral expression

$$Z = \int_{-\infty}^{\infty} N\tan\phi\,\mathrm{e}^{-nbK|1-x|}\frac{(xN\tan\phi)^{N-\frac{1}{2}}\,\Gamma\left(\frac{1}{2}\right)(2K)^{\frac{1}{2}}}{\Gamma(N)L}\mathcal{K}_{N-\frac{1}{2}}(xNK\tan\phi)\,\mathrm{d}x. \tag{4}$$

We can now compute the $N\to\infty$ asymptotic behaviour by utilizing known asymptotic expansions

$$\Gamma(N) \sim N^{N-\frac{1}{2}}\,\mathrm{e}^{-N}\,(2\pi)^{\frac{1}{2}} \tag{5}$$

$$\mathcal{K}_{N-\frac{1}{2}}(xN\tan\phi K) \sim \frac{\pi^{\frac{1}{2}}\,\mathrm{e}^{-(N-\frac{1}{2})\sqrt{1+x^2K^2\tan^2\phi}}}{(2N-1)^{\frac{1}{2}}(1+x^2K^2\tan^2\phi)^{\frac{1}{4}}}\left(\frac{1+\sqrt{1+x^2K^2\tan^2\phi}}{xK\tan\phi}\right)^{N-\frac{1}{2}}. \tag{6}$$

Stirlings formula and an expansion for large order and argument[9]. These expansions result in a lengthy form for the partition function. Ultimately the expression of interest is the free energy of the system, defined by

$$\mathcal{F} = -\lim_{N\to\infty}\left[\frac{1}{N}\ln Z\right] \tag{7}$$

and hence the dominant contribution to the integral will be provided from terms proportional to N which are exponentiated in Z. Z is of the form

$$Z \sim \int_{-\infty}^{\infty} g(x)\,\mathrm{e}^{-Nf(x)}\,\mathrm{d}x \tag{8}$$

with

$$f(x) = b\tan\phi K|1-x| + \sqrt{1+x^2K^2\tan^2\phi} - \ln\left(1+\sqrt{1+x^2K^2\tan^2\phi}\right). \tag{9}$$

This expression has two competing minima for different values of the parameters. At certain values of the parameters this is the cusp minima induced by the modulus around $x=1$ and there also exists a local minima at the point

$$x = \frac{2b}{(1-b^2)K\tan\phi} \tag{10}$$

[3] At this stage it is equally possible to make progress in both this problem and the full problem by substituting the expression in (2) directly into (1) and switching the order of integration. The resulting problem is easily solved by direct integration. However, subsequent interpretation is clearer by utilizing the steps followed in the text.

which is present if this value is less than unity. The two minima are thus mutually exclusive. The phase boundary can be determined as the solution of the transcendental equation

$$\sqrt{1+K^2\tan^2\phi}-\ln\left(1+\sqrt{1+K^2\tan^2\phi}\right)-1=bK\tan\phi+\ln\left(\frac{1-b^2}{2}\right) \tag{11}$$

which can be solved by inspection to give the critical value of the weakening parameter, b, as

$$b^*_{\mathrm{SOS}}=\frac{\sqrt{1+K^2\tan^2\phi}-1}{K\tan\phi} \tag{12}$$

which may be compared to the exact Ising result

$$b^*_{\mathrm{Ising}}=\frac{1}{2K_1}\log\left(\frac{\tan\phi\cosh 2K_1+\sqrt{1+\tan^2\phi\sinh^2 2K_1}}{\tan\phi+1}\right) \tag{13}$$

in small $K, \phi\sim\pi/2$ limit. The formal *horizontal* SOS limit must also be taken ($K_2\to\infty$, $2K_1\to K$). The correspondence to this scaling regime can be understood in two ways, firstly the small K limit is required because of our continuity assumptions about the variables j prior to our taking the limit $\to\infty$. The assumption that $\phi\sim\pi/2$ is required to ensure that the fluctuations on the opposing side of the mid-point are suppressed as they are not included in the SOS, but *are* included in the Ising calculation. This calculation explicitly assumes that the interface is independent of its partner on the other side of the defect line. Though this is manifestly obvious in this half calculation, we shall see that this is unaltered when we consider the full system below and that this assumption is actually implicit.

3. Full system

We shall now show how the results for the phase boundary, and other results, are unaltered by considering the full SOS problem, depicted in figure 2. The partition function for this situation is given by

$$Z=\sum_{j_1,j_2}\langle 0|\mathcal{T}^N|j_1\rangle\,\mathrm{e}^{-bK|j_1-j_2|}\langle j_2|\mathcal{T}^N|2n\rangle. \tag{14}$$

The unknown intermediate function can be expressed as a sum of two Bessel functions

$$\begin{aligned}\langle j_2|\mathcal{T}^N|2n\rangle=\frac{\Gamma\left(\frac{1}{2}\right)(2K)^{\frac{1}{2}}}{2\Gamma(N)L}\Big\{&(2n+j_2)^{N-\frac{1}{2}}\mathcal{K}_{N-\frac{1}{2}}((2n+j_2)K)\\&+(2n-j_2)^{N-\frac{1}{2}}\mathcal{K}_{N-\frac{1}{2}}((2n-j_2)K)\Big\}.\end{aligned} \tag{15}$$

We can now, by taking a continuum limit ($2nx\leftrightarrow j_1, 2ny\leftrightarrow j_2$) once more, write the expression for the partition function in the form

$$Z\sim\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}g(x,y)\,\mathrm{e}^{-Nf(x,y)}\,\mathrm{d}x\,\mathrm{d}y \tag{16}$$

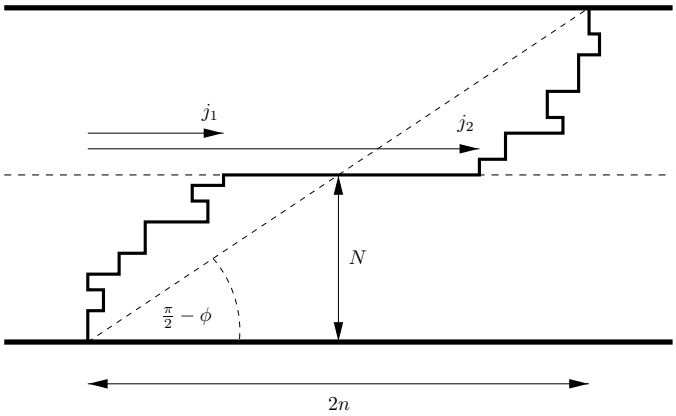

Figure 2. The full system. The boundary condition described in the text can be seen explicitly. The direct correspondence of the results from this system and that of the half system are strong evidence for the two interfaces behaving independently in the SOS approximation.

with

$$f(x, y) = 2b \tan\phi K|x - y| + \sqrt{1 + 4x^2K^2 \tan^2\phi} - \ln\left(1 + \sqrt{1 + 4x^2K_2 \tan^2\phi}\right) + \sqrt{1 + 4(1 - y)^2K^2 \tan^2\phi} - \ln\left(1 + \sqrt{1 + 4(1 - y)^2K^2 \tan^2\phi}\right) \tag{17}$$

where we have made a mapping $x \mapsto -x$, $y \mapsto -y$ in one of the integrations. Analysis of the function $f(x, y)$ proceeds in an analogous way to the half problem, though care must be taken to verify the nature of any minima. The two solutions are

$$x = y = \tfrac{1}{2} \qquad \text{and} \qquad x = \frac{b}{(1 - b^2)K \tan\phi} \qquad y = 1 - \frac{b}{(1 - b^2)K \tan\phi} \tag{18}$$

which are the competing local minima. Comparison of the energies yields the identical result for the phase boundary as the half problem, thus justifying our previous analysis.

The free energy can now be written, using definition (7), as

$$\mathcal{F} = \begin{cases} 2\sqrt{1 + K^2 \tan^2\phi} - 2\ln\left(1 + \sqrt{1 + K^2 \tan^2\phi}\right) & b > b^*_{\mathrm{SOS}} \\ 2bK \tan\phi + 2 - 2\ln 2 + 2\ln(1 - b^2) & b < b^*_{\mathrm{SOS}} \end{cases} \tag{19}$$

showing the change in behaviour at the transition explicitly. The obvious choice of order parameter is the number of broken bonds on the defect line [1] which can be computed with the identity

$$\langle |j_1 - j_2| \rangle = -\frac{1}{KN}\frac{\partial}{\partial b} \ln Z = \begin{cases} 0 & b > b^*_{\mathrm{SOS}} \\ 2\tan\phi - \frac{4b}{(1-b^2)K} & b < b^*_{\mathrm{SOS}}. \end{cases} \tag{20}$$

In the thermodynamic limit we thus have a second-order phase transition with the order parameter increasing continuously from zero. The discontinuity in $\partial^2\mathcal{F}/\partial T^2$ is also present, in common with the established behaviour at the wetting transition [10].

4. Layered system

The advantage of this SOS approach over an Ising calculation is we can now use our established methodology to extend to more general situations. Here we will consider the equilibrium

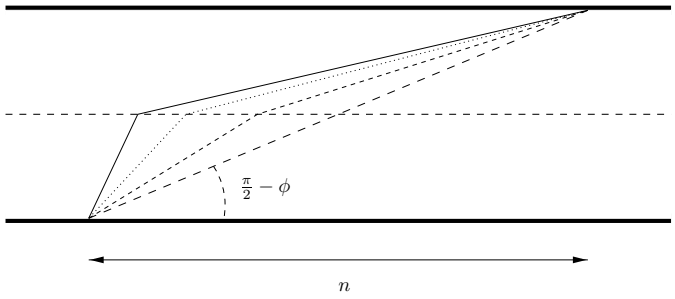

Figure 3. A system showing some sample configurations when the stiffness above and below the bonds differ. n has been set to 1 for convenience. The configurations shown are all taken with $K_t = 1$, and $\tan\phi = 12/5$. The values of K_b are 2 (solid line), 1.5 (dotted line), 1.2 (short dashed line) and 1 (long dashed line).

behaviour of the same model but where the effective stiffness of the SOS model varies on either side of the defect. This change is simple to implement in a way parallel to the analysis above. We denote the new stiffnesses K_b and K_t in an obvious manner to avoid confusion with any Ising quantities. We denote the weakened bond strength as bH, where H is the algebraic mean of K_b and K_t. This choice maintains the link with the motivating model, where the weakened tier joins the two differing regions. The partition function is thus

$$\begin{aligned} Z &= \sum_{j_1, j_2} \langle 0|\mathcal{T}_b^N|j_1\rangle \, \mathrm{e}^{-bH|j_1 - j_2|} \langle j_2|\mathcal{T}_t^N|2n\rangle \\ &\sim \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g(x, y)\, \mathrm{e}^{-Nf(x,y)}\, \mathrm{d}x\, \mathrm{d}y \end{aligned} \tag{21}$$

with

$$\begin{aligned} f(x, y) = {} & 2b\tan\phi H|x - y| + \sqrt{1 + 4x^2\tan^2\phi K_b^2} - \ln\left(1 + \sqrt{1 + 4x^2\tan^2\phi K_b^2}\right) \\ & + \sqrt{1 + 4(1 - y)^2\tan^2\phi K_t^2} - \ln\left(1 + \sqrt{1 + 4(1 - y)^2\tan^2\phi K_t^2}\right) \end{aligned} \tag{22}$$

the new expression for the dominant term in the energetics. The location of the minima proceeds in an identical fashion. For the pinned state we find

$$x = \frac{bH}{\left(K_b^2 - b^2H^2\right)\tan\phi} \qquad \text{and} \qquad y = 1 - \frac{bH}{\left(K_t^2 - b^2H^2\right)\tan\phi} \tag{23}$$

whereas for the diagonal state the analysis is now more complex. We let $z = x = y$ and then minimize the function $h(z) \equiv f(z, z)$ to find the crossing point. The solution is found to be the solution of the quartic equation

$$z^2K_b^2 + (1 - z)^2K_t^2 - z(1 - z)\left[K_t^2 + K_b^2\right] = z^2(1 - z)^2\tan^2\phi\left[K_t^2 - K_b^2\right]^2 \tag{24}$$

which reproduces the known result, $z = 1/2$ when $K_t = K_b$. Due to the lengthy nature of (24) it is regrettable that a simple direct comparison with Snell's Law is not possible analytically. This should not be surprising, as we have fully included all the fluctuations (upto the SOS approximation) which contribute to the mean position whereas previous authors have made the comparison in a mean-field approximation [3]. Although this is of course entirely appropriate for rays, it is well established that for interfaces in two dimensions, fluctuations are extremely important in determining equilibrium properties, especially contact angles [11].

Numerically however the roots of (24) are simple to determine and we include a plot showing some sample results, see figure 3. Care must be taken to select the correct root by using the condition $z < 1/2$ when $K_t < K_b$.

5. Summary

In this paper we have shown how an approach using a horizontal SOS model can successfully recover results in the appropriate scaling limit that have previously been obtained in an exact calculation. The SOS model enables one to approach the problem in a greater degree of generality without losing the essential features of the physics. We also emphasize the weakness in the model: it is unable to treat fluctuations that dominate around the mid-position. A fact that should be readily apparent due to the precise correspondence of the results in a half model to those in a full model. These faults are however compensated by the fact that we are able to compute the equilibrium position of the interface when it experiences different interfacial stiffnesses in the top and bottom halves of the system.

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