COMMENT

Interface refraction at a grain boundary

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Abstract. We consider an interface between co-existing phases embedded in an inhomogeneous sample which consists of two (or more) grains separated by a grain boundary. Using microscopic considerations we show that, under appropriate circumstances, the different inclination angles inside two grains are related by a law reminiscent of Snell's in geometrical optics. The role of the refraction index is played by the surface stiffness coefficient. This picture breaks down for rigid interfaces and in situations where the grain boundary pins the interface.

The behaviour of interfaces between two co-existing equilibrium phases in anisotropic systems, e.g. solids, have been the subject of many recent investigations, ranging from experiments [1] and Monte Carlo simulations [2] to theoretical studies [1, 3, 4]. One particularly interesting aspect concerns the roughening transition [5] where interfaces aligned with special orientations (such as crystallographic axes) display critical behaviour. One characteristic of this behaviour lies in τ, the energy per unit area, also referred to as the surface tension, which would be a singular function of the temperature. Other singular behaviour persists below the transition, so that τ is not an analytic function of the orientation of interfaces. Studying interfaces tilted slightly away from alignment allows us to probe this type of singularity.

In previous studies only *homogeneous* systems were used, in which an inclined interface is introduced by the choice of appropriate boundary conditions [4]. However, real experimental samples are *inhomogeneous* (polycrystalline), consisting of uniform regions (grains) separated by grain boundaries. In this work we analyse the behaviour of an inclined interface in the inhomogeneous Ising system which, we expect, models the experimental situation more realistically. Specifically, we consider a system which is made of two (or more) regions joined by the grain boundary, as shown in figure 1. In addition, we impose the boundary conditions in such a way that a tilted interface is forced across the whole system. Our purpose is to analyse the effect of inhomogeneity on the inclination of the interface in the two grains. The new result of this comment is that under appropriate circumstances, the rough interface behaves as a light ray refracted at the boundary between two optical media. Although in this study we concentrate on the 2D systems (line interfaces), appropriate generalisations to 3D samples is straightforward (see below).

Consider a 2D square lattice of Ising spins, with boundary conditions as shown in figure 1. Such boundary conditions pin the interface by its endpoints at $A = (0, 0)$ and $B = (L, m_2)$, with $L = L_1 + L_2$. The interior of the sample consists of two *different* Ising systems, with nearest-neighbour ferromagnetic interactions J_1 and J_2, respectively. In
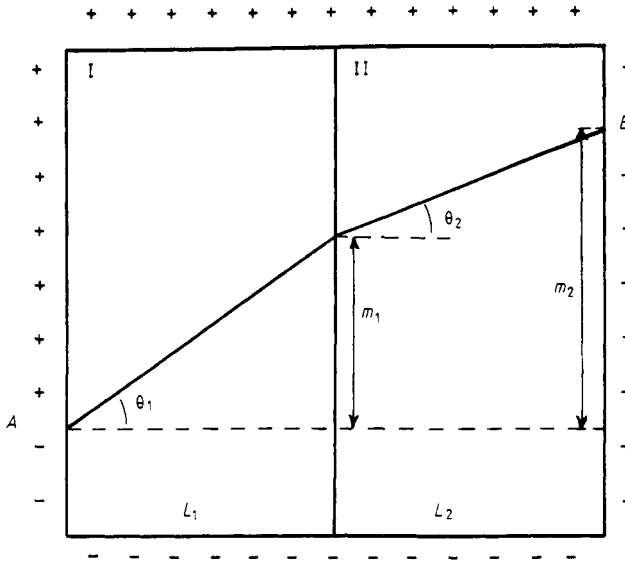
Figure 1. Schematic illustration of the inhomogeneous model considered. The boundary conditions (denoted by + and −) around the edge force a tilted interface across the whole system. In the interior of the grains I and II, the tilt angles are θ_1 and θ_2. In the absence of pinning at the grain boundary, the angles are related by the optical law of refraction.

the particular case when $J_1 = J_2$, the boundary conditions force a tilted interface, with the average inclination angle $\theta = \tan^{-1}(m_2/L)$, with respect to the horizontal axis. In the general case, when $J_1 \neq J_2$, the tilt in the two regions will be different, and must be described by two angles, θ_1 and θ_2, as shown in figure 1. The magnitude of θ_1 and θ_2 depends on the properties inside each system. Furthermore, the two inclinations are not independent, and the relation between them is obtained from thermodynamic considerations.

In order to determine the relation between the two inclination angles, consider the partition function for the system in figure 1. Let us suppose that the interface at the grain boundary passes through the intermediate point (L_1, m_1), and consider first, for simplicity, the case when the interface crosses the grain boundary only once. (Later, an interface with more than one crossing will be discussed.) Under these assumptions, the single point, (L_1, m_1), suffices to specify the position of the interface at the boundary. The total partition function, for the compound system of length L, with the interface crossing the grain boundary at a height m_1, is

$$Z(L, m_1) = \mathscr{Z}(L_1, m_1)\mathscr{Z}(L_2, |m_2 - m_1|) \tag{1}$$

where $\mathscr{Z}(X, Y)$ denotes the partition function for the system with the interface pinned by its endpoints, $(0, 0)$ and (X, Y), and inclined by the angle $\tan^{-1}(Y/X)$. Thus, the determination of $Z(L, m_1)$ is reduced to calculation of $\mathscr{Z}(X, Y)$ for the *homogeneous* sample. The values of X and Y are specified by (1). When the inclination angle $\tan^{-1}(Y/X)$ is small, $\mathscr{Z}(X, Y)$ has the Gaussian form [6, 7]

$$\mathscr{Z}(X, Y) = \exp(-\tau X)\left(\frac{\kappa}{2\pi X}\right)^{1/2} \exp\left[-X\frac{\kappa}{2}\left(\frac{Y}{X}\right)^2\right] \tag{2}$$

where τ and κ are the surface tension and the surface stiffness coefficient, respectively, of the inclined interface. Note that (2) is valid for small inclination angles, and we

assume X large, so that the finite-size corrections for τ and κ [6, 7] can be neglected. Using the result (2), with (1), we obtain

$$Z(L, m_1) = \exp(-\tau_1 L_1 - \tau_2 L_2) \left(\frac{\kappa_1 \kappa_2}{4\pi^2 L_1 L_2} \right)^{1/2} \exp\left(-\frac{\kappa_1 m_1^2}{2L_1} - \frac{\kappa_2 (m_2 - m_1)^2}{2L_2} \right). \tag{3}$$

The precise form of τ and κ will depend on the specific model. In this work we consider Ising, solid-on-solid (sos), and restricted solid-on-solid (rsos) models for interfacial properties. In these cases, the surface tension and the surface stiffness coefficient are known exactly [7]. Specifically, denote by $K_i = J_i/k_B T$, with $i = 1, 2$, the nearest-neighbour interactions in the two subsystems. Then

$$\tau_i = \begin{cases} 2(K_i - K_i^*), & \text{for the Ising model} \\ 2(K_i - K_i^*) & \text{for the sos model} \\ 2K_i - \ln(1 + 2e^{-2K_i}) & \text{for the rsos model} \end{cases} \tag{4}$$

and

$$\kappa_i = \begin{cases} \sinh 2(K_i - K_i^*) & \text{for the Ising model} \\ 2\sinh^2 K_i & \text{for the sos model} \\ 1 + \tfrac{1}{2}e^{2K_i} & \text{for the rsos model} \end{cases} \tag{5}$$

with the dual coupling K_i^* defined by $\sinh 2K_i \sinh 2K_i^* = 1$.

The partition function $Z(L, m_1)$, given by (3), depends on the intermediate interface height m_1. This height is fixed by the variational requirement that the interfacial free energy is minimal. That is

$$\frac{\partial}{\partial m_1} Z(L, m_1) = 0 \tag{6}$$

which yields

$$m_1 = \frac{\kappa_2 L_1}{\kappa_1 L_2 + \kappa_2 L_1} m_2. \tag{7}$$

This result can be further expressed in terms of the inclination angles as

$$\kappa_1 \tan \theta_1 = \kappa_2 \tan \theta_2. \tag{8}$$

For small angles we use the approximation $\tan \theta_i \simeq \sin \theta_i$. Therefore, equation (8) relating the two inclination angles is analogous to Snell's law of geometrical optics: it describes the refraction of a light ray at the boundary of two optical media, with indices of refraction κ_1 and κ_2. The minimisation (6) is equivalent to Fermat's principle. Note also that the above procedure can be easily generalised to the situation when the sample consists of more than two grains.

If the angles are not small, then the full anisotropic surface tension function $\tau_i(\theta)$ comes into play. The generalisation of (8) is

$$x_{W1}(\theta_1) = x_{W2}(\theta_2) \tag{9}$$

where $x_{Wi}(\theta) = \sin(\theta)\tau_i + \cos(\theta)[\partial \tau_i/\partial \theta]$ is nothing but the x coordinate of the Wulff shape associated with τ_i [8, 9]. To obtain the appropriate reduction, recall that $\kappa_i \equiv \tau_i + \partial^2 \tau_i/\partial \theta^2$ and, for *rough* interfaces near a symmetry orientation, that τ_i is analytic in θ^2. Equations like (9) will be useful in constructing the *general* equilibrium shape of a bubble (of a third phase, e.g. disordered) embedded at the boundary of two solids.

There has been previous work [10, 11] along these lines, though all assume special circumstances.

The derivation leading to (8) was performed under the assumption that the interface crosses the grain boundary only once. (For the RSOS model this assumption is always true since this model prevents vertical steps longer than one lattice spacing). Physically, this means the boundary is *not* pinning. In the case of pinning, e.g. when the couplings at the grain boundary are weaker than those in either of the two grains, the situation is more complicated. In order to gain energy, the interface will first reach the boundary at some height m_a, then run vertically along the grain boundary up to a height m_b and, finally, extend from (L_1, m_b) to (L, m_2). Such an interface will not, in general, obey 'Snell's law' (8). We believe that the proper description in this case can be formulated in the framework of the recently developed path integral decomposition expansion [12]. Furthermore, it may prove possible to use this expansion more generally [13] and derive rigorously the range of validity of the optical law (8) for rough interfaces. Within this formalism, the minimisation of the appropriate action is equivalent to minimising the free energy.

We now discuss the tilt angles in the corresponding 3D systems. In this case it is essential to distinguish the behaviour below and above the roughening transition temperature T_R. For $T > T_R$, the interface is *rough* and the partition function, in the absence of pinning, has the form [6] similar to (3). (In 2D systems the interface is rough for all $T > 0$.) Thus, an appropriate 'Snell's law' can be derived for 3D systems, provided care is taken to properly parametrise interface inclinations and introduce principal stiffness coefficients [6]. However, when $T < T_R$, the interface is *rigid* and the Gaussian form (3) is not valid. Recall that a rigid interface tilts in steps [5], and the tilt angles will depend on the *step free energy* within each grain. In this case 'Snell's law' is not expected to apply.

Acknowledgments

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