Comment on "Universal Jump of Gaussian Curvature at the Facet Edge of a Crystal"

In a recent Letter,[1] Akutsu, Akutsu, and Yamamoto (AAY) demonstrate that, for short-range interactions, there is a universal jump in the Gaussian curvature at the facet edge of a crystal. In this Comment, I provide a new derivation of their result which casts more light on its physical origin. Further, I demonstrate that their result is altered by the presence of elastic and dipolar forces, which are long ranged.

The well-known universal curvature jump[2] at a roughening transition may be clearly understood as a consequence of the universality of a correlation-function exponent at the transition. This correlation function is

$$C(x,y) = \langle e^{i[z(x,y)-z(0,0)]}\rangle \approx e^{-\langle [z(x,y)-z(0,0)]^2/2\rangle}, \qquad (1)$$

where $z(x,y)$ is the height of the surface at the point $\mathbf{r}=(x,y)$. Orient the coordinates so that the x and y axes are principal axes of curvature. Then the principal curvatures are given by[3]

$$\kappa_{ii} = -\tfrac{1}{2}\beta\lambda \int d\mathbf{r}\, \partial^2 \langle [z(\mathbf{r})-z(0)]^2\rangle / \partial x_i^2 , \qquad (2)$$

where λ scales the size of the crystal and $\beta = 1/k_B T$. If $C(x,y)$ has the asymptotic form

$$C(x,y) \propto 1/[k_x^2 x^2 + k_y^2 y^2]^\eta , \qquad (3)$$

the combination of Eqs. (1)-(3) readily yields, for the Gaussian curvature $K = \kappa_{xx}\kappa_{yy}$,

$$(k_B T/\lambda)\sqrt{K} = 4\pi\eta . \qquad (4)$$

At a roughening transition η takes on the universal value $1/2\pi^2$.

Now, the correlation function $C(x,y)$ is perfectly well defined on the curved surface away from the facet edge, and, in the context of commensurate-incommensurate transitions, it has been calculated by Shultz[4] for the case of short-ranged interactions. In the limit that the facet edge is approached, Eq. (3) holds with $\eta = 1/4\pi^2$, which, when inserted in Eq. (4) yields the result of AAY, who derived it by connecting the coefficient B of the cubic term in the expansion of the surface free energy in powers of the slope with the step stiffness.

Elastic interactions and, in metals, dipolar interactions lead to a long-range interaction between steps varying as g/l^2, where l is the step separation[5] and g is a constant. These interactions affect B and thus could invalidate the universal result of AAY if the step stiffness is not affected in a compensating way. The effect of $1/l^2$ interactions on the step stiffness is now known. Fortunately, relevant results for the correlation function $C(x,y)$ exist. In Ref. 5 the connection between steps on crystal surfaces and the ground-state properties of spinless fermions in one dimension is discussed. In particular, a computation of the pair correlation function for fermions is equivalent to a calculation of the slope-slope correlation function $S(x) = \langle S_x(x,0)S_x(0)\rangle$, where $S_x = \partial z/\partial x$. As is clear from Eqs. (1)-(3), the coefficient of $1/x^2$ in $S(x)$ is 2η. Using the fermion results of Sutherland,[6] one finds the AAY result $\eta = 1/4\pi^2$ for $g=0$, $\eta = 1/2\pi^2$ for $g=-t/4$, and $\eta = 1/8\pi^2$ for $g = 2t$. Here $t = \beta^{-1} \times e^{-\beta\Gamma}$, where Γ is a kink energy.[5]

The result for general g is not available, but these partial results make it clear that the universality of the curvature jump K fails in the case of the physically relevant long-range elastic and dipole forces. This failure will be most manifest at low temperatures. Near roughening, entropic effects dominate the long-range forces, and the universal-curvature-jump prediction of AAY will obtain.[5]

This work was partially supported by the National Science Foundation under Grant No. DMR-84-04961. Discussions with David Edwards and Sebastien Balibar are gratefully acknowledged, and special thanks goes to C. Jayaprakash for key conversations and a critical reading of the manuscript.

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Received 6 March 1989
PACS numbers: 61.50.Jr, 05.70.Jk, 68.35.Rh, 82.65.Dp

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