Free-fermion solution for overall equilibrium crystal shape
L. Mikheev, V. Pokrovsky

To cite this version:

HAL Id: jpa-00246337
https://hal.archives-ouvertes.fr/jpa-00246337
Submitted on 1 Jan 1991

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Free-fermion solution for overall equilibrium crystal shape

L. V. Mikheev (1, *) and V. L. Pokrovsky (2,3)

2) Landau Institute for Theoretical Physics, Ul. Kosygina 2, Moscow 117940, U.S.S.R.
3) Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, Postfach 1913 D-5170 Jülich, Germany.

(Received 16 July 1990, accepted in final form 8 November 1990)

Abstract. — We generalize the random walk or free-fermion method of Yamamoto, Akutsu and Akutsu to obtain a simple explicit solution for the overall equilibrium crystal shape of a simple cubic crystal at temperatures, T, low with respect to the nearest-neighbour coupling, E. The thermal rounding of the corners and of the edges of the cube appears to be qualitatively different: at the corners the width of the rounded, vicinal surface and its radius of curvature are estimated to be of order $\left(k_b T/E\right)R$, where $2R$ is the diameter of the crystal. As the distance $\ell$ from the corner along an edge increases, the width of the vicinal surface and transverse radius of curvature decrease as $\exp(-\ell k_b T/ER)$ reaching an exponentially small value at the middle of the edge. On the other hand, the radius of curvature parallel to an edge grows as $\exp(\ell k_b T/ER)$, so that the product of two principal curvatures remains constant up to a numerical factor. A qualitative explanation of the results is presented, based on the strong dependence of the stiffness of the steps on their orientation with respect to the axes of the crystal.

1. Introduction.

The problem of the statistical mechanical description of equilibrium crystal shapes (ECS) has recently attracted considerable attention [1]. However, most authors have restricted themselves to (i) the close vicinity of a facet and (ii) high symmetry directions. A noticeable exception is the work of Abraham [2] in which the ECS of a BCC crystal has been found for a wide range of directions normal to (110). Beyond that some advances have been achieved in two directions:

(i) Kashubaa and one of us [3] have found an interpolation expression for the ECS at an arbitrary angle along a high symmetry direction (for example, perpendicular to the (100) plane in a simple cubic crystal);

(*) Now at: Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742, U.S.A.
(ii) Yamamoto, Akutsu and Akutsu (YAA) [4-6] investigated the vicinity of a facet edge scanning over azimuthal angles. In the framework of the free-fermion approximation (i.e. noncrossing random walks) they found that the Gaussian curvature, $K$, has a jump across the facet edge from zero to a universal value $K = \lambda^2 \beta^2 \pi^{-2} d^4$, where $\lambda$ is the Lagrange multiplier in the Wulff construction (see Ref. [5] and the next section), $\beta \equiv 1/k_B T$, and $d$ is the height of an elementary step. Later Saam [7] pointed out that the universal value of $K$ is related to the universal properties of correlations in the free-fermion system or in a dilute ensemble of steps.

In this paper we show that the random walk approach of YAA yields a very simple explicit expression for the overall ECS if the fugacity of a kink, $\exp(-\beta E)$, is small.

Another approach to the calculation of the overall ECS, similar to that of reference [2], has been developed by Kashuba [8].

2. The model.

We consider the simplest possible model of a simple cubic crystal which still captures the essential features of real crystals: lattice symmetry and strong fluctuations of steps.

We ascribe an energy $E$ to each nearest-neighbour bond in the crystal. In the bulk, all the bonds are in their low-energy or satisfied state, while some bonds are broken by the surface. Thus, the energy of the crystal is equal to $E \times \text{(number of broken bonds)}$. We consider a surface tilted on average at an angle $\theta < \frac{\pi}{2}$ to the z-axis and specify its configurations by the (in general, multiple-valued) height function $z_0(x, y)$. The length of a bond is taken to be unity, so both the local height $z_0$ and the lateral coordinates $x, y$ are integers. We define steps as lines separating sites with local heights differing by unity. Then any configuration can be represented as a set of steps. We will ascribe a direction to each step. The direction may be indicated by an arrow, so that the z-coordinate is larger to the right of the arrow (Fig. 1). We consider the low-temperature limit in which the fugacity $\exp(-\beta E) = \exp(-\varepsilon) \ll 1$. This is typically realized for crystal-vapor interfaces at temperatures below the melting point. All effects of order $\exp(-2\varepsilon)$ will be neglected. In particular, if one step passes over another one, two additional vertical bonds have to be broken and the probability is diminished by a factor $\exp(-2\varepsilon)$. Thus configurations with overlaps may be ignored, so that $z_0$ is a single-valued function of $x$ and $y$. Now it is easy to see that the energy of a configuration is:

$$H = \text{Const.} + EL$$

(1)

where $L$ is the total length of all steps. Note that two steps may run along the same link: in our nearest-neighbour approximation the energy of steps is additive. Now following YAA [4, 6] we represent a step as a random walk. The direction of the step becomes the time direction of the walk. At any lattice vertex the step has four possibilities to move (Fig. 1). We ascribe a weight $\eta_{2j} = \exp(-\varepsilon \pm \mu_j)$ to a jump along the positive (negative) direction of the $j$-axis ($j = x, y$). We will see below that at the rounded parts of the surface the largest $\eta_j$ is of order unity (otherwise a flat facet is more favourable). The probability of two consecutive jumps back and forth, namely, $\eta_{+j} \eta_{-j} = \exp(-2\varepsilon) \ll 1$, will be neglected, so that there is no double counting in our approach. We consider two regimes:

A. $\eta_{-x} \ll \eta_{-y} \ll \eta_{+y} \ll \eta_{+x} \approx 1$. In this case the probability of two consecutive jumps forwards and back along the $y$ axis is $O(\eta_y^2) = O(\exp(-2\varepsilon))$ and thus negligible. The step goes along the $x$-axis with rare jumps in the perpendicular direction (Fig. 2a).

B. $\eta_{-x} \ll \eta_{-y} \ll \eta_{+y} \ll \eta_{+x} \sim O(1)$. In this case $\mu_j \approx \varepsilon$, so that both probabilities of jumps in the negative direction $\eta_{-x}, \eta_{-y}$ are $O(\exp(-2\varepsilon)) \ll 1$ and thus negligible (Fig. 2b).
Fig. 1. — Representation of a single step as a random walk.

Fig. 2. — Representations of steps as fermionic world lines: a) Regime A; b) Regime B.

The crossover between regime A and B occurs when \( \eta_+^2 = \eta_-^2 \) which corresponds to \( \mu_y = \epsilon/3 \); both \( \eta_+^2 \) and \( \eta_-^2 \) are then of order \( \exp \left( -\frac{4}{3} \epsilon \right) \) which is negligible at our level of precision. The crucial point is that at low temperatures (\( \epsilon \gg 1 \)) the two regimes A and B have a domain where they overlap. All other cases are obtained from these two by the use of symmetry. Thus the simple explicit expressions which we obtain below for these two regimes will allow for a description of the overall ECS. It should be noted that in both cases our model satisfies the usual terrace-step-kink conjecture. Thus we arrive at the grand partition sum \( \Xi = \sum \exp \left[ \sum_{j = -x,y} (\mu_j - \epsilon) \times (\text{total number of } j \text{-type jumps}) \right] \), where the first sum runs over all the configurations of the steps. Only sets of nonintersecting steps are considered. The chemical potentials \( \mu_j \) are adjusted so as to provide the desired mean orientation of the surface. It is easily shown that the derivatives of the free energy \( f = -\log (\Xi/N_x N_y) \) with respect to the \( \mu_j \) yield the mean slopes of the surface:

\[
\partial_{\mu_j} f = p_j = \langle \partial z_0/\partial y \rangle; \quad \partial_{\mu_x} f = -p_x = -\langle \partial z_0/\partial x \rangle.
\]

Here \( N_x \) and \( N_y \) are the lateral sizes of the system. The chemical potentials \( \mu_j \) introduced above are, thus, simply related to the commonly defined chemical potentials \([1]\), conjugate to the slopes. Thus Andreev's duality transformation (see in \([1]\)) \( f \rightarrow \lambda Z, \mu_x \rightarrow \lambda y, \mu_y \rightarrow \lambda x \) allows us to convert the partition sum \( \Xi(\mu_x, \mu_y) \) into the ECS function \( Z(x, y) \). Here \( \lambda \) is the common scale factor proportional to the size of the crystal.
3. Equilibrium crystal shape : the explicit solution.

The partition sum corresponding to the Hamiltonian (1) is explicitly evaluated within our assumptions by the transfer-matrix method of YAA. The representations needed for the regimes A and B are a bit different.

**REGIME A.** Here the x-axis is taken as the time direction. The lines \( x = \text{Const.} \) are crossed by each step once and only once (Fig. 2a). When the time goes from \( x \) to \( x + 1 \), a step either rests at the same site, \( y \), with the probability \( \eta_{+x} = \eta_x \) or it jumps to a neighbouring site, \( y + 1 \), with probability \( \eta_{+y} = \eta_{x+1} \). In order to account for the nonoverlapping of steps we introduce an additional row of sites between each pair of steps so that for a state of \( m \) steps \( N_y \rightarrow N_y + m \) and forbid steps to meet on the same site. Thus we arrive precisely at the system considered in reference [4]. The transfer-matrix used by YAA is

\[
\hat{T} = \prod_k \begin{pmatrix} a_k^+ & \eta_x + \eta_{+y} \eta_x \exp(ik) + \eta_{-y} \eta_x \exp(-ik) \\ \eta_x + \eta_{+y} \eta_x \exp(ik) + \eta_{-y} \eta_x \exp(-ik) & a_k \end{pmatrix}
\] (2)

where \( a_k^+ \), \( a_k \) are the fermion creation and annihilation operators. Note that after the extraction of a common scale factor, \( \eta_x \), the values \( T(k) - 1 \) are the eigenvalues of the nonhermitian Hamiltonian

\[
\sum_y \left[ \eta_{+y} a^+(y + 1) a(y) + \eta_{-y} a^+(y) a(y + 1) \right]
\] (3)

which is a natural generalization of the Hamiltonian used in reference [3].

The partition sum \( \Xi \) is determined by the eigenvalue of \( T \) of largest modulus. For a fixed number of steps \( m \) it corresponds to filling all fermion states with \( |k| < k_F = \pi m/(m + N_y) \). Then \( f(\eta_x, \eta_y) \) is obtained by the minimization of the function

\[
f(m, \mu_x, \mu_y) = -\log \left( \frac{\Xi(m)}{N_x N_y} \right)
\] over \( m \). Thus we find

\[
f(m, \mu_x, \mu_y) = \min_{k_F} \frac{(-1)}{\pi - k_F} \int_0^{k_F} \log |T(k)| \, dk = \min_{k_F} \frac{(-1)}{\pi - k_F} \left[ k_F (\lambda y - \epsilon) + 2 e^{-\epsilon} \cosh(\lambda x) \sin(k_F) \right]
\] (4)

where the assumption \( \eta_{\pm y} \ll 1 \) has been used in (5).

**REGIME B.** Now the time axis goes along the diagonal \( x = y \) (Fig. 2b). At each instant of time a step jumps either to the right or to the left with probability \( \eta_{+y} = \eta_y \), \( \eta_{-x} = \eta_{x+1} \), respectively. We introduce again additional « time » rows between each pairs of steps to arrive at the system of reference [6] with \( T(k) \) defined by

\[
T(k) = [\eta_x \exp(ik/2) + \eta_y \exp(-ik/2)].
\] (6)

Now (4) yields \( f = 0 = \text{Const.} \) when \( |T(0)| < 1 \), which corresponds to the flat (001) facet. Hence the boundary of the facet is given by \( |T(0)| = 1 \). On combining the two expressions, (2) and (6), and using the result in (4), we obtain an interpolative equation for the facet boundary, namely,

\[
\eta_{+x} + \eta_{-x} + \eta_{+y} + \eta_{-y} = 2 \exp(-\epsilon) (\cosh \lambda x + \cosh \lambda y) = 1,
\] (7)

which satisfies all the symmetries of the system. Note that we have proved a posteriori the conjecture \( \max \eta_y = O(1) \) used when defining regimes A and B in the previous section.
Thus we have developed a method of constructing the rounded surface adjacent to an (100) facet. However, this approach clearly breaks down near another (say (010)) facet, where many steps run along the same edge and overhangs cannot be neglected. The natural way of avoiding this difficulty is to match the constructions starting from the (100) and (010) facets. The mirror plane of the crystal parallel to (110) should be crossed by the surface at a right angle, i.e.\( \partial_y Z = - \partial_x f = -1 \) at the intersection. The last equality defines a curve on the surface \( f(\mu_x, \mu_y) \) defined by (4), (5), (6). It must be a plane curve. Straightforward calculations (see the Appendix) prove that this is indeed so: up to corrections of order \( e^{-\varepsilon} \), the curve lies in the plane

\[
\log(\eta_x) + f = \lambda y + \lambda Z - \varepsilon = 0
\]

which is parallel to (011) \((Z + y = 1, \text{if we take the scale factor } \lambda = \varepsilon)\). Thus we can smoothly match the surface \( Z(x, y) \) with \( X(y, z) \) and others obtained by permutations and changes of sign of the three coordinates. In this way the overall crystal shape is obtained. Note that (8) defines the absolute size of the crystal: the center lies at a distance \( \varepsilon/\lambda \) below the (001) facet. Thus \( \lambda = \varepsilon/R \), where \( R \) is the distance from the center of the crystal to a facet.

We have up to now set the origin of z-axis at the (001) plane. It is more natural to shift the origin to the center which requires the additive redefinition: \( Z = (f + \varepsilon)/\lambda \).

For small \( \eta_y \) (regime A), (8) corresponds to \( k_F = \pi/2 \) (see the Appendix). Therefore, \( \eta_x \) changes across the curved region from \( 1 - (\eta_{+y} + \eta_{-y}) \) at the facet edge to \( 1 - (\eta_{+y} + \eta_{-y})/\pi \) at the middle of the region. Thus it is close to unity everywhere which provides a smooth crossover between regimes A and B. Now it is easily checked that by introducing the new variables \( \Pi_j = \eta_{+j} + \eta_{-j}, \ \text{(} j = x, y \text{)} \), we may use the interpolative expression

\[
f = \min_{k_F} \frac{-1}{\pi - k_F} \int_0^{k_F} \log \left( \Pi_x^2 + \Pi_y^2 + 2 \Pi_x \Pi_y \cos k \right) \, dk/2
\]

for all values of \( \Pi_x, \Pi_y \), thus defining a universal function \( f(\Pi_x, \Pi_y) \). After that, for any given \( \varepsilon = E/k_B T \), the ECS for \( x > y > 0, \ Z > z \) is obtained through the mapping:

\[
\lambda x = \cosh^{-1}(e^{\varepsilon} \Pi_x/2), \quad \lambda y = \cosh^{-1}(e^{\varepsilon} \Pi_y/2), \quad \lambda z = f + \varepsilon
\]

and then the rest by rotations and reflections. The whole procedure is accurate up to corrections of order \( \exp(-4\varepsilon/3) \). The results for the projection of the ECS onto the (110) plane for \( \varepsilon = 3, 5 \) and \( 10 \) are shown in figure 3.

4. The correlation functions and Gaussian curvature.

We start by calculating the density-density correlation function for our random walkers. The standard transfer matrix technique [9] yields

\[
\langle \rho(x_1) \rho(x_2) \rangle = \langle 0 | : a^+(x_1) a(x_1) \hat{T}^t a^+(x_2) a(x_2) : | 0 \rangle / \langle 0 | \hat{T}^t | 0 \rangle
\]

where \( \langle 0 | \) stands for the ground state corresponding to the largest eigenvalue of \( \hat{T} \), while \( x_i = (r_i, t_i) \), where \( r \) labels the sites in the «space-direction» rows \( x = \text{Const. in the A-regime and } x = y = \text{Const. in the B-regime} \), and \( t \) (time) counts these rows; the symbol \( : \) denotes time-ordering of the operators and \( t = |t_2 - t_1| \). For \( \hat{T} \) given by (2) the correlation of
the density fluctuations $\delta \rho \equiv \rho - \langle \rho \rangle = \rho - k_F / \pi$ is determined by the creation-annihilation of particle-hole pairs which yields

$$\langle \delta \rho (x_1) \delta \rho (x_2) \rangle = \sum_{k_1, k_2} \exp[i (k_2 - k_1) (x_2 - x_1)] (1 - \rho_{k_2} \rho_{k_1} [T(k_2) / T(k_1)]^4).$$  \hspace{1cm} (12)

After setting $\delta \rho (x) = \sum_q \rho_q \exp(i q x)$ it is easily seen that the asymptotic form of $G(q) = \langle |\delta \rho_q|^2 \rangle$ for small $q$ is determined by the close vicinity of $k = \pm k_F$. Introducing $w = -d \log T(k)/dk|_{k_F}$ (so that $w^* = -d \log T(k)/dk|_{-k_F}$) we get

$$G(q) = k_F^2 \text{Re} \left( \frac{w^2}{\pi} \left( k_F^2 w^2 + k_F^2 + 2 k_F k_1 \text{Im} w \right) \right).$$ \hspace{1cm} (13)

Fig. 3. — Projections of the ECS onto the (110) plane. Solid lines represent the profile of the shape; dashed lines denote facet edges. a) $\varepsilon = \beta E = 3$; b) $\varepsilon = 5$; c) $\varepsilon = 10$. 
Since each step crosses each space-row only once one finds \( \rho = (\partial z/\partial r)_r \). Hence one obtains
\[
\langle |z_0|^2 \rangle^{-1} = [G(q)/k^2]^{-1} = \left[ \pi (k^2 + 2 k^2 r_k + \text{Im} w) \right]/\text{Re} w
= \Gamma_{i,j} k_i k_j
\]
(14)
which implies
\[
\det \Gamma_{i,j} = \pi^2
\]
(15)
So even though the transfer-matrix \( \hat{T} \) is nonhermitian and \( w \) is not real, the value of \( \det \Gamma \) is real and universal. Now, following the arguments of YAA and Saam [7] we find that the correlation function given by (14) can be obtained from the capillary Hamiltonian
\[
H = \frac{1}{2} \int \text{d}^2 r \Gamma_{ij} \partial_i z \partial_j z
\]
(16)
where \( z \) denotes the fixed \( z \)-axis rather than the normal to the given average orientation of surface. Hence \( \Gamma_{ij} = \partial_i g(p^j) \), where \( g \) is the Legendre transform of the grand potential \( \log \Xi/N_t(N_r + m) \) and depends on the mean tangent slope \( p^j = \langle \partial z/\partial x_i \rangle \) of the auxiliary \( N_t \times (N_r + m) \) lattice, \( p^j = k_r/\pi \). Finally
\[
f(\mu) = \min_{\rho_j} (1 - \rho_j)^{-1}[p_j \mu_j + p^j \mu_r - g(p^j)],
\]
so that
\[
\det \partial_i \partial_j f = \det \Gamma_{ij}^{-1}/(1 - \rho_j)^4 = (1 + \rho_j)^4 \pi^{-2},
\]
(17)
where \( \rho_j = p_j/(1 + p_j) \) are the real slope variables conjugate to \( \mu_j \). Combining (17) and (1) and keeping in mind that for both regimes \( (1 + \rho_j)^2/(1 + p^j)^2 \approx (\sum n_j)^2, j = x, y, z, \) we get
\[
K = \lambda^2 \beta^2 (|n_x| + |n_y| + |n_z|)^4/\pi^2 = R^{-2} (|n_x| + |n_y| + |n_z|)^4 (\beta E/\pi)^2
\]
(18)
where \( R \) is the distance from the center to the (100) plane. Note the explicit cubic symmetry of the final expression in contrast to the asymmetric way in which it was derived.

5. Discussion.

Equations (9) and (10) contain a complete solution of the ECS problem for the nearest neighbour simple cubic crystal in the low-temperature limit. Some examples of shapes are presented in figure 3. The model clearly involves two major simplifications: (i) the total neglect of the long-range interatomic forces other than NN bonds. This precludes the formation of facets other than of (100) type. (ii) The low-temperature approximation, i.e. the expansion in powers of fugacity \( \exp(-\varepsilon) \). Because of this we have completely neglected all overhangs, particularly the appearance of closed finite terraces which renormalize the step free energy and the effective step-step interaction.

These assumptions are physically justified for a range of temperatures \( T_{R_2} < T < T_{R_1} \), where \( T_{R_{1,2}} \) are the roughening temperatures of (100) and (110) faces respectively. For the crystal-vapor system \( T_{R_i} \) is usually higher than the melting temperature. The effect of a sea of closed step loops on the free energy of a single (infinitely long) step has been recently considered by Holzer and Wortis [10]. In this way the shape of a single facet has been determined at temperatures closer to \( T_{R_1} \). The effect of the loops on the step-step interaction,
which determines the shape of the vicinal surface connecting adjacent facets, was not investigated to our knowledge. The appearance of a « devil’s staircase » of higher order faces provided by long-range step-step (equivalently, fermion-fermion) interaction was demonstrated by Kashuba and one of us [3].

To summarize, the main results of the present work are:

(i) If \( 2R \) is the distance between the opposite faces, the width of the rounded vicinal surface between the facets obeys the exponential law \( (R/\beta E) \exp(-\beta E\ell/R) \), where \( \ell \) is the distance along the edge to the nearest corner. Thus while the edges of the cube are smeared at \( T = 0 \) with a small relative width \( \alpha (R/\beta E) \exp(-\beta E) \) [3], the corners are smeared with a much larger relative width \( \alpha R/\beta E \).

(ii) The model under consideration cannot be reduced to an equivalent fermionic system because the transfer-matrix and the Hamiltonian are not Hermitian. Nevertheless the determination of the generalized stiffness matrix \( \Gamma \) is universal, determining the critical exponent \( \eta = 1/4\pi \) [7].

(iii) The Gaussian curvature \( K \) is given by the rather simple expression (18). It is clearly seen that \( K^{1/2} = (K_1 K_2)^{1/2} = O(\beta E/R) \) varies by a factor 9 on the rounded, vicinal surface, while the principal curvatures \( K_{1,2} \) vary more strongly from \( K_1 = K_2 \approx R^{-1}\beta E \) at the corners to \( K_1 = \exp(\beta E)\beta E/R \) and \( K_2 = \exp(-\beta E)\beta E/R \) at the edges. The numerical prefactor in (18) is obviously model-dependent. Its experimental determination could serve to check the applicability of the model.

(iv) The shape of the vicinal surface near the (001) facet edge is well described by the simple expression

\[
1 - z = (2^{3/2}/3\pi) (\Pi_x - \Pi_y - 1)^{3/2}/(\Pi_x \Pi_y)^{1/2}
\]

(19)

which follows from (9) and (10). Thus the universal law \( \Delta z = C\rho^{3/2} \) [11], \( \rho \) being the normal distance from the facet edge, is fulfilled everywhere. However the coefficient \( C \) depends on the location along the edge of the facet, varying from of order \( (\beta E)^{3/2} \) at the \( x = \pm y \) corners to much larger values, of order \( (\beta E)^{3/2} \exp(\beta E) \), at the middle of an edge. Thus the vicinal surface rises much more steeply near the center of the facet edges than near the corners.

The qualitative picture arising from our explicit calculation can be obtained by simple physical arguments. First, the form of the surface along the edge of the cubical crystal is qualitatively similar to the form of the boundary of the facet: see (7). The left hand side of this relation simply reproduces the free energy of a single step.

At low temperatures it is convenient to represent any configuration of the step as a perturbation of the lowest energy configuration in which the step runs parallel to the edge (i.e. the \( x \)-axis). The elementary excitations are « kinks », that is, links of perpendicular, \( y \)-orientation. Each kink carries a quantum of slope, \( dy/dx = \pm 1 \). According to the duality transformation which we are exploiting, the coordinate along the edge, \( x \), is proportional to the chemical potential of a kink. The chemical potential is conjugate to the slope: it is of opposite sign for kinks of opposite slopes.

The exponential dependence describing most parts of the curve (7) corresponds to the Boltzman statistics describing a gas of kinks of one sign, dominating at a given part of the edge. Both near the centers of the edges and near the corners these exponential curves join smoothly owing to the mixing of two different sorts of kinks.

Second, the form of the vicinal surface transverse to an edge is given by the free energy of the system of many steps compressed by an external « pressure » proportional to the transverse coordinate \( \rho \). The compressibility is determined by the entropic repulsion of the steps, which for large step-step separations, \( L_4 \), varies like \( Dk_B T/L_4^2 \). Here \( D \) is the
diffusivity (proportional to inverse stiffness) of a single step, determining its mean square wandering \( \langle w_{1}^{2} \rangle = DL_{1} \), as a function of the distance \( L_{1} \) along the step. The law \( \Delta Z = C \rho^{3/2} \), cited above, immediately follows with \( C \propto D^{-1/2} \). The width \( \Delta \rho \) of the rounded region may be estimated by simple scaling arguments as \( \Delta \rho \propto C^{-2} \propto D^{-2} \): if the repulsion is weak/strong the compressibility is large/small and the characteristic «pressure», \( \Delta \rho \), necessary to compress the system to the density of order unity is small/large.

Now the steps diffuse by propagation of kinks and \( D \) is easily shown to be merely proportional to the average number density of kinks (not to the «slope density» \( = \) slope : kinks of both signs contribute to the diffusion). The crucial point here is that if the average slope of the steps with respect to the edge, \( q \), is smaller than the fugacity of a kink, \( \exp(-\beta E) \), then the diffusivity is determined by the thermally activated kinks. So one has \( \Delta \rho \propto D \propto \exp(-\beta E) \) which is very small at low temperatures. On the other hand, for \( q \gg \exp(-\beta E) \), the finite density of kinks, which is of order \( q \), is determined just by the geometrical constraint. In particular, near the corners \( q = O(1) \) and \( \Delta \rho \propto q \) is relatively large. Finally, combining the \( \Delta \rho \propto q \) dependence with the exponential approximation \( q \propto \exp(-\beta E/|R|) \) from (7), we obtain the exponential dependence of \( \Delta \rho \) on the distance along the edge from the corner that was noted above.

Finally, notice that the only quantity determining the results of the preceding discussion is the fugacity of a kink on a step. In our case this is just \( \exp(-\beta E) \), but it can be defined more generally for any lattice, interaction, or facet orientation, and is expected to be a small parameter at low temperatures. In this way our results can be applied much more widely, to a vicinal surface between any two facets well below their roughening temperatures (provided the direct long-range repulsion between steps [12] is negligible). The major problem here is that in most of the cases, the facets are not equivalent, so that two different fugacities of kinks determine the behavior from the opposite sides of the rounded zone. The description of such an asymmetric situation remains a task for future work.

Acknowledgments.

One of us (LM) is indebted to Noriko Akutsu for drawing his attention to references [4-6]. The kind help of Curtis A. Doty and especially of Michael E. Fisher in the final stage of work on this paper is gratefully acknowledged. The work was completed with the aid of financial support from the National Science Foundation (under Grant NO. DMR 90-07811).

Appendix.

Here we prove that the points satisfying the equation \( \partial f / \partial \mu_{x} = 1 \) lie, within the prescribed accuracy, on the plane (8). In regime B we find

\[
\frac{\partial f}{\partial \mu_{x}} = \frac{\partial f}{\partial \log \eta_{x}} = (\pi - k_{F})^{-1} \int_{0}^{k_{F}} \frac{1 + \chi \cos k}{1 + \chi^{2} + 2 \chi \cos k} \, dk
\]

\[
= (\pi - k_{F})^{-1} \left[ \frac{k_{F}}{2} + \tan^{-1} \left( \frac{1 - \chi}{1 + \chi} \tan \frac{k_{F}}{2} \right) \right]
\]

where \( \chi = \eta_{y} / \eta_{x} \). On the other hand the condition for an extremum to be present in (5) is equivalent to

\[
\frac{1}{2} \log \left[ \eta_{x}^{2} + \eta_{y}^{2} + 2 \eta_{x} \eta_{y} \cos k_{F} \right] + f = \log \eta_{x} + f + \frac{1}{2} \log \left( 1 + \chi^{2} + 2 \chi \cos k \right) = 0.
\]
Setting the r.h.s. of (A1) to unity we find \( \chi + 2 \cos k_F = 0 \) and after substitution into (A2) obtain (9).

The corresponding calculations for the regime A are much simpler. Setting \( \partial f/\partial \log \eta_x = k_F/(\pi - k_F) = 1 \), we obtain \( k_F = \pi/2 \), while minimization of (6) leads to

\[
\frac{f}{2} + \log \eta_x + \frac{1}{2} \log [1 + 2(\eta_x + \eta_y) \cos k_F] = 0,
\]

which for \( k_F = \pi/2 \) again reduces to (9).

References


also Kolomeisky B. E., unpublished.


