A new exponent in the equilibrium shape of crystal surfaces[*]

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Abstract. A new exponent characterizing the rounding of crystal facets is found by mapping a crystal surface onto the asymmetric six-vertex model (i.e. with external fields h and v) and using the Bethe ansatz to obtain appropriate expansions of the free energy close to criticality. Leading order exponents in δh, δv are determined *along the whole phase boundary and in an arbitrary direction.* A possible experimental verification of this result is discussed.

Keywords: integrable spin chains and vertex models, surface effects

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[*] This paper is dedicated in fond remembrance of our PhD advisor Vladimir Rittenberg.

Contents

1. Introduction

Crystals are believed to be entirely faceted at $T = 0$, i.e. be polyhedral. Research—both theoretical as well as experiments—on these so-called quantum crystals has increased at an accelerated pace in the last few years. This is due to a miriad of prospective applications and experimental advances [1] which allows us to conduct experimental at those extreme temperatures. To name a few applications, quantum computing, high-pressure synthesis, nanoelectronics, and ferroelectrics whose Curie temperature is very close to absolute zero are among the most prominent ones [2, 3]. Moreover, since some of the most prototypical quantum crystals are rare-gases like He and Ne or molecular crystals as H_2 or CH_4, their availability make them particularly suited for experimental studies. As the temperature of a quantum crystal is raised, thermal fluctuations bring about a rounding of the edges where planes with different indices (hkl) meet. At the roughening transition temperature T_R the remaining planar portion of (hkl) disappears entirely and the face becomes rough. Different facets may have different T_R's. This smoothing that occurs at the edge where two facets meet can be visualized in a simple geometrical way [4]: near the edge there is a curving of the interface (see figure 1) which varies as

$$z(x) \sim (x - x_c)^\theta + \text{higher-order terms} \tag{1}$$

where x_c is the position of the edge and z measures height perpendicular to the facet. θ is the roughening exponent. Understanding how this rounding occurs is key to knowing how crystals' properties change and any questions concerning the exact value of T_R or exponents characterizing the macroscopic smoothing out of the edges cannot be addressed in a satisfactory way unless one has a microscopic model from which these quantities can be derived from first principles. However, from thermodynamics one can show that if a solid is in thermal equilibrium with its surrounding fluid, the free energy $F(T)$ is given by the same equation (up to an overall constant) which defines the geometrical form of the crystal. The implication of this result is straightforward: if one is able from first principles to calculate explicitly $F(T)$ and find its singularities, one is directly determining the singularities of the crystal shape, as the equations are the same. In other words, the singularities of the surface free energy gives us directly the roughening exponent θ. Before we present the main content of this paper, which
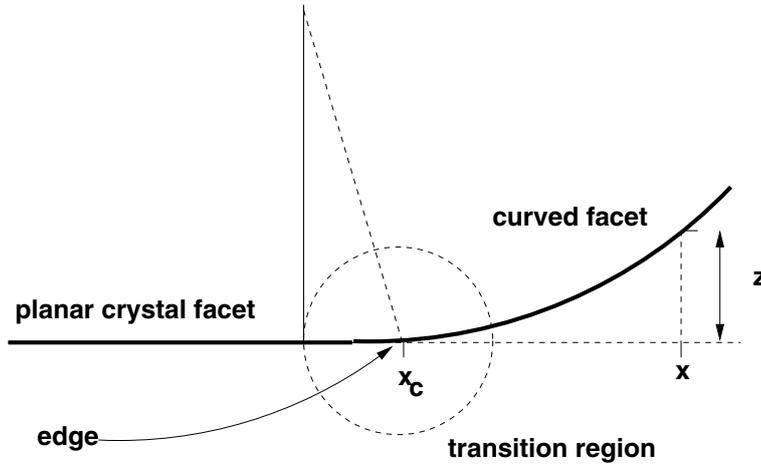
Figure 1. The profile of the smooth edge of an ideal crystal facet in the transition region where it becomes rounded. Based on [4].

applies to both quantum as well as classical crystals, we briefly discuss the thermodynamics of equilibrium crystal shapes (ECS) to better elucidate our results.

2. Thermodynamics of ECS

Along a first-order coexistence line the shape of a solid inclusion in equilibrium with its fluid is determined by the Gibbs–Curie constrained minimization condition: for a fixed volume V of the inclusion, the equilibrium surface $\Omega = z(x, y)$ is such as to minimize the surface free energy

$$F(T) = \int_\Omega \tau(\vec{n}, T) \mathrm{d}\Omega = \text{minimum} \tag{2}$$

where the surface tension τ depends on the orientation of Ω, $\vec{n} = \vec{\nabla} z(x, y)$ and temperature T. To solve the constrained variational problem to determine $z(x, y)$ one introduces a Lagrange multiplier 2ν

$$\delta\left\{ \int [f(p, q) - 2\nu z(x, y)] \mathrm{d}x \mathrm{d}y \right\} = 0$$

$p = \frac{\partial z}{\partial x}$, $q = \frac{\partial z}{\partial y}$ are the slopes of the surface and $f(p, q, T) = \tau(p, q, T)\sqrt{1 + p^2 + q^2}$ is the specific surface free energy projected onto the (x, y)-plane. The solution reads [5, 6]

$$\nu z = \overline{f}(-\nu x, -\nu y) \tag{3}$$

where the Legendre transformed potential $\overline{f}$ is defined through [6]

$$\overline{f}(\eta_x, \eta_y) = f(p, q) - p\eta_x - q\eta_y \tag{4}$$

with $\eta_x = \frac{\partial f}{\partial p}$, $\eta_y = \frac{\partial f}{\partial q}$ the surface tilting fields conjugate to the slope variables p and q. Thus the determination of $\overline{f}$ yields the equilibrium surface $z(x, y)$ directly, up to some

overall irrelevant constant. The main question however is how much of the physics can be captured by this description.

3. The free energy of the six-vertex model and ECS

Since both the free energy and the ECS of a crystal are given by the same mathematica formula equation (3), it is clear that questions concerning the exact value of T_{R} or exponents characterizing the macroscopic smoothing out of the edges cannot be addressed in a satisfactory way unless one has a microscopic model from which the surface tension τ can be derived from first principles. This problem has been tackled with success by several authorseq mainly by using a connection between the theory of equilibrium shapes and two-dimensional lattice models, with the asymmetric six-vertex model playing a major role [7–10]. This system of interacting dipoles on a lattice is the natural extension of the symmetric problem through the inclusion of external fields h and v [11]. It is a classical paradigm of models soluble through the Bethe ansatz and an exact expression for its free energy has been known for many years [12]. Originally introduced in the context of equilibrium crystal shape problems (ECS) to describe the $(0\,0\,1)$ facet of a bcc crystal [7], it was later extended to cover other facets on different lattices as well. In this way very comprehensive results have been obtained regarding the form of the equilibrium surface as well as its thermal evolution [9]. In particular there is a region in the (h, v) plane bounded by a curve Γ and containing the origin $(h = 0, v = 0)$, which defines the loci of points where the free-energy retains its zero-field value [12]. This implies that z is a constant over an entire region of the parameter space. Beyond Γ the free energy changes continuously as a function of the fields. Appropriate expansions of the surface free energy around Γ show a leading order exponent for the scaling of $z(x, y)$ as one approaches the boundary of the $(1\,1\,0)$ fcc facet along the $y = 0$ direction [9]

$$z \sim (x - x_c)^{\frac{3}{2}} + \mathcal{O}(x - x_c)^2. \tag{5}$$

This result has been confirmed experimentally [4, 13]. However, even though a great deal has been learned from exact analytical methods, their handling is no trivial matter and previous results were somewhat limited in their scope by rather involved technical difficulties. In spite of the fact that it had already been conjectured that (5) should hold on *the entire facet boundary* a proof of this result still eluded us [9]. In this letter we give such a proof based on the expansion of the free energy of the asymmetric six-vertex model via the Bethe ansatz, introduced in [14, 15] as a generalization of previous methods [10, 11]. The main results can be summarized as follows: the exponent $\frac{3}{2}$ dominates the rounding in all directions *but* the tangential one, in which case a new exponent 3 dominates. These results hold for the whole boundary.

For the sake of clarity, we consider one particular geometry, namely that of the $(1\,1\,0)$ facet of an *fcc* lattice[4]. One may associate an energy to the surface arising from the cleavage of an infinite ideal crystal through the plane (hkl) based solely on the number and type of bonds broken per primitive cell. This is the simplest model possible and yet one which allows an exact handling of the equations that follow. Consider an fcc

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[4] The results here presented can be easily extended to other geometries.

lattice (figure 1) with energies $-J_1$ and $-J_2$ assigned to nearest—and next-to-nearest neighbor bonds respectively ($J_1 > J_2 > 0$). The $T = 0$ surface tension reads [16]

$$\tau(\vec{n}_{hkl}) = \frac{\vec{n}_{hkl}}{V^{\mathrm{pc}}|\vec{n}_{hkl}|} \cdot \left(J_1[2\,1\,0] + J_2[1\,1\,1] \right) \tag{6}$$

where $\vec{n}_{hkl} = h\widehat{x} + j\widehat{y} + k\widehat{z}$ is the vector normal to the plane (hkl) and V^{pc} is the volume of the primitive fcc cell. Voids (excitations in the bulk) as well as overhangs (height differences between neighboring columns of atoms bigger than some unit length) are strictly forbidden (solid-on-solid condition). The connection between the $(1\,1\,0)$ facet and the vertex model is shown in figure 1.

From (6) one may associate the following energies to the vertices [9]

$$
\begin{aligned}
e_1 &= J_2 + \frac{A}{\eta}{}_x = J_2 - H - V \\
e_2 &= J_2 - \frac{A}{\eta}{}_x = J_2 + H + V \\
e_3 &= J_1 - \frac{A}{\sqrt{2}}\eta_y = J_1 - H + V \\
e_4 &= J_1 + \frac{A}{\sqrt{2}}\eta_y = J_1 + H - V \\
e_5 &= e_6 = 0.
\end{aligned}
\tag{7}
$$

Here $A = \frac{a^2}{\sqrt{2}}$ is the area of a vertex (for a lattice constant a) and

$$
\begin{aligned}
H &= -\frac{A}{2}\left(\eta_x - \frac{\eta_y}{\sqrt{2}} \right) \\
V &= -\frac{A}{2}\left(\eta_x + \frac{\eta_y}{\sqrt{2}} \right).
\end{aligned}
\tag{8}
$$

Note that this parametrization is slightly different than the one used in [9] but is consistent with figure 1.

The free energy (4) follows straightforwardly [9]

$$\overline{f}(\vec{\eta}, T) = f(1\,1\,0) + f_{6-\mathrm{vertex}}(J_1, J_2, H, V, T). \tag{9}$$

A configuration of alternating vertices 5 and 6 corresponds to the macroscopically smooth $(1\,1\,0)$ plane. The twofold degeneracy (exchanging vertices $5 \leftrightarrow 6$) represents the invariance of the crystal surface by the removal of the top layer of atoms. In terms of the original dipoles, this configuration of vertices has a zero net dipole moment (which trivially translates to the facet $(1\,1\,0)$ having zero slope, being the reference plane). Regions of net dipole moment different from zero (nonzero slopes p, q) correspond to tilts away from the reference plane. To find f (or equivalently $\overline{f}$) of this system of interacting dipoles attached to the links of a square grid, we consider a lattice of $N \times M$ sites and impose periodic boundary conditions on both directions. Define the row-to-row transfer matrix

$$T(u)_{\{\underline{\alpha}\},\{\underline{\alpha}'\}} = \sum_{\{\underline{\beta}\}} \prod_{k=1}^{N} R_{\alpha_k \alpha_k'}^{\beta_k \beta_{k+1}}(u) \tag{10}$$

where $\{\underline{\alpha}\} = \alpha_1, \cdots, \alpha_N$ are the arrows on a row of N vertical links (the α''s are one row above) and β_k (β_{k+1}) is the arrow to the left (right) of the kth vertex. $R_{\alpha_k \alpha_k'}^{\beta_k \beta_{k+1}}$ is the Boltzmann weight associated to a given configuration $\{\alpha_k, \alpha_k', \beta_k, \beta_{k+1}\}$ of the kth vertex (see figure 2). It is more conveniently described in terms of the so-called spectral parameter u and anisotropy γ, whose explicit relation to the original parameters reads

$$\sinh u = e^{-J_1/k_B T} \sqrt{\cosh^2 \gamma - 1} \tag{11}$$

$$\cosh \gamma = -\cosh \frac{1}{k_B T}(J_1 - J_2) + \frac{1}{2} e^{\frac{1}{k_B T}(J_1 + J_2)} \tag{12}$$

and k_B is the Boltzmann constant. We also incorporate the Boltzmann factors in new definitions for H and V, namely $h = \beta H$ and $v = \beta V$ (see figure 2).

The transfer matrix can be diagonalized exactly with the Bethe ansatz. Its eigenvalues read [12]

$$
\begin{aligned}
\Lambda(u, \gamma, h, v) &= e^{v(N-2n)} e^{hN} \left[\frac{\sinh(\gamma - u)}{\sinh \gamma} \right]^N \prod_{j=1}^{n} \frac{\sinh(\frac{\gamma}{2} + u - \frac{i\alpha_j}{2})}{\sinh(\frac{\gamma}{2} - u + \frac{i\alpha_j}{2})} \\
&+ e^{v(N-2n)} e^{-hN} \left[\frac{\sinh u}{\sinh \gamma} \right]^N \prod_{j=1}^{n} \frac{\sinh(\frac{-3\gamma}{2} + u - \frac{i\alpha_j}{2})}{\sinh(\frac{\gamma}{2} - u + \frac{i\alpha_j}{2})}
\end{aligned}
\tag{13}
$$

where the α_j are the roots of the Bethe ansatz equations

$$\left[\frac{\sinh(\frac{\gamma}{2} + \frac{i\alpha_k}{2})}{\sinh(\frac{\gamma}{2} - \frac{i\alpha_k}{2})} \right]^N = (-1)^{n+1} e^{2hN} \prod_{l=1}^{n} \frac{\sinh(\gamma + \frac{i}{2}(\alpha_k - \alpha_l))}{\sinh(\gamma - \frac{i}{2}(\alpha_k - \alpha_l))} k = 1, 2, \cdots, n \tag{14}$$

n represents the number of arrows in a row of N vertical links which are reversed with respect to the reference ferroelectric state $|\uparrow\uparrow \cdots \uparrow\rangle$.

The specific free energy is given by $f = -\lim_{N,M\to\inf} \frac{k_B T}{NM} \ln \mathbf{Z}$ where $\mathbf{Z} = Tr(T^M)$ is the partition function. In the thermodynamic limit this expression is dominated by the largest eigenvalue Λ_0 of T and and the free energy reduces to

$$f(u, \gamma, h, v) = -\lim_{N\to\infty} k_B T \frac{\ln \Lambda_0(u, \gamma, h, v)}{N}.$$

At this point it is interesting to discuss some already known facts about the physics of the asymmetric six-vertex model before solving the Bethe ansatz equations explicitly. The phase diagram and the nature of the phase transitions are well understood when $h = v = 0$ (symmetric six-vertex), or when $h = 0$ and $v \neq 0$ [11].

The $T = 0$ phase diagram for $(h, v) \neq 0$ is trivial [12]. In this case the ground state wanders, as a function of the external fields, through each one of the different regions composed exclusively of vertices of type 1, 2, $\cdots$, 5 + 6. The boundaries between each region are sharply defined. In figure 3 a plot of the free energy both in the (h, v)-plane
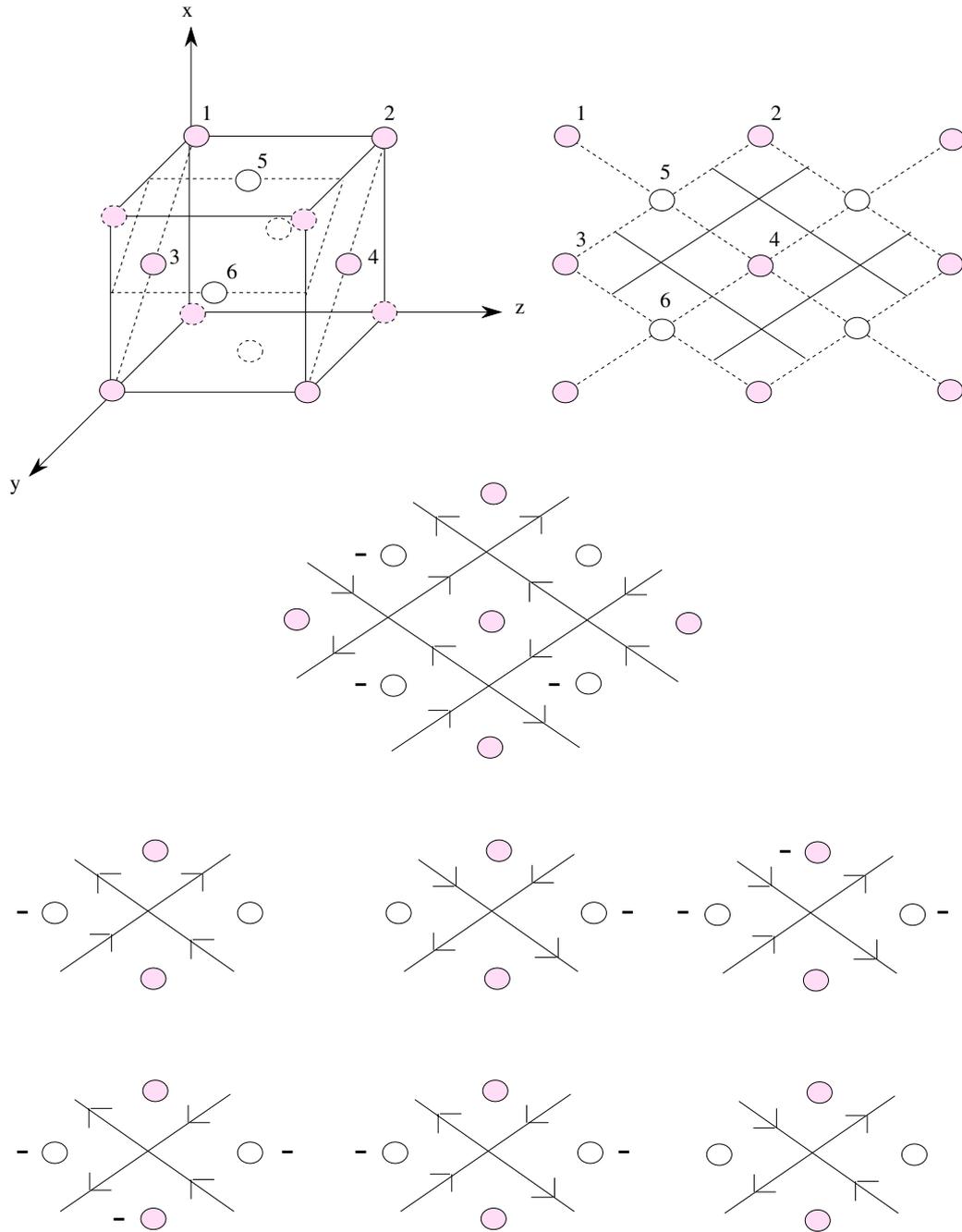
Figure 2. The fcc cell and vertices. On the top left the $(1\,1\,0)$ plane is depicted (full circles). Atoms in the plane immediately above are represented by empty circles. Two such planes combined define the macroscopically smooth $(1\,1\,0)$ crystal surface. Vertices (full lines, top right) are defined for each group of 4 atoms (two filled and two empty circles). In the middle, a particular configuration of 4 vertices is depicted, a—sign indicating an atomic vacancy. The exact correspondence between vertices and configurations of the crystal plane is shown in the bottom figure. Vertices 1 through 4 represent tilts away from the $\langle 1\,1\,0 \rangle$ direction, and correspond locally to planes $(1\,1\,\bar{1})$, $(1\,1\,1)$, $(1\,0\,0)$ and $(0\,1\,0)$ respectively. An alternating configuration of vertices 5 and 6 correspond to the $(1\,1\,0)$ surface.

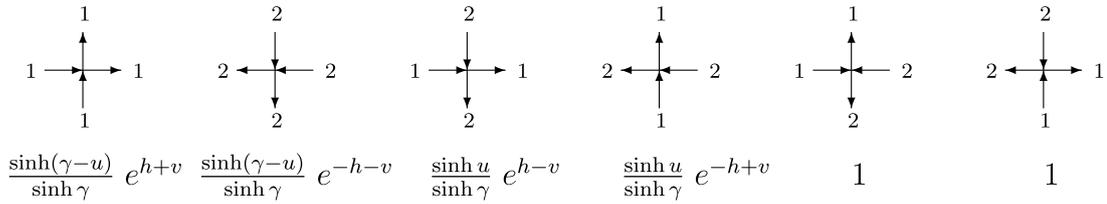**Figure 3.** The vertices and their corresponding Boltzmann weights.

as well as in the (η_x, η_y)-plane are presented. The crystal facets to which each region corresponds are accordingly indicated [9].

As the temperature is raised, thermal excitations bring about a rounding of edges [7]. When $T \neq 0$ (γ finite) the free energy $f(h, v)$ remains constant as function of the field ('flat phase') in a region of the (h, v) plane containing $h = v = 0$ and bounded by a curve Γ. Beyond this, the field is sufficiently strong to destroy the antiferroelectric order of the system, but not strong enough to impose ferroelectric order, and an incommensurate phase appears where the polarization (or surface slope), which is zero in the flat phase, changes continuously with the field. The spectrum of the transfer matrix is gapless with finite size corrections typical of the gaussian model [17]. The curve Γ has been investigated only at a few points [9, 11] and the nature of the phase transition was found to be of a Pokrovskii–Talapov type [18]. To study this curve in more detail, one has to solve the Bethe ansatz equations in their limiting form for arbitrary values of h, v and determine the free energy. This is a non trivial problem. A detailed exposition of the methods used to tackle (14) can be found in [10, 14, 15]. Here we point out only the main results which are of relevance to the questions addressed. Since the Boltzmann factor is inessential to the forecoming discussion, we drop it out of our analysis. The vertical polarization y is defined through

$$y = \lim_{N \to \infty} \frac{2S^z}{N} = \lim_{N \to \infty} \left(1 - \frac{2n}{N}\right). \tag{15}$$

Inside the boundary curve Γ in the (h, v)-plane the polarization is constant at its $y = 0$ value; the free energy does not depend on the field and is given by [12]

$$f(u, \gamma, h, v) = -2 \sum_{n=1}^{\infty} \frac{e^{-2\gamma n}}{n \cosh \gamma n} \sinh(nu) \sinh n(\gamma - u). \tag{16}$$

The parametric equation $(h(b), v(b))$ of Γ is given by [10, 14]

$$h(b) = -\frac{b}{2} - \sum_{n=1}^{\infty} (-)^n \frac{\sinh nb}{n \cosh n\gamma} \tag{17}$$

and

$$v(b) = \frac{\gamma}{2} - \frac{|\gamma - 2u - b|}{2} + \sum_{n=1}^{\infty} \frac{(-)^n}{n} \frac{\sinh[n(\gamma - |\gamma - 2u - b|)]}{\cosh n\gamma} \qquad -\gamma \leqslant b \leqslant \gamma. \tag{18}$$

These equations reproduce only half of the curve Γ. The other half can be recovered from the symmetry $f(-h, -v) = f(h, v)$. Figure 4 depicts Γ in the (h, v)-plane along with the same plot in the (η_x, η_y)-plane (the latter being the boundaries of the $(1\,1\,0)$
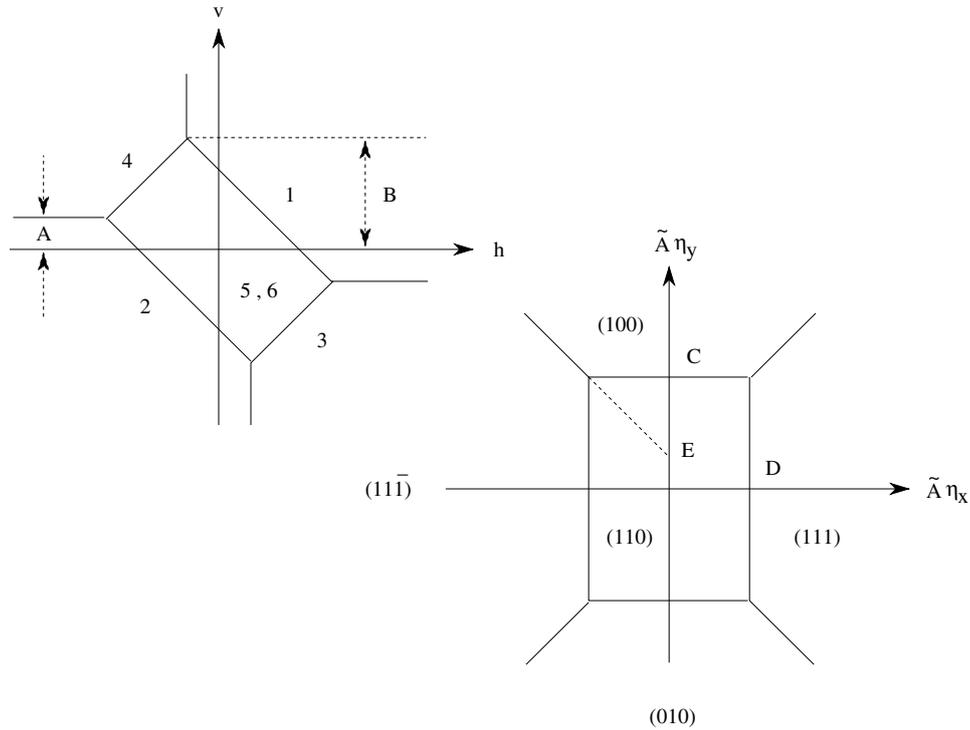
Figure 4. $T = 0$ view of the free energy in the (h, v)—and (η_x, η_y)-plane. The values of the parameters are $A = \frac{J_1 - J_2}{2}$, $B = \frac{J_1 + J_2}{2}$, $C = J_1$, $D = J_2$ and $E = \sqrt{2}(J_1 - J_2)$; $\widetilde{A}$ is the area of a vertex.
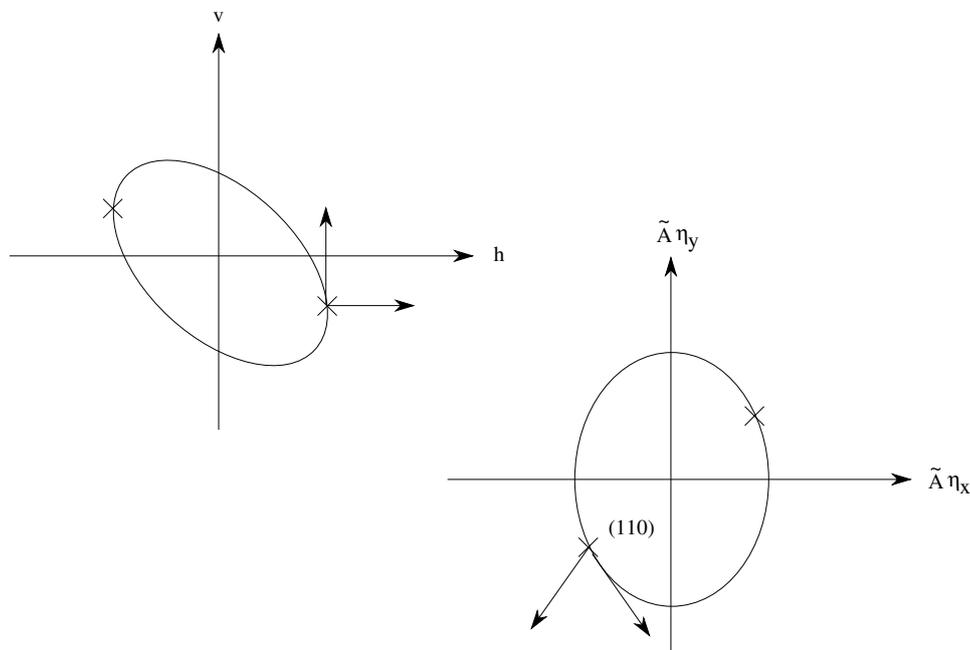

Figure 5. Parametric plot of Γ for $\cosh \gamma = 21$ and spectral parameter $u = \frac{1}{2}$ in the (h, v)—and (η_x, η_y)-plane respectively. The latter corresponds to the boundaries of the $(1\,1\,0)$ fcc facet. The points (h_c, v_c) (lower half-plane) and $(-h_c, -v_c)$ (upper half-plane) are singled out.

facet) obtained numerically for $\cosh\gamma = 21$, $u = 0.5$ (non zero, finite temperature, see figure 5). Two points, (h_c, v_c) and $(-h_c, -v_c)$ are singled out: the reason for this is explained in what follows.

It is believed [7, 9, 10] that the free energy singularity should be governed by a universal exponent $\frac{3}{2}$. A calculation performed for $\eta_y = 0$ gives [9]

$$\overline{f} \sim \overline{f_0} + \text{constant} \times (\eta_x - \eta_x^{\text{crit}})^{3/2} + \mathcal{O}(\delta\eta_x^2).$$

From this result, it follows straightforwardly that

$$z = z_0 + \text{constant} \times (x - x_0)^{3/2}.$$

An earlier result also support this observation, the direction of approach being however tilted relative to the normal of the surface [11]. It remains however to be proven that such results apply irrespective of the direction of approach and for the whole facet boundary. In order to prove this, one has to perform expansions on the free energy by means of an extension of previous techniques so as to allow an arbitrary angle of approach [14, 15]. Consider first the points (h_c, v_c). Here the equations simplify significantly and the increments δh, δv are perpendicular and tangential to the boundary, respectively. One obtains, when approaching Γ from the incommensurate phase

$$f(u, \gamma, h_c + \delta h, v_c) = f(u, \gamma, h_c, v_c) - 2c_2 \left(\frac{2}{c_1}\delta h\right)^{3/2}$$

$$f(u, \gamma, h_c, v_c + \delta v) = f(u, \gamma, h_c, v_c) - \frac{2}{c_2^2}\left(\frac{c_1}{6\pi}\right)^3 |\delta v|^3$$

where c_1 and c_2 are functions of γ and u only. These results are not related to the unique geometrical character of the points. They hold over the whole boundary curve and can be expressed using the parametric equation of Γ, $(h(b), v(b))$ given by equations (17) and (18). We introduce the following notation [15]

$$
\begin{aligned}
v_t(b) &= \frac{\mathrm{d}}{\mathrm{d}b}v(b) \quad h_t(b) = \frac{\mathrm{d}}{\mathrm{d}b}h(b) \\
v_1(b) &= \frac{\mathrm{d}}{\mathrm{d}b}v_t(b) \quad h_1(b) = \frac{\mathrm{d}}{\mathrm{d}b}h_t(b) \\
\Delta &= v_t h_1 - h_t v_1
\end{aligned}
\tag{19}
$$

and approach the curve Γ from the outside along straight lines $h = h(b) + \delta h$, $v = v(b) + \delta v$ where $\delta v = k\delta h$ and k fixes a slope not tangential to Γ. The free energy singularity reads in this case [15]

$$\delta f(\delta h) = \left(\frac{h_t}{\Delta}\right)^{1/2}\frac{h_t}{3\pi}[2(k - \frac{v_t}{h_t})\delta h]^{3/2}. \tag{20}$$

These results clearly show that the exponent $3/2$ is obtained for all directions except the tangential one, that is when $\delta v = \frac{v_t}{h_t}\delta h$. Here the singularity is

$$\delta f(\delta h) = \begin{cases} c_+\delta h^3 & \text{if} \quad \delta h > 0 \\ c_-\delta h^3 & \text{if} \quad \delta h < 0 \end{cases} \tag{21}$$

where $c_+ \neq c_-$ are constants depending on the parameter b of the curve.

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The result of our long calculation is that one has two critical exponents $\theta_1 = 3/2$ corresponding to the rounding off of a crystal facet when the facet boundary is approached in all other directions except the tangential one and $\theta_2 = 3$ if the facet boundary is approached tangentially. Experiments on small Pb-crystals [4] which looked for θ_1 have found $\theta_1 = 1.60 \pm 0.15$ whereas experiments on large He^4-crystals [13] have found $\theta_1 = 1.55 \pm 0.06$ confirming the theoretical predictions. More recent results on Pb were presented in [19]. According to Babkin [20] and Henrich [21] measurements to put in evidence the second critical exponent θ_2 are feasible. An open problem common to the measurements in both exponents is the effect of gravity. These effects have been discussed in [22] and more extensively in the reviews [23–25].

Acknowledgments

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