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Universal properties in the free energy of the asymmetric N-state vertex model

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Abstract. Electric-field-dependent free energy of the exactly solvable asymmetric N-state vertex model (i.e. in an arbitrary vertical and an arbitrary horizontal electric field v and h) in the low-temperature antiferroelectric phase is obtained in the form of the expansion in terms of small but nonzero polarization p. Exact mapping onto a microscopic surface model (solid-on-solid (SOS) model) is employed to study the vicinal-surface free energy below the roughening temperature T_R which determines the equilibrium crystal shape (ECS) near the facet edge of a crystal.

The obtained expansion of the free energy is of the well-established Gruber–Mullins–Pokrovsky–Talapov (GMPT) type: $f(p,h) = f(0,h) + a(h)p + b(h)p^3 + \mathrm{O}(p^4)$. It is found that the coefficients $a(h)$ and $b(h)$ are identical with those of the asymmetric six-vertex model. Based on this expansion, in cooperation with the Andreev construction of the ECS, universal properties are verified *along the whole facet contour*. First, directly from the GMPT-type expansion, the critical exponents governing the rounding of the crystal facet are obtained; the exponent is $\frac{3}{2}$ in all direction *except* the tangential one in which case it is 3. Second, the universal relation between $a(h)$ and $b(h)$ is verified, leading to the universal Gaussian curvature jump at the facet edge and a universal relation between the critical amplitudes of the ECS profiles of the vicinal surface.

1. Introduction

Exact solution of the two-dimensional (2D) classical statistical systems has a long history [1,2]. Most of the solutions concern 2D models without an external electric field. Exact solvability of models in an electric field is not a trivial problem. In 1967 Yang [3] and Sutherland *et al* [4] solved a general six-vertex model (called the asymmetric six-vertex model) when arbitrary horizontal and vertical electric fields, h and v, are present. They obtained the phase diagram as well as the exact expression of the free energy for zero polarization. Later, the solvability condition (a commutation relation: the Yang–Baxter relation) between the transfer matrices of the asymmetric N-state vertex model has been found [5]. In this paper we obtain the exact expansion of the free energy of the asymmetric N-state vertex model in the low-temperature antiferroelectric phase for small polarization as a generalization of previous works [6–9]. Comparison among these works and the present one is listed in table 1. Asymmetric models should be used to study the properties of models in an arbitrary direction. Expanding the free energy up to the third order gives the small-polarization properties of the vertex models. This calculation for the asymmetric model was first done in [9]. ([7] refers to the expansion up to the first order.) We verify that the same universal properties hold for the asymmetric N-state vertex model as those for the asymmetric six-vertex model [9]. We further find that the higher-order terms of the expansion exhibit a non-universal property.

Among applications of 2D classical statistical systems is analysis of the equilibrium crystal shape (ECS). As a pioneering work of exact analysis of the ECS, van Beijeren [10] mapped the

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Table 1. List of the works on expansion of the free energy of vertex models for nonzero polarization.

	Six-vertex (two-state vertex) model	N-state vertex model
Symmetric	[6]	[8, 12]
Asymmetric	[7, 9]	this work

six vertex model onto the microscopic surface model (body-centred solid-on-solid (BCSOS) model) to discuss the roughening transition exactly. By virtue of this correspondence the asymmetric six vertex model has played a major role in studying properties of the roughening transition at T_R as well as the thermal evolution of facet shapes of a crystal for temperatures $T < T_R$ [7,10,11]. Exact mapping onto a surface model is also possible for the N-state vertex model [5]. We perform this mapping to study the surface free energy of the corresponding generalized SOS model exactly.

Below the roughening temperature T_R, the ECS near the facet edge is viewed as a vicinal surface (i.e. a crystal surface with small average gradient). It was believed that the vicinal surface for $T < T_R$ belongs to the Gruber–Mullins–Pokrovsky–Talapov (GMPT) universality class [13] and that the vicinal-surface free energy $f(p)$ as a function of surface gradient p ($\sim$polarization of the vertex model) takes the well-established form of the expansion [13, 14], $f(p) = f(0) + ap + bp^3 + \mathrm{O}(p^4)$, which determines the ECS near the facet edge of a crystal via the Wulff construction [15]. Some universal properties are associated with this vicinal-surface free energy. The rounding off of a crystal facet is governed by two kinds of the universal critical exponents $\frac{3}{2}$ and 3 [16,18]; the ECS behaves as $Z \sim (\Delta X)^{3/2}$ in a 'normal' direction [6,11,17] and as $Z \sim (\Delta Y)^3$ in the tangential direction [18]. (We have chosen the Z-axis to be facet normal, and ΔX to be the 'normal' distance (perpendicular to the facet contour).) The universal relation holds between the coefficients a and b [19]. This leads to the universal relation between the critical amplitudes of the normal and the tangential ECS profile near the facet edge [16], and also to the universal Gaussian curvature jump at the facet edge [9, 19, 20], which thus has a different physical origin [21] from that of the universal curvature jump at T_R [11].

Andreev [22] showed that the surface free energy as a function of fields directly gives the ECS. In this paper we verify the GMPT-type expansion as well as the universal properties along the whole facet contour, based on the field-dependent vicinal-surface free energy $f(p, h)$ of our SOS model. The expansion of $f(p, h)$ up to the third order is N-independent, as is stated above. The result is of special interest since another calculation on this SOS model shows that the curvature jump at T_R is N-dependent [12].

2. Free energy of the asymmetric N-state vertex model

The exactly-solvable N-state vertex model (spin-s model) is an extension of the six vertex model [5]. The edge valuables of a vertex take any one of $\{-s, \ldots, s\}$ ($N = 2s + 1$) under the 'charge conservation' condition (figure 1). In this paper we concentrate on the low-temperature antiferroelectric phase (hyperbolic regime for the Boltzmann weights). We employ the Boltzmann weights with the normalization $X^{ss}_{ss}(u) = \prod_{l=1}^{N-1} \sinh(l\lambda - u)$ and with the crossing symmetry $X^{ij}_{kl}(\lambda - u) = X^{-ki}_{l-j}(u)$. Introducing a certain gauge transformation [5], we can construct the Boltzmann weights $\hat{X}^{ij}_{kl}(u)$ of the asymmetric model (in a horizontal electric field h) from those of the symmetric one $X^{ij}_{kl}(u)$:

$$\hat{X}^{ij}_{kl}(u) = H^{(j+k)/2} X^{ij}_{kl}(u) \qquad H = \exp(2\beta h) \tag{1}$$

$$i + j = k + l \qquad i, j, k, l = -s, \ldots, s. \tag{2}$$

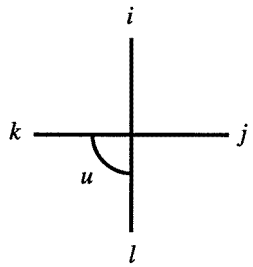

Figure 1. The Boltzmann weight $X_{kl}^{ij}(u)$. The nonvanishing weights are allowed for the vertex configuration under the 'charge conservation' condition $i + j = k + l$.

We should note that the Boltzmann weights $\hat{X}_{kl}^{ij}(u)$ themselves do not satisfy the factorization (Yang–Baxter) equation, but that there exists a commutation relation associated with the transfer matrices of the model which ensure the solvability of the asymmetric model.

Diagonalization of the transfer matrix of the asymmetric N-state vertex model is worked out by using the algebraic Bethe ansatz method [23, 24]. The resulting Bethe ansatz equation is

$$\exp(\mathrm{i}p_j L) = H^L \prod_{l=1}^{n} \exp(\mathrm{i}\Theta(p_j, p_l)) \qquad 1 \leqslant j \leqslant n \tag{3}$$

where

$$\mathrm{e}^{\mathrm{i}p} = \frac{\mathrm{e}^{2s\lambda} - \mathrm{e}^{-\mathrm{i}\alpha}}{\mathrm{e}^{2s\lambda - \mathrm{i}\alpha} - 1} \tag{4}$$

$$\Theta(p_j, p_l) = 2 \arctan\left[\coth\lambda \tan\left(\frac{\alpha - \beta}{2}\right)\right]. \tag{5}$$

In the thermodynamic limit we write the Bethe ansatz integral equation for the continuous root density $R(\alpha)$:

$$\begin{aligned} R(\alpha) + \int_C K(\alpha - \beta) R(\beta)\, \mathrm{d}\beta &= \xi(\alpha) \\ \pi(1 - y) &= \int_C R(\beta)\, \mathrm{d}\beta \end{aligned} \tag{6}$$

where

$$\xi(\alpha) = \sum_{k=1}^{2s} \frac{\sinh(2k-1)\lambda}{\cosh(2k-1)\lambda - \cos\alpha} \tag{7}$$

$$K(\alpha) = \frac{\sinh 4s\lambda}{\cosh 4s\lambda - \cos\alpha} + 2 \sum_{k=1}^{2s-1} \frac{\sinh 2k\lambda}{\cosh 2k\lambda - \cos\alpha}. \tag{8}$$

The phase shift function $\Theta(x)$ and the kernel $K(x)$ are related to each other as $K(x) = \mathrm{d}\Theta(x)/\mathrm{d}x$, and the vertical polarization y is defined by

$$y = \lim_{L\to\infty} \frac{2s^z}{L} = \lim_{L\to\infty} \frac{L - 2n}{L}. \tag{9}$$

The parameter λ scales the temperature. The integration path C is, unlike the symmetric case, shifted from the real axis to the interval [4, 7]

$$C : [-a + \mathrm{i}b, a + \mathrm{i}b]. \tag{10}$$

Note that a and b depend implicitly on the two variables y and h, and vice versa. In terms of the new variable $u = \alpha - \mathrm{i}b$ ($v = \beta - \mathrm{i}b$), the equations (6) are rewritten ($0 \leqslant a(y,h) \leqslant \pi$)

$$\begin{aligned} &R(u,b) + \int_{-a}^{a} K(u-v)R(v,b)\,\mathrm{d}v = \xi(u,b) \\ &\pi(1-y) = \int_{-a}^{a} R(u,b)\,\mathrm{d}u \end{aligned} \tag{11}$$

with the normalization

$$p^0(a,b) - \int_{-a}^{a} \theta(a-v)R(v,b)\,\mathrm{d}v = \frac{\pi}{2}[1-y(a,b)] - \mathrm{i}\ln H(a,b) \tag{12}$$

where $p^0(a,b)$ is a (complex) wavenumber. Once the solution $R(\alpha)$ is known, the per-site field-dependent free energy as a function of vertical polarization, $f(y,h)$, is given by

$$\begin{aligned} -\beta f(y,h) &\equiv g(y,h) \\ &= -\frac{1}{2}\ln H + \ln \hat{X}_{ss}^{ss}(u) + \frac{1}{\pi}\int_{-a}^{a} \Phi(u,b)R(u,b)\,\mathrm{d}u \end{aligned} \tag{13}$$

with ($\varphi = \lambda + \phi_0 - b$, $\phi_0 < b < \lambda$)

$$\Phi(u,b) = \sum_{-\infty}^{\infty} \hat{\Phi}_n(b)\mathrm{e}^{\mathrm{i}nu} \tag{14}$$

$$\hat{\Phi}_n(b) = \begin{cases} 2s(\Delta + \mathrm{i}u) & (n=0) \\ \dfrac{1}{n}\mathrm{e}^{-2s\lambda|n|}\dfrac{\sinh 2s\lambda n}{\sinh \lambda n} & (n \neq 0) \end{cases} \tag{15}$$

where the parameter ϕ_0 is defined by

$$\mathrm{e}^{\phi_0} = \frac{1+\mathrm{e}^{\lambda}\eta}{\mathrm{e}^{\lambda}+\eta} \qquad 0 \leqslant \phi_0 \leqslant \lambda. \tag{16}$$

For small vertical polarization y we obtain the free energy in its expansion form in terms of y:

$$g(y,h) = g(0,h) + \sum_{n=1}^{\infty} \frac{g_n(h)}{n!}y^n. \tag{17}$$

Calculations can be performed in a similar way to that of Lieb and Wu [6], but the asymmetry of the Boltzmann weights makes the analysis rather complicated although straightforward. To obtain the expansion (17), we need the derivatives of various quantities with respect to y at $y = 0$. Define

$$R^{(j)}(u,b) \equiv \left.\frac{\partial^j R(u,b)}{\partial y^j}\right|_{h:fixed, y=0}. \tag{18}$$

We denote the partial derivatives of a function F with respect to t at $y = 0$ by F_t, F_{tt}, and so on. $R^{(0)}(u,b)$ and $R_b^{(0)}(u,b)$ have been obtained in [7]. We expand (11) in terms of y and obtain $R^{(j)}(u,b)$'s recursively. After some calculations, we obtain

$$\begin{aligned} R^{(1)}(u,b) &= R^{(1)}(u) = R_{sym}^{(1)}(u) \\ R^{(2)}(u,b) &= R_b^{(0)}(u,b)b_{yy} \\ R^{(3)}(u,b) &= R_{sym}^{(3)}(u,b) + 2\mathrm{i}R^{(1)}(u)'b_{yy} + R_b^{(0)}(u,b)b_{yyy} \end{aligned} \tag{19}$$

where the quantities with subscript sym stands for those for the symmetric case which are given in [8]. Note that the solutions (19) are of the same form of the functional relations as

those in the $N = 2$ case (six-vertex model), but are actually N-dependent. In the derivation of (19) we have used the following relations at $y = 0$ ($a = \pi$) which are derived through (11) and (12):

$$\begin{aligned}
&\check{H} \equiv \ln H = 2\beta h = -b - 2\sum_{n=1}^{\infty} \frac{(-1)^n}{n} \frac{\sinh bn}{\cosh \lambda n} \\
&\check{H}_a = 0 \qquad \check{H}_{aa} = 4sR_b^{(0)}(\pi, b) \qquad \check{H}_{aaa} = \frac{R^{(1)}(\pi)}{s\pi} \check{H}_{aa} \\
&b_{\check{H}} = -\frac{1}{2R^{(0)}(\pi, b)} \qquad b_{\check{H}\check{H}} = -\frac{\check{H}_{bb}}{\check{H}_b} b_{\check{H}}^2 \\
&b_y = 0 \qquad b_{yy} = -\frac{a_y^2}{\check{H}_b} \check{H}_{aa} \qquad b_{yyy} = \frac{1}{4sR^{(0)}(\pi, b)} (3\check{H}_{aa} a_y a_{yy} + \check{H}_{aaa} a_y^3).
\end{aligned} \tag{20}$$

Noting that $b_{yy} = b_{yyy} = 0$ for $h = 0$ ($b = 0$), we observe in (19) that $R^{(j)}(u, b)$ ($j \leqslant 3$) reduce to the results for the symmetric model [8].

Substituting the solutions (19) into (13), after a lengthy calculation using (20), we obtain the expansion (17). It is convenient to scale the polarization by $2s$:

$$(p, q) = (2sy, 2sx) \qquad f(y, h) \to \hat{f}(p, h) \tag{21}$$

(x is the horizontal polarization) in association with the Legendre transformation ($\hat{f}(p, q) \equiv f(p/2s, q/2s)$)

$$\hat{f}(p, q) = \hat{f}(p, h) + hq \tag{22}$$

with

$$q = -\left.\frac{\partial \hat{f}(p, h)}{\partial h}\right|_p. \tag{23}$$

We then finally have

$$\begin{aligned}
-\beta \hat{f}(p, h) &\equiv \hat{g}(p, h) \equiv g(p/2s, h) \\
&= \hat{g}(0, h) + \sum_{n=1}^{\infty} \frac{\hat{g}_n(h)}{n!} p^n \\
&= \hat{g}(0, h) + \hat{g}_1(h) p + \tfrac{1}{6} \hat{g}_3(h) p^3 + \mathrm{O}(p^4)
\end{aligned} \tag{24}$$

with

$$\begin{aligned}
&\hat{g}_1(h) = -\Xi(\varphi) \\
&\hat{g}_3(h) = \left[\frac{\pi}{R^{(0)}(\pi, b)}\right]^2 \left[\Xi''(\varphi) + \frac{R_b(\pi, b)}{R^{(0)}(\pi, b)} \Xi'(\varphi)\right]
\end{aligned} \tag{25}$$

where the function $\Xi(x)$ is defined by

$$\Xi(x) = \cosh^{-1}\left[\mathrm{nd}\left(\frac{\boldsymbol{K}(k)}{\pi} x \middle| 1 - k\right)\right] \qquad (\geqslant 0) \tag{26}$$

where $\boldsymbol{K}(k)$ denotes the complete elliptic integral of the first kind with modulus k, and nd is the Jacobi elliptic function. The result verifies the GMPT-type expansion without the p^2 term [13, 14] for the asymmetric N-state vertex model. We further derive a simple relation between $\hat{g}_1(h)$ and $\hat{g}_3(h)$ as follows. Since

$$\begin{aligned}
\frac{\mathrm{d}^2}{\mathrm{d}h^2}(\Xi(\varphi)) &= (\Xi''(\varphi)(b_h)^2 - \Xi'(\varphi) b_{hh}) \\
&= \left[\Xi''(\varphi) + \frac{R_b(\pi, b)}{R^{(0)}(\pi, b)} \Xi'(\varphi)\right] (b_h)^2
\end{aligned} \tag{27}$$

with

$$b_h = -\frac{\beta}{R^{(0)}(\pi, b)} \tag{28}$$

we obtain

$$\hat{g}_3(h) = -\frac{\pi^2}{\beta^2} \cdot \hat{g}_1''(h). \tag{29}$$

We find, as for the expansion up to the third order, that the results (24) and (29) are N-independent and are given in [9]. This is understood from the fact that the N-state vertex model is a special case of the 'Z-invariant' inhomogeneous six vertex model with suitable boundary conditions [2, 8]. The present calculation shows that this property holds when an arbitrary electric field is present.

We carry out a further calculation of the expansion to obtain higher-order terms than the third one. In what follows in this section only we deal with the symmetric N-state model for simplicity. The Bethe ansatz integral equation is given in [8] and can be obtained by letting $b = 0$ (i.e. $h = 0$) in (13) (with $\phi_0 = -2\Delta u$). The free energy $\hat{g}(p, h)$ in (24) is now a function only of p (and u). A calculation up to the fifth order gives

$$\hat{g}_4 = \hat{g}_4(0) = -\frac{16\pi^2}{R^{(0)}(\pi)^3}\Phi(s)\Xi''(\lambda - 2\Delta u) \tag{30}$$

$$\hat{g}_5 = \hat{g}_5(0) = \frac{240\pi^2}{R^{(0)}(\pi)^4}\Phi^2(s)\Xi''(\lambda - 2\Delta u) + \left[\frac{\pi}{R^{(0)}(\pi)}\right]^4 \times \left[-\frac{4R^{(0)''}(\pi)}{R^{(0)}(\pi)}\Xi''(\lambda - 2\Delta u) + \Xi^{(4)}(\lambda - 2\Delta u)\right] \tag{31}$$

where the function $\Phi(s)$ is defined by

$$\Phi(s) = \sum_{n=1}^{\infty}\left(1 - \frac{\mathrm{e}^{2s\lambda n}}{2\sinh(2s\lambda n)}\tanh(\lambda n)\right). \tag{32}$$

We find that the p^4 term does not vanish, whereas the p^2 terms do. This distinguishes the model from the free fermion model. Recalling that the higher-order terms of the free energy reflect contributions due to the higher-order (high-energy) processes of the interaction between the multi-valued variables (multipoles) (or, steps in the TSK picture (see section 3)), the result shows that the difference between the N-state vertex model and the free fermion model appears in the forth and higher orders of the free energy. We also remark that $\hat{g}_4$ and $\hat{g}_5$ are definitely *s-dependent*, while the coefficients $\hat{g}_n$ for $n \leqslant 3$ are s-independent, as is shown in the analysis of the asymmetric model. We generally argue, from the derivation of our results, that $\hat{g}_n$ for even n is intrinsically s-dependent and that $\hat{g}_n$ for odd n consists of both the s-dependent and s-independent terms.

3. Vicinal-surface free energy for $T < T_R$

Below the roughening temperature T_R, the ECS consists of both facets (flat faces) and a rounded surface. Choose the Cartesian coordinates (X, Y, Z) with the Z-direction being facet normal and give the ECS at a temperature T by an equation $Z = Z(\vec{R}) = Z(X, Y)$. The surface free energy per projected (X, Y)-area is given by $f(\vec{p}) = \gamma(\vec{p})\sqrt{1 + \vec{p}^2}$, where $\gamma(\vec{p})$ is the surface tension, and $\vec{p}$ is the surface gradient vector: $\vec{p} = (p_X, p_Y) = (\partial Z/\partial X, \partial Z/\partial Y)$. Andreev [22] showed that the ECS is given by the equation

$$Z = \frac{1}{\lambda}\tilde{f}(-\lambda\vec{R}) \tag{33}$$

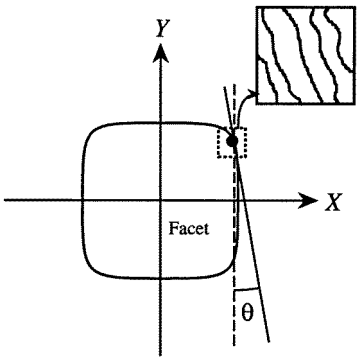

Figure 2. Top view of a facet. θ is the direction angle of the tangential line along the facet contour. 'Atomic scale' view of a vicinal surface as an assembly of wandering steps is also shown. The angle θ corresponds to the mean running direction of the steps.

where the the Legendre transformed free energy $\tilde{f}(\vec{\eta})$ is defined by

$$\tilde{f}(\vec{\eta}) = f(\vec{p}) - \vec{\eta} \cdot \vec{p} \tag{34}$$

with $\vec{\eta} = \partial f(\vec{p})/\partial \vec{p}$ the surface tilting 'field' conjugate to $\vec{p}$. (We consider the 'normalized' ECS when we set $\lambda = 1$.) Thus the calculation of the Andreev free energy $\tilde{f}(\vec{\eta})$ directly determines the ECS.

A rounded surface with small gradient near the facet edge is the vicinal surface. The vicinal surface is suitably described by the terrace–step-kink (TSK) picture where a surface is regarded to be composed of terraces (flat areas) connected by non-crossing steps (linear objects). Properties of the vicinal surface at temperatures $T < T_R$ is determined by the small-$|\vec{p}|$ behaviour of the free energy $f(\vec{p})$. For systems with short-range step–step interactions the GMPT-type expansion [13, 14] of the surface free energy (= step free energy in the TSK picture) has been known

$$f(\vec{p}) = f(0) + \gamma_s(\theta)|\vec{p}| + B(\theta)|\vec{p}|^3 + \mathrm{O}(|\vec{p}|^4) \tag{35}$$

where $\gamma_s(\theta)$ is the step tension. We take account the anisotropy of a crystal with the angle θ, defined by $\vec{p} = |\vec{p}|(-\cos\theta, -\sin\theta)$. The variable θ measures the angle between the Y-axis (crystal axis) and the mean running direction of steps, and is also the direction angle of the tangential line along the facet contour (figure 2). In association with the expansion (35), the universal relation between the coefficients $\gamma_s(\theta)$ and $B(\theta)$ is known in the coarse-grained TSK picture [19],

$$B(\theta) = \frac{\pi^2}{6\beta^2\tilde{\gamma}_s(\theta)} \tag{36}$$

where $\tilde{\gamma}_s(\theta) = \gamma_s(\theta) + \partial^2\gamma_s(\theta)/\partial\theta^2$ is the step stiffness. We will verify (35) and (36) by an exact calculation for a microscopic surface model associated with the N-state vertex model.

The solid-on-solid (SOS) model is a microscopic model for crystal surfaces, excluding overhangs and voids (the SOS condition). The shape of a surface is described by the heights at each site on the square lattice. As a generalization of [10], we can consider a certain SOS model which is exactly mapped onto the N-state vertex model [5]. The vertex model is defined on the dual lattice of that of the SOS model. The mapping is depicted in figure 3. In our case the $N(= 2s + 1)$ values of differences $\{-s, -s+1, \ldots, s-1, s\}$ are allowed between the nearest-neighbour heights (integers or half-odd integers, depending on N) of the surface. The vertical and horizontal polarizations (p, q), and the vertical and horizontal electric fields (v, h) of the vertex model correspond to the surface gradients (p_X, p_Y) and to the surface tilting 'fields' (η_X, η_Y) of the SOS model, respectively. Then, knowledge of the free energy as a function v

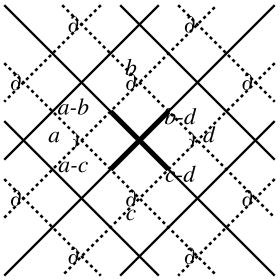

Figure 3. Correspondence between the vertex model (solid lines) and the SOS model (dotted lines). A single vertex is indicated by the thick line. The Boltzmann weight $W(a, b, c, d)$ for a (local) hight configuration $\{a, b, c, d\}$ in the SOS model is identified with the Boltzmann weight $X_{a-c\ c-d}^{a-b\ b-d}(u)$ of the corresponding vertex configuration as $W(a, b, c, d) = X_{a-c\ c-d}^{a-b\ b-d}(u)$.

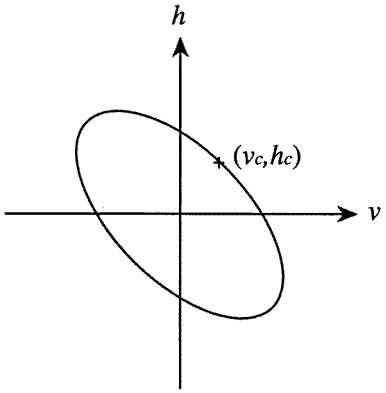

Figure 4. Example of facet contour (v_c, h_c) in the (v, h)-plane. Inside the contour the free energy is constant as a function of fields (facet is formed).

and h enables us to determine the ECS via (33). We rewrite (24) as

$$-\beta\hat{f}(p,h) \equiv \hat{g}(p,h) = \hat{g}(0,h) + \hat{\gamma}(h)p + \hat{B}(h)p^3 + \mathrm{O}(p^4). \tag{37}$$

In what follows we perform our explicit calculations on the free energy $\hat{f}(p, h)$, or $\hat{g}(p, h)$, instead of the Andreev free energy $\tilde{g}(v, h)$, which is given by the Legendre transformation

$$\tilde{g}(v,h) = \hat{g}(p,h) - vp \tag{38}$$

where

$$v = \left.\frac{\partial\hat{g}(p,h)}{\partial p}\right|_h \tag{39}$$

which describes the ECS. Hence the calculation of the field-dependent free energy $\hat{g}(p, h)$ leads to the ECS at any point on a crystal surface. It then follows that the h-dependent free energy $\hat{f}(p, h)$ is equivalent to the θ-dependent free energy (35). For $p = 0$, in fact, equation (39) reads

$$v_c = \hat{\gamma}(h_c). \tag{40}$$

This is the equation which determine the (2D) facet contour (v_c, h_c) from the field-dependent (one-dimension) surface tension $\hat{\gamma}(h)$ [26]. An example of facet contour in the (v, h)-plane is given in figure 4. The parametric equation $(v_c(b), h_c(b))$ is identical with that in the six vertex model case and is given in [4, 7].

The relation between the coefficients (29) now reads

$$\hat{B}(\tilde{h}) = -\frac{\pi^2}{6\beta^2}\cdot\hat{\gamma}''(h) \tag{41}$$

which is equivalent to (36) and is crucial in verifying the universal properties.

The 'normalized' Gaussian curvature [25], a product of two principal curvatures $K_X \approx \partial^2 Z/\partial X^2$ and $K_Y \approx \partial^2 Z/\partial Y^2$, is now calculated to be [9]

$$\hat{K} = -\left\{1 + p^2 + \left(\frac{\partial\hat{f}(p,h)}{\partial h}\right)^2\right\}^{-2}\left(\frac{\partial^2\hat{f}(p,h)}{\partial h^2}\Big/\frac{\partial^2\hat{f}(p,h)}{\partial p^2}\right)\Bigg|_{\hat{Z}=\hat{f}(-v,-h)} \tag{42}$$

in terms of $\hat{f}(p,h)$. Substituting (37) into (42) and taking the limit $p \to 0$, we obtain the limiting value of K approached from the curved region,

$$\hat{K} = -\frac{\hat{\gamma}''(h)}{6\hat{B}(h)}. \tag{43}$$

From (41) and (43) we conclude that the Gaussian curvature takes the values,

$$\hat{K} = \begin{cases} (\beta/\pi)^2 & \text{at the facet edge} \\ 0 & \text{on a facet} \end{cases} \tag{44}$$

irrespective of the field. We have then verified the universal Gaussian curvature jump $\sqrt{\Delta\hat{K}}/\beta = 1/\pi$ [19,20] *at any point* on the facet edge for our generalized SOS model.

The rounding off of a crystal facet is governed by the critical exponent with respect to displacement $(\Delta v, \Delta h)$ from the facet edge (v_c, h_c). The well known universal exponent $\frac{3}{2}$ of the ECS near the facet edge is shown for the BCSOS model in a 'normal' direction (perpendicular to the facet contour), or $h = 0$ direction as [6,11]

$$\hat{g}(v_c + \Delta v, h_c) - \hat{g}(v_c, h_c) \sim (\Delta v)^{3/2}. \tag{45}$$

This exponent has been confirmed experimentally [17]. Recently, it is shown that in the tangential direction along the facet contour a different critical exponent 3 dominates instead of $\frac{3}{2}$ [16,18].

As the vicinal-surface free energy for $T < T_R$ is already obtained, the calculation of critical exponents is straightforward. We derive the values of universal critical exponents as well as the critical amplitudes of the ECS profiles near the facet edge *at any position* of the facet edge and *in all direction* as follows.

Expanding (39) with respect to Δh and p ($\Delta h \ll 1$ and $p \ll 1$) gives

$$\begin{aligned} v &= v_c + \Delta v \\ &= \hat{\gamma}(h_c) + \hat{\gamma}'(h_c)\Delta h + \tfrac{1}{2}\hat{\gamma}''(h_c)(\Delta h)^2 + 3\hat{B}(h_c)p^2. \end{aligned} \tag{46}$$

The deviation of the free energy $\Delta\hat{g}(v,h) \equiv \hat{g}(v_c + \Delta v, h_c + \Delta h) - \hat{g}(v_c, h_c)$ is expanded to be

$$\begin{aligned} \Delta\hat{g}(v,h) &= -(v_c + \Delta v)p + (\hat{\gamma}(h_c) + \hat{\gamma}'(h_c)\Delta h + \tfrac{1}{2}\hat{\gamma}''(h_c)(\Delta h)^2)p + \hat{B}(h_c)p^3 \\ &= (-\Delta v + \hat{\gamma}'(h_c)\Delta h + \tfrac{1}{2}\hat{\gamma}''(h_c)(\Delta h)^2)p + \hat{B}(h_c)p^3. \end{aligned} \tag{47}$$

In a general direction of displacement $(\Delta v, \Delta h)$ away from the facet edge (v_c, h_c), we have from (46) (neglecting the $(\Delta h)^2$ term)

$$p = \frac{1}{\sqrt{3\hat{B}(h_c)}}(\Delta v - \hat{\gamma}'(h_c)\Delta h)^{1/2} \tag{48}$$

giving, from (47),

$$\begin{aligned} \Delta\hat{g}(v,h) &= -\frac{2}{3\sqrt{\hat{B}(h_c)}}(\Delta v - \hat{\gamma}'(h_c)\Delta h)^{3/2} \\ &\equiv A_n(h_c)(\Delta v - \hat{\gamma}'(h_c)\Delta h)^{3/2} \end{aligned} \tag{49}$$

with the well known exponent $\frac{3}{2}$ for a 'normal' profile.

On the tangential line: $\Delta v = \hat{\gamma}'(h_c)\Delta h$ ('tangential' means that $\partial v/\partial h = \hat{\gamma}'(h_c)$ at the facet edge, which is read off from (39)), (49) vanish and the rounding has a different critical exponent. In this case (46) gives

$$p = \sqrt{-\frac{\hat{\gamma}''(h_c)}{6\hat{B}(h_c)}} \cdot \Delta h \tag{50}$$

for which (47) results in

$$\Delta\hat{g}(v,h) = \frac{\hat{\gamma}''(h_c)}{3}\sqrt{-\frac{\hat{\gamma}''(h_c)}{6\hat{B}(h_c)}}(\Delta h)^3 \equiv A_t(h_c)(\Delta h)^3 \tag{51}$$

with the exponent 3 for the 'tangential' profile. These shows that the critical exponents which govern the rounding of the facet are obtained at any position of the facet edge and in all direction. We have, in addition, a universal relation between the critical amplitudes $A_n(h_c)$ and $A_t(h_c)$ of the ECS profiles near the facet edge. From (49) and (51) with the help of (41) we have

$$[A_n^2(h_c)A_t(h_c)]^{1/3} = \frac{2\beta}{3\pi} \tag{52}$$

which is constant along the facet contour, in connection with the Gaussian curvature jump (44). We should note that the results obtained here are direct consequences of the GMPT-type expansion of the vicinal-surface free energy for $T < T_R$ and are thus universal [16].

4. Summary

We have obtained the exact expansion with respect to small polarization p of the electric-field-dependent free energy of the asymmetric N-state vertex model (in an arbitrary vertical electric field v and an arbitrary horizontal electric field h) in the low-temperature antiferroelectric phase. As a generalization of the work of van Beijeren on the six-vertex model, we have mapped the vertex model onto a microscopic surface model (SOS model) to study exactly the vicinal-surface free energy below the roughening temperature which governs properties of the ECS near the facet edge of a crystal.

We have obtained the expansion of the well-established GMPT type: $f(p,h) = f(0,h)+a(h)p+b(h)p^3+\mathrm{O}(p^4)$, where the coefficients $a(h)$ and $b(h)$ are identical with those of the asymmetric six vertex model. The field-dependent free energy directly gives the ECS via the Andreev construction. We have verified, based on the obtained expansion of the free energy, universal properties *along the whole facet contour*. First, directly from the GMPT-type expansion, we have obtained the critical exponents which govern the rounding off of the crystal facet; the well known exponent $\frac{3}{2}$ dominates in all direction *except* the tangential one in which case the exponent 3 is dominating. Second, we have verified the universal relation between the coefficients $a(h)$ and $b(h)$ which leads to the universal Gaussian curvature jump and the universal relation between the critical amplitudes of the ECS profiles near the facet edge.

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