Universal Quantization of Curvature Jump at the Roughening Transition

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For a sequence of solvable solid-on-solid models, an exact analysis of the faceting transition is performed. It is shown that the curvature of the equilibrium crystal shape jumps at the roughening temperature with an amplitude given by an integer (≥ 1) multiple of the universal value predicted by Jayaprakash, Saam, and Teitel. An interpretation of this phenomenon, *universal quantization of curvature jump*, is presented from the viewpoint of the non-Abelian bosonization theory.

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The roughening transition of two-dimensional interfaces has attracted much attention.[1] For theoretical analyses, a class of lattice models called *solid-on-solid* (SOS) models has been introduced. The solid-on-solid approximation, which neglects bubbles in the bulk and overhangs of the interface, has been justified from the fact that the roughening temperature T_R is well below the bulk melting temperature. It has been believed that any SOS model belongs to the Kosterlitz-Thouless (KT) universality class[2] which consists of U(1) models [models with U(1) symmetry] such as the XY-spin model and the Coulomb gas. This SOS-U(1) equivalence implies the following: (1) The free energy of the SOS models should show the essential singularity at T_R; (2) in the high-temperature phase or the rough phase, the height-height correlation function $\mathcal{G}(\mathbf{R})\equiv\langle(h_i-h_j)^2\rangle$ (h_i denotes interface height; $\mathbf{R}=\mathbf{i}-\mathbf{j}$) behaves as $\mathcal{G}(\mathbf{R}) \sim A(T)\ln|\mathbf{R}|$ as $|\mathbf{R}|\to\infty$, where the amplitude $A(T)$ takes a universal value $A(T_R)=2/\pi^2$ at T_R [the $\ln|\mathbf{R}|$ divergence of $\mathcal{G}(\mathbf{R})$ corresponds to the algebraic decay of the spin-spin correlation of the U(1) models in the low-temperature phase, and the value $2/\pi^2$ to the universal decay exponent $\eta=\frac{1}{4}$ at the transition temperature $T_{\rm KT}$].

The SOS-U(1) equivalence has been confirmed in several ways. For example, the duality transformations map the partition functions of the SOS models to those of the Coulomb gas[3] or XY-type–spin models.[4] Monte Carlo calculations of the interface width[5] and the height-height correlation function[6] also support the equivalence. The most convincing one is provided by van Beijeren's body-centered-cubic SOS (BCSOS) model,[7] which allows exact analyses. The model, which is equivalent to the F-model case of the six-vertex model,[8] shows the essential singularity at the roughening temperature T_R. The height-height correlation function $\mathcal{G}(\mathbf{R})$ at a special temperature in the rough phase has been explicitly calculated[9] to verify the $\ln|\mathbf{R}|$ divergence of $\mathcal{G}(\mathbf{R})$. Although an exact calculation of $\mathcal{G}(\mathbf{R})$ of the BCSOS model at general T has not been performed yet, the exact value of the amplitude $A(T)$ can be drawn from the calculation of the surface stiffness or the curvature κ of the equilibrium crystal shape (ECS) made by Jayaprakash, Saam, and Teitel.[10] In particular, the universal jump of the ECS curvature $\Delta\kappa=2/\pi k_BT_R$ at the faceting transition, which was explicitly verified for the BCSOS model, confirms the amplitude $A(T_R)=2/\pi^2$. This curvature jump has also been observed experimentally.[11] All the existing evidence seems to support the SOS-U(1) equivalence.

Have we seen a happy end of a story? The answer is *no*. In this Letter, we show that there exists a sequence of SOS models which are *not* in the KT universality class. As a result, what we should expect for general interface models is not a single "universal" value of $\Delta\kappa$, but *universal quantization* of $\Delta\kappa$ with the quantization unit given by the value of Jayaprakash, Saam, and Teitel.

We analyze here a series of multistate vertex models and their equivalent SOS models proposed by Sogo, Akutsu, and Abe (SAA).[12] The $(\mathcal{N}+1)$-state vertex model ($\mathcal{N}$ is an integer ≥ 1) in the series is the one where each edge variable takes one of $\mathcal{N}+1$ states $\{-\mathcal{N}/2,-\mathcal{N}/2+1,\ldots,\mathcal{N}/2\}$. We write the Boltzmann weight for a vertex configuration $(ijkl)$ by $w(ij|kl)$. The model is then characterized by the "charge-conservation" condition: $w(ij|kl)=0$ unless $i+j=k+l$. Under this condition, the number of nonzero vertex weights is $(\mathcal{N}+1)[2(\mathcal{N}+1)^2+1]/3$. For example, cases with $\mathcal{N}=1$, $\mathcal{N}=2$, and $\mathcal{N}=3$ correspond to the 6-vertex, 19-vertex (Ref. 13) (see Fig. 1), and 44-vertex models,[12] respectively. The Boltzmann weights $\{w(ij|kl)\}$

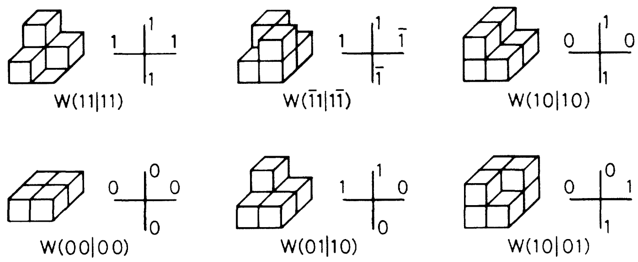

FIG. 1. Mapping between configurations of local heights and those of vertex for $\mathcal{N}=2$ (19-vertex model). Among 19 possible configurations, only representative ones are shown. For $u=\lambda/2$, the Boltzmann weights are given by $w(11\,|\,11) = \rho_0 \sin(\lambda/2)\sin(3\lambda/2)$, $w(\bar{1}1\,|\,1\bar{1}) = \rho_0 \sin\lambda \sin(2\lambda)$, $w(10\,|\,10) = \rho_0 \sin^2(\lambda/2)$, $w(00\,|\,00) = \rho_0[\sin\lambda\sin(2\lambda) - \sin^2(\lambda/2)]$, and $w(01\,|\,10) = w(10\,|\,01) = \rho_0 \sin(\lambda/2)\sin(2\lambda)$ (ρ_0 is an arbitrary normalization factor). Other weights, which correspond to $\pm 90°$- and $180°$-rotated configurations of the ones shown in the figure, are given through the *CPT* invariances, $w(ij\,|\,kl) = w(\bar{i}\bar{j}\,|\,\bar{k}\bar{l}) = w(ji\,|\,lk) = w(kl\,|\,ij)$, and the crossing symmetry, $w(ij\,|\,kl) = w(j\bar{k}\,|\,l\bar{i})$.

are parametrized in terms of the spectral parameter u so that they satisfy the Yang-Baxter relation to ensure the solvability. In terms of an auxiliary parameter λ which appears in the actual parametrization, the "crossing symmetry" is expressed as $w(ij\,|\,kl;u) = w(j\bar{k}\,|\,l\bar{i};\lambda - u)$ ($\bar{i} = -i$). Physically, u represents the anisotropy, and λ gives a temperature scale such that the roughening temperature corresponds to $\lambda = 0$. The crossing symmetry is related to a 90° rotation of the lattice. Explicit parametrization has been given recursively[12] or by the fusion procedure.[14]

Mapping of the vertex model into the SOS model has been made by a generalization of van Beijeren's mapping, called the generalized Wu-Kadanoff-Wegner tranformation.[12] In the SOS model mapped from the $(\mathcal{N}+1)$-state vertex model, the nearest-neighbor height difference can take one of the following $\mathcal{N}+1$ integer values:

$$h_i - h_j = -\mathcal{N}/2, -\mathcal{N}/2+1, \ldots, \mathcal{N}/2\,. \tag{1}$$

We simply call the SOS model the $(\mathcal{N}+1)$-state SOS model. Since the Boltzmann weights are assigned not to each bond but to each face, the Hamiltonian of the model is not of the nearest-neighbor pair-interaction type. The Hamiltonian contains next-nearest-neighbor interactions and four-body interactions[15] which invalidate the duality transformation; the argument for the U(1)-SOS equivalence based on the duality transformation does not hold for the present SOS model. The vertical polarization ρ_x and the horizontal polarization ρ_y of the vertex model relate to the surface gradient $\boldsymbol{\rho} = (\rho_x, \rho_y)$ of the SOS model. In an SOS model, it is natural to expect a symmetry with respect to the 90° rotation of the height configurations. The crossing symmetry assures this rotation symmetry if we put $u=\lambda/2$. The free energy for $\boldsymbol{\rho}=0$ has been calculated[12] to show the essential singularity at $\lambda = 0$.[16]

To obtain the surface stiffness or the ECS curvature, we should calculate the per-site free energy with fixed surface gradient $\boldsymbol{\rho}$, denoted by $f(\boldsymbol{\rho})$, or its Legendre transform $\tilde{f}(\boldsymbol{\eta}) = \min_{\boldsymbol{\rho}}\{f(\boldsymbol{\rho}) - \boldsymbol{\eta}\cdot\boldsymbol{\rho}\}$. From Andreev's reformulation[17] of the Wulff construction, the ECS $z=z(x,y)$ (x,y,z are Cartesian coordinates) is given by

$$vz(x,y) = \tilde{f}(-vx, -vy)\,, \tag{2}$$

where v stands for a Lagrange multiplier necessary to fix the crystal volume. In what follows we consider the *normalized* ECS with $v=1$. For $\mathbf{x}\approx 0$ ($\boldsymbol{\rho}\approx 0$), we can calculate the curvature tensor κ_{ij} $[=(\partial^2 z/\partial x_i\,\partial x_j)_{\mathbf{x}=0},\ x_{1,2}=x,y]$ as the inverse of the stiffness matrix $f^{(2)}$:

$$f^{(2)}_{ij} = \left[\frac{\partial^2 f(\boldsymbol{\rho})}{\partial\rho_i\,\partial\rho_j}\right]_{\boldsymbol{\rho}=0} \quad (\rho_{1,2} = \rho_x, \rho_y)\,, \qquad \kappa_{ij} = [f^{(2)-1}]_{ij}\,. \tag{3}$$

We calculated $f(\boldsymbol{\rho})$ via the (algebraic) Bethe *Ansatz* method for the model.[18] In the low-temperature phase,[19] $f(\boldsymbol{\rho})$ has the Gruber-Mullins-Pokrovsky-Talapov-type expansion:

$$f(\boldsymbol{\rho}) = f(0) + \gamma_s\,|\boldsymbol{\rho}| + B\,|\boldsymbol{\rho}|^3 + \text{higher-order terms}\,. \tag{4}$$

The coefficients γ_s and B are $\mathcal{N}$ independent;[19] hence, they are given by those of the BCSOS model.[8,10] The form (4) confirms the existence of a facet, a region where $\kappa_{ij}\equiv 0$, around the origin $(x,y)=(0,0)$ in the low-temperature phase of the $(\mathcal{N}+1)$-state SOS model. As $T\to T_R - 0$, the step tension γ_s (>0 for $T<T_R$) vanishes and the facet area shrinks to zero.

In the high-temperature phase or the rough phase, we obtain

$$f(\boldsymbol{\rho}) = f(0) + k_B T \frac{\pi - \mathcal{N}\lambda}{4\mathcal{N}} \sin\left(\frac{u\pi}{\lambda}\right) |\boldsymbol{\rho}|^2 + \text{higher-order terms}\,. \tag{5}$$

To be precise, in (5) [also in (4)] we have calculated only the case $\boldsymbol{\rho} = (\rho_x, 0)$. We believe, however, that (5) holds for general $\boldsymbol{\rho}$ due to the isotropy in the rough phase and also to the invariance of (5) under the crossing transformation $u\to\lambda - u$. Putting $u=\lambda/2$ (isotropic limit) and making $T\to T_R + 0$ ($\lambda\to +0$) in (5), we obtain, via (3), the curvature jump at T_R:

$$\Delta\kappa = 2\mathcal{N}/\pi k_B T_R\,. \tag{6}$$

Remarkably, this is precisely $\mathcal{N}$ times the value of Jayaprakash, Saam, and Teitel (the $\mathcal{N}=1$ case). We have thus shown the existence of an infinite series of SOS models labeled by an integer (≥ 2) which *does not* belong to the KT [or U(1)] universality class. An intriguing conjecture which naturally arises is that the sequence of universality classes represented by the multistate SOS models should exhaust all the SOS models, predicting that the curvature jump is *universally quantized* in the units of $2/\pi k_B T_R$.

To give an interpretation of the curvature-jump quantization, let us consider the models in the critical limit ($\lambda \to +0$) to which the non-Abelian bosonization theory[20] is applicable. The curvature jump (6) implies, through the capillary-wave theory,[21] the following asymptotic form of the height-height correlation function

$$\mathcal{G}(x'-x,y'-y) = \langle [h(x',y') - h(x,y)]^2 \rangle$$

at $T \approx T_R$:

$$\mathcal{G}(x,y) = \frac{2\mathcal{N}}{\pi^2} \ln(x^2+y^2)^{1/2} . \qquad (7)$$

To calculate $\mathcal{G}(x,y)$, we work on an equivalent spin-chain, spin-$\mathcal{N}/2$ massless Heisenberg-like model, whose Hamiltonian $\mathcal{H}$ is given from the transfer matrix of the $(\mathcal{N}+1)$-state vertex model $\mathcal{T}(u)$ through Baxter's formula, $\mathcal{H} = -[d \ln \mathcal{T}(u)/du]_{u=0}$.[22] We use the representation of spin operators in terms of fermion operators with $\mathcal{N}$ colors:[20]

$$\sum_{i,f,g} S^a = (\psi^\dagger)^{if} (\sigma^a)_g^f \psi_{ig} , \qquad (8)$$

where σ^a ($a = x,y,z$) is the Pauli matrix, $i \in \{1, \ldots, \mathcal{N}\}$, and $f,g \in \{\text{up,down}\}$. An antiferromagneticlike structure of the ground state [which gives the maximum eigenvalue of $\mathcal{T}(u)$] requires the fermion system to be half filled. In terms of the spin-spin correlation function $\mathcal{G}_s^{\alpha\beta}(\zeta,\zeta') = \langle S^\alpha(\zeta) S^\beta(\zeta') \rangle$, $\mathcal{G}(x,0)$ is expressed as

$$\mathcal{G}(x'-x,0) = 4 \sum_{\zeta=x}^{x'} \sum_{\zeta'=x}^{x'} \mathcal{G}_s^{zz}(\zeta,\zeta') . \qquad (9)$$

Since relevant excitations are those near the Fermi surface, we can decompose the fermion field into a right one (ψ_R) and a left one (ψ_L):

$$\psi = e^{-ik_F x} \psi_L + e^{ik_F x} \psi_R . \qquad (10)$$

The resulting model possesses three kinds of conserved currents J ($\bar{J}$), $\{J^a\}$ ($\{\bar{J}^a\}$), and $\{J^A\}$ ($\{\bar{J}^A\}$), which are associated with U(1), SU(2), and SU($\mathcal{N}$) symmetry, respectively. Expression (8) is then rewritten as

$$S^a(x) = J^a(x) + \bar{J}^a(x) + (-1)^x G^a(x) , \qquad (11)$$

where

$$G^a(x) = \sum_i \psi_L^{\dagger i}(x) \sigma^a \psi_{Ri}(x) + L \leftrightarrow R$$

denotes the mass operator. Accordingly, $\mathcal{G}_s^{\alpha\beta}$ is given by J^α-J^β, J^α-G, and G-G correlation functions. Through the non-Abelian bosonization,[20] we have three bosonic fields. The ground-state spin structure freezes two of these fields. The remaining field denoted by g is that of the SU(2) level-$\mathcal{N}$ Wess-Zumino-Witten (WZW) model,[23] which was shown[20] on the basis of the renormalization-group argument; the mass operator is essentially given by $G^a = \text{tr}[(g - g^\dagger)\sigma^a]$. Working with the WZW field, the G-G correlation is easily evaluated[20] to give a term $\sim (-1)^{\zeta-\zeta'}/(\zeta-\zeta')^\Delta$ with $\Delta = 3/(2+\mathcal{N})$. The oscillatory behavior implies that it originates from the antiferromagnetic part of the fluctuation, and hence the term does not contribute to $\mathcal{G}$; only the ferromagnetic part of the fluctuation contributes to $\mathcal{G}$.[9] Recalling that the WZW model possesses a symmetry with respect to the change $g \to -g$, we see that the J^α-G correlations vanish identically. The remaining J^α-J^β correlations can be evaluated from the current algebra:[20,23]

$$\mathcal{G}_s^{\alpha\beta}(\zeta,\zeta') = \langle J^\alpha(\zeta) J^\beta(\zeta') \rangle + \langle \bar{J}^\alpha(\zeta) \bar{J}^\beta(\zeta') \rangle$$
$$= \frac{\delta_{\alpha\beta}\mathcal{N}}{4\pi^2} \frac{1}{(\zeta-\zeta')^2} . \qquad (12)$$

Inserting (12) with $\alpha = \beta = z$ into (9), we obtain (7) (for $y = 0$) confirming (6).

As was discussed by Zamolodchikov and Fateev,[24] the current in the WZW model can be written in terms of a U(1) field plus $Z_\mathcal{N}$ parafermion fields. This means that the SAA model in its gapless regime possesses $Z_\mathcal{N}$ symmetry in addition to the basic U(1) symmetry. This additional $Z_\mathcal{N}$ symmetry is the source of the $\mathcal{N}$-dependent curvature jump. The $Z_\mathcal{N}$ symmetry of the model has been partly verified by numerical calculation[25] on the spin-$\mathcal{N}/2$ chain, and by explicit construction[26] of the modular-invariant partition function for $\mathcal{N} = 2$.

We have thus demonstrated the breakdown of the SOS-U(1) equivalence; the $\mathcal{N}$-state SOS model for general $\mathcal{N}$ does not belong to the KT [U(1)] universality class but represents its own universality class. The curvature jump at T_R, or equivalently, the prelogarithm factor of the height-height correlation function at T_R is $\mathcal{N}$ times the U(1) value. Naturally, one may expect a similar $\mathcal{N}$ dependence also in the low-temperature phase. In fact, the interface width shows a nontrivial $\mathcal{N}$ dependence,[27] while the correlation length and the step tension do not depend on $\mathcal{N}$.[27] The Gaussian curvature jump[28] at the facet edge does not depend on $\mathcal{N}$ either,[19] which sharply contrasts with the curvature jump at T_R. A detailed account of this Letter, including a derivation of (5), will be published elsewhere.

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[15]For example, a Hamiltonian corresponding to vertex weights ($\mathcal{N}=2$, $u=\lambda/2$) defined by $w(i,j\,|\,k,l)=\exp[-\mathcal{H}(i,j\,|\,k,l)/k_BT]$ is given as follows:

$$\frac{\mathcal{H}(i,j\,|\,k,l)}{k_BT}=K_1(ik+jl)+K_2[(ij)^2+(jk)^2+(kl)^2+(li)^2]+K_3[(ik)^2+(jl)^2]+K_4ijkl\,.$$

The coupling constants K_1-K_4 stand for $K_1=\frac{1}{4}\ln([\lambda][2\lambda]/[\lambda/2][3\lambda/2])>0$, $K_2=\ln(\rho/[2\lambda][\lambda/2])>0$, $K_3=\ln(\rho/[\lambda/2]^2)-K_1>0$, and $K_4=\ln([\lambda/2]^7[2\lambda]^4/\rho^5[3\lambda/2])<0$, where $[x]=\sin(x)$ and $\rho=[\lambda][2\lambda]-[\lambda/2]^2$. The appearance of terms proportional to K_2 and K_3 is a novel feature of the 19-vertex ($\mathcal{N}=2$) model. Around a vertex, four height variables are assigned to dual sites. We number them, starting from the lower-left sites, in an counterclockwise direction, as (h_1,h_2,h_3,h_4). Apparently they are related to arrow variables by $i=h_2-h_1$, $j=h_1-h_4$, $k=h_3-h_4$, $l=h_2-h_3$. To get a feeling, we may replace $i,k\rightarrow a\,\partial_xh(x)$, $j,l\rightarrow -a\,\partial_yh(x)$ in the "continuum limit" (a signifies lattice spacing). In this limit, $\mathcal{H}$ can be written in the following form:

$$\mathcal{H}/k_BT=\tilde{K}_1[(\partial_xh)^2+(\partial_yh)^2]+[4\tilde{K}_2+\tilde{K}_4(\partial_xh\,\partial_yh)^2]+\tilde{K}_3[(\partial_xh)^4+(\partial_yh)^4]\,.$$

One should note, however, that the restrictions on height configurations in the original vertex model become obscure in this representation.

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