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Hard-Hexagon Model: Anisotropy of Correlation Length and Interfacial Tension

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The directional dependence of the correlation length of the hard-hexagon model is calculated by a new method which introduces the shift operator into the usual transfer matrix method. This method is also applied to the calculation of the interfacial tension of the hard-hexagon model, which is anisotropic. In addition, the equilibrium droplet shape of one phase embedded inside another is obtained from the analysis of the interfacial tension by the use of Wulff's construction.

KEY WORDS: Hard-hexagon model; correlation length; interfacial tension; equilibrium shape.

1. INTRODUCTION

The hard-hexagon model is a model of particles placed on the site of a triangular lattice in such a way that no two particles occupy the same site or adjacent ones.[1] Due to this constraint, one particle excludes other particles from the hexagonal region around it (Fig. 1). Hence this model is called the hard-hexagon model. Because the hard-hexagon model does not have an interaction energy, we can determine its thermal equilibrium state for a given value of one-particle activity z. As z increases, this model undergoes a phase transition from a homogeneous phase to an inhomogeneous one, where densities of three sublattices ρ_A, ρ_B, ρ_C are not equal to each other.

In 1980 Baxter[1,2] exactly calculated the free energy of this model and the order parameter, which is the difference between the sublattice densities. According to Baxter's exact calculation, the critical activity is

$$z_c = (11 + 5\sqrt{5})/2 \sim 11.09 \tag{1.1}$$

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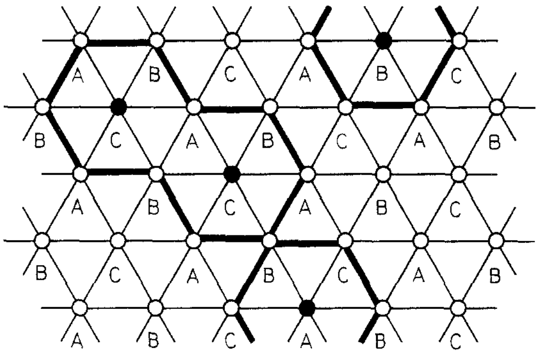


Fig. 1. A typical configuration of the hard-hexagon model. Occupied sites are denoted by solid circles and unoccupied sites are denoted by open circles.

and the critical exponents are

$$\alpha = \alpha' = 1/3 \tag{1.2}$$

$$\beta = 1/9 \tag{1.3}$$

Later, in 1982 Baxter and Pearce[3] also analyzed the correlation length and the interfacial tension using the transfer matrix method, where they determined other critical exponents,

$$\nu = \nu' = 5/6, \qquad \mu = 5/6 \tag{1.4}$$

We note here that this analysis assumed a specific orientation of the line connecting two particles. We generally expect that the correlation length and the interfacial tension are anisotropic. It is difficult, however, to find the anisotropy using the usual transfer matrix method.

Recently the interface and crystal shape problem has attracted much attention.[4–7] This revival is due to the roughening transition phenomena. The analysis of the anisotropic interfacial tension is very important there. For example, from its anisotropy we can find the equilibrium droplet shape of one phase embedded inside another, using Wulff's construction. Moreover, the disappearance of facets in the equilibrium crystal shape is an indication of the roughening transition.[8,9]

This paper has two purposes. First, using the shift operator, we extend the analysis by Baxter and Pearce to find the anisotropy of the correlation length and the interfacial tension of the hard-hexagon model. Second, the equilibrium shape of the hard-hexagon crystal is derived from the anisotropy of the interfacial tension by the use of Wulff's construction.

The outline of this paper is as follows. In Section 2 we deal with the disordered state of the hard-hexagon model. First, in Section 2.1 a new method to calculate the anisotropic correlation length is explained, and in Section 2.2 we use this method to extend the analysis of the correlation length of the hard-hexagon model by Baxter and Pearce. In Section 3 the ordered state of this model is considered. In Sections 3.1 and 3.2 we calculate the anisotropic interfacial tension by the use of a similar technique to that given in Section 2.1. The result of this calculation is used to derive the equilibrium shape of the hard-hexagon crystal in Section 3.3. In Section 3.4 we analyze the correlation length in the ordered state. Section 4 is devoted to a summary and discussion.

2. DISORDERED STATE

2.1. Correlation Length 1

We start by reviewing the usual analysis of the correlation length, where its anisotropy does not enter.[1,3] We assume the square lattice with M columns and N rows which is obtained by deforming the triangular lattice (Fig. 2a). We impose on it the cyclic boundary condition in both directions (the toroidal boundary condition). At each site labeled (i, j) there is an occupation number σ_{ij}, which takes 1 if the site (i, j) is occupied by a particle and 0 otherwise. To each face consisting of four lattice sites we assign a Boltzmann weight $W(a, b, c, d)$ if the occupation numbers around a face are a, b, c, d counterclockwise starting from the southwest corner (Fig. 2b).

Then two operators are introduced. One is the row–row transfer matrix $\mathbf{V} = \{V(\sigma_i, \sigma_j)\}$, which is defined as

$$V(\sigma_i, \sigma_{i+1}) = \prod_{j=1}^{M} W(\sigma_{ij+1}, \sigma_{ij}, \sigma_{i+1,j}, \sigma_{i+1,j+1}) \tag{2.1}$$

where the occupation numbers of the ith row $\{\sigma_{i1},..., \sigma_{iM}\}$ are represented by σ_i. We define also

$$S_k(\sigma_i, \sigma_{i+1}) = \sigma_{ik} \prod_{j=1}^{M} \delta(\sigma_{ij}, \sigma_{i+1,j}) \tag{2.2}$$

where $\delta(\sigma_{ij}, \sigma_{i+1,j})$ is the Kronecker delta. These operators can be used to represent the correlation between the site (0, 0) and the site (l, m),

$$\langle \sigma_{00}\sigma_{lm} \rangle = \frac{\mathrm{tr}[\mathbf{S}_0 \mathbf{V}^l \mathbf{S}_m \mathbf{V}^{N-l}]}{\mathrm{tr}[\mathbf{V}^N]} \qquad \text{for} \quad N > l > 0 \tag{2.3}$$

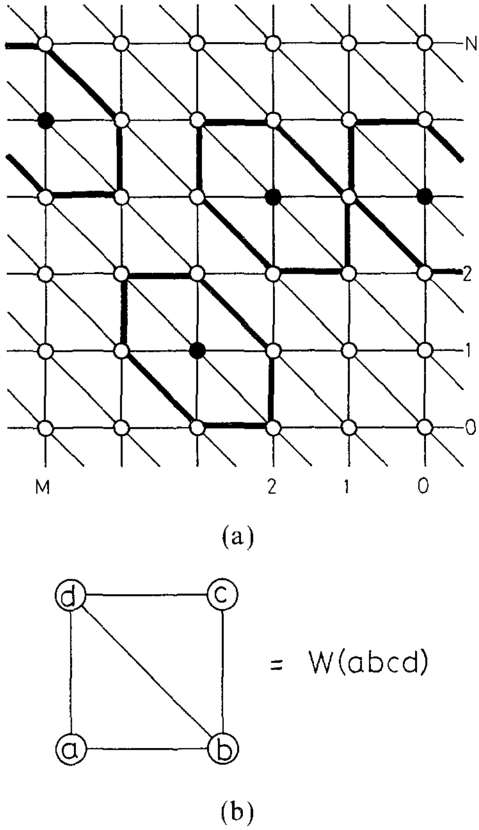


Fig. 2. (a) The deformed triangular lattice. (b) Boltzmann weight around a face.

(Since $\langle \sigma_{00}\sigma_{-l-m}\rangle = \langle \sigma_{00}\sigma_{lm}\rangle$, it is sufficient to consider the case of $l>0$.) Applying the similarity transformation which diagonalizes $\mathbf{V}$, and letting N, $M\to\infty$, we get

$$\langle \sigma_{00}\sigma_{lm}\rangle = \sum_p \tilde{S}_0(1, p)\,\tilde{S}_m(p, 1)\left[\frac{V(p)}{V(1)}\right]^l \qquad \text{for} \quad l>0 \tag{2.4}$$

where $\tilde{\mathbf{S}}_k$ is the matrix transformed from $\mathbf{S}_k$ by the matrix of eigenvectors of $\mathbf{V}$, and $V(p)$ is the pth eigenvalue of $\mathbf{V}$ in decreasing order of absolute value. For simplicity we assumed that

$$|V(1)| > V(p)| \qquad \text{for} \quad p\neq 1 \tag{2.5}$$

Since

$$\langle \sigma_{00}\rangle\langle \sigma_{lm}\rangle = \tilde{S}_0(1, 1)^2 = \tilde{S}_0(1, 1)\,\tilde{S}_m(1, 1) \tag{2.6}$$

the correlation function between the site (0, 0) and the site (l, m) is given by

$$\langle\sigma_{00}\sigma_{lm}\rangle - \langle\sigma_{00}\rangle\langle\sigma_{lm}\rangle = \sum_{p\neq 1} S_0(1, p)\, S_m(p, 1)\left[\frac{V(p)}{V(1)}\right]^l \qquad \text{for} \quad l>0 \tag{2.7}$$

When m is fixed and l becomes large, the rhs of (2.7) exponentially decays. Analyzing this decay rate, which can be calculated from the ratios between the largest and next-largest eigenvalues of **V**, we can find the correlation length ξ along the vertical axis. In the simplest case, for example, ξ can be represented as

$$-1/\xi = \ln[V(2)/V(1)] \tag{2.8}$$

This is the usual method.

Now we try to find the anisotropy. The behavior of the correlation function, when the ratio m to l is fixed and l becomes large, comes into question. We expect that it also decays exponentially, and the correlation length alqong the direction designated by the ratio m to l can be calculated from the rate of this decay. In the rhs of (2.7), however, this decay is determined by the matrix elements $\tilde{S}_0(1, p)\, \tilde{S}_m(p, 1)$, as well as the ratios between the eigenvalues. A difficulty arises here: the direct calculation of the matrix elements is very complex. Fortunately, it can be done without calculating the matrix elements. In the following we explain this.

Here we introduce the third operator, which is the shift operator **T** defined by

$$T(\sigma_i, \sigma_{i+1}) = \prod_{j=1}^{M} \delta(\sigma_{ij}, \sigma_{i+1, j-1}) \tag{2.9}$$

The shift operator connects $\mathbf{S}_m$ with $\mathbf{S}_0$ by the relation

$$\mathbf{S}_m = \mathbf{T}^m \mathbf{S}_0 \mathbf{T}^{-m} \tag{2.10}$$

The relation (2.10) can be used to rewrite (2.3) as

$$\langle\sigma_{00}\sigma_{lm}\rangle = \frac{\mathrm{tr}[\mathbf{S}_0 \mathbf{V}^l \mathbf{T}^m \mathbf{S}_0 \mathbf{T}^{-m} \mathbf{V}^{N-l}]}{\mathrm{tr}[\mathbf{V}^N]} \qquad \text{for} \quad N>l>0 \tag{2.11}$$

Noting that the transfer matrix can be diagonalized simultaneously with the shift operator due to the translational invariance of this system, we find in the $N, M \to \infty$ limit

$$\langle\sigma_{00}\sigma_{lm}\rangle - \langle\sigma_{00}\rangle\langle\sigma_{lm}\rangle = \sum_{p\neq 1} \tilde{S}_0(1, p)\, \tilde{S}_0(p, 1)\left[\frac{V(p)}{V(1)}\left(\frac{T(p)}{T(1)}\right)^v\right]^l \qquad \text{for} \quad l>0 \tag{2.12}$$

where $T(p)$ is the pth eigenvalue of **T**, and $v = m/l$.

Let v be fixed and l large. The rhs of (2.12) shows that the correlation function decays exponentially, and that the decay rate is determined by $[V(p)/V(1)][T(p)/T(1)]^v$. From the knowledge of the eigenvalues of **V** and the corresponding ones of **T**, we can find the correlation length along the direction designated by v.

A new problem arises: is the calculation of the eigenvalues of **T** practicable? We finish this section by mentioning that in the case of the hard-hexagon model it is a simple problem. In Baxter's method of calculating the eigenvalues of the transfer matrix, finding a series of models whose transfer matrices commute with each other, the commuting family, has an important meaning.(1,2) Then a functional equation holding among the eigenvalues of the commuting family is derived. Using this, we obtain the eigenvalues of all the commuting family. The shift operator is always a member of the commuting family, being simultaneously diagonalized with the others. In the case of the hard-hexagon model we can get the necessary information from the analysis by Baxter and Pearce.(3)

2.2. Correlation Length 2

Baxter and Pearce assumed the continuous distribution of the eigenvalues in (2.7), and calculated ξ along the vertical axis by the method of steepest descent. We introduce the shift operator into their analysis to find the anisotropy of ξ. When v is fixed and l is large, the correlation function is represented as

$$\langle \sigma_{00}\sigma_{lm}\rangle - \langle \sigma_{00}\rangle\langle \sigma_{lm}\rangle$$

$$\sim \frac{1}{2\pi i}\oint_{|a|=1} \frac{da}{a}\,\rho(a)[\phi(ax^{-2})\,\phi(a)^v]^l \qquad \text{for} \quad -\infty < v < \infty \tag{2.13a}$$

where

$$\phi(a) = -\frac{1}{a}\frac{f(ax, x^6)\,f(ax^2, x^6)}{f(a^{-1}x, x^6)\,f(a^{-1}x^2, x^6)} \tag{2.13b}$$

and

$$f(p, q) = (1-p)\prod_{n=1}^{\infty}(1-pq^n)(1-p^{-1}q^n)(1-q^n) \tag{2.13c}$$

The functions $\phi(ax^{-2})$ and $\phi(a)$ correspond to $V(p)/V(1)$ and $T(p)/T(1)$ in (2.12), respectively, and the summation in (2.12) becomes an integral along a unit circle due to the continuous distribution of the eigenvalues. The function $\rho(a)$ is to be determined from the distribution of the eigenvalues and the matrix elements $\tilde{S}_0(1, P)\,\tilde{S}_0(P, 1)$. Its explicit form is unknown. In this analysis it is sufficient to assume its analyticity. The parameter x is related to the one-particle activity z by

$$z = -x \prod_{n=1}^{\infty} \left[\frac{(1-x^{5n-4})(1-x^{5n-1})}{(1-x^{5n-3})(1-x^{5n-2})}\right]^5 \qquad \text{for} \quad -1 < x < 0 \qquad (2.14)$$

In the present analysis the triangular lattice is deformed into the square lattice. The parameter v is related to $\theta_{||}$, which is the argument of the site (l, m) on the triangular lattice, by the relation

$$v = \frac{1}{2} - \frac{\sqrt{3}}{2 \tan \theta_{||}} \qquad \text{for} \quad 0 < \theta_{||} < \pi \qquad (2.15)$$

We estimate the integral in the rhs of (2.13a) by the method of steepest descent. For example, when $\theta_{||} = \pi/3$ (this is the case of Baxter and Pearce), from the derivative of $\ln \phi(a)$,

$$\begin{aligned} \frac{d}{da} \ln \phi(a) & \\ &= -f(x^2, x^6)\, f(x^3, x^6) \\ &\quad \times \frac{1}{a} \frac{f(a^{-1}x^{3/2}, x^6)\, f(-a^{-1}x^{3/2}, x^6)\, f(ax^{3/2}, x^6)\, f(-ax^{3/2}, x^6)}{f(a^{-1}x, x^6)\, f(a^{-1}x^2, x^6)\, f(ax^2, x^6)\, f(ax, x^6)} \end{aligned} \qquad (2.16)$$

two saddle points of $|\phi(ax^{-2})|$ are found at $a = \pm x^{1/2}$. After the contour is deformed without crossing the singular points of the integrand, the integral can be estimated around these two saddle points. Since the contributions from these two saddle points are complex conjugate to each other, we get

$$\langle \sigma_{00} \sigma_{lm} \rangle - \langle \sigma_{00} \rangle \langle \sigma_{lm} \rangle \sim \alpha \exp(-l/\xi) \cos(l\eta + \delta) \qquad (2.17a)$$

$$-1/\xi = \ln |\phi(x^{1/2})| \qquad (2.17b)$$

$$\eta = \mathrm{Arg}[\phi(x^{1/2})] \qquad (2.17c)$$

where α and δ are to be determined from ρ and the second derivative of $\ln \phi(a)$ at $a = x^{1/2}$.

For $\theta_{||} \neq \pi/3$ the situation remains unchanged: two saddle points which are complex conjugate are found, and the rhs of (2.13a) can be estimated around them. The equation which determines the saddle points a_s is

$$\frac{d}{da} [\ln \phi(ax^{-2}) + v \ln \phi(a)]_{a = a_s} = 0 \qquad (2.18)$$

or from (2.15) and (2.16), after some calculations,

$$\frac{\sqrt{3}-\tan\theta_{||}}{\sqrt{3}+\tan\theta_{||}}=a\frac{f(ax,x^3)\,f(a^{-1}x^{1/2},x^3)\,f(-a^{-1}x^{1/2},x^3)}{f(a^{-1}x,x^3)\,f(ax^{1/2},x^3)\,f(-ax^{1/2},x^3)},\qquad a=a_s \tag{2.19}$$

Using (2.19) with the condition

$$a_s=x^{1/2}\qquad \text{for}\quad \theta_{||}=\pi/3 \tag{2.20}$$

we can uniquely determine the saddle point in the upper half-plane as a continuous function of $\theta_{||}$. (Hereafter we denote it by a_s.) For large l the correlation function can be represented as

$$\langle\sigma_{00}\sigma_{lm}\rangle-\langle\sigma_{00}\rangle\langle\sigma_{lm}\rangle\sim\alpha\exp(-r/\xi)\cos[(l+m)\eta+\delta] \tag{2.21a}$$

$$-\frac{1}{\xi}=\frac{2}{\sqrt{3}}\left[\sin\theta_{||}\ln|\phi(a_sx^{-2})|+\sin\left(\theta_{||}-\frac{\pi}{3}\right)\ln|\phi(a_s)|\right] \tag{2.21b}$$

$$\eta=\{\operatorname{Arg}[\phi(a_sx^{-2})]+v\operatorname{Arg}[\phi(a_s)]\}/(1+v) \tag{2.21c}$$

where

$$r=(l^2+m^2-lm)^{1/2} \tag{2.21d}$$

Now we investigate the case $x\to -1$ to find the behavior of ξ near the critical point. We derive also some simple relations satisfied by a_s. To do this, it is convenient to introduce the conjugate modulus transformation[1,3]

$$\theta_1(u,\exp-\varepsilon)=\frac{1}{2}\left(\frac{2\pi}{\varepsilon}\right)^{1/2}\exp\left(\frac{\varepsilon}{8}-\frac{\pi^2}{2\varepsilon}+\frac{2u(\pi-u)}{\varepsilon}\right)\times f\left(\exp-\frac{4\pi u}{\varepsilon},\exp-\frac{4\pi^2}{\varepsilon}\right) \tag{2.22}$$

$$\theta_1(u,-\exp-\varepsilon)=-\frac{1}{2}\left(\frac{\pi}{\varepsilon}\right)^{1/2}\exp\left(\frac{\varepsilon}{8}-\frac{\pi^2}{8\varepsilon}-\frac{u(2u+\pi)}{\varepsilon}\right)\times f\left(\exp\frac{2\pi u}{\varepsilon},-\exp-\frac{\pi^2}{\varepsilon}\right) \tag{2.23}$$

where

$$\theta_1(u,q^2)=\sin u\prod_{n=1}^{\infty}(1-2q^{2n}\cos 2u+q^{4n})(1-q^{2n}) \tag{2.24}$$

The transformation (2.23) can be used in (2.19) to expand it into a power series of $\exp(-5\varepsilon/6)$ for large ε (or near the critical point), where the new variable ε is related to x by

$$x = -\exp(-\pi^2/5\varepsilon) \tag{2.25}$$

Keeping the dominant term in the $\varepsilon \to \infty$ limit, and assuming the region of $0 < \mathrm{Arg}[a] < \pi$, we obtain

$$\frac{\sqrt{3} - \tan\theta_{||}}{\sqrt{3} + \tan\theta_{||}} = \exp\left(\frac{\pi}{3} i\right) \frac{A_0^2 - \exp(-5\varepsilon/3)\exp(-\pi i/3)}{A_0^2 - \exp(-5\varepsilon/3)\exp(\pi i/3)} \tag{2.26}$$

where A_0 is the asymptotic form of A near the limit $\varepsilon \to \infty$ defined by

$$A = \exp\left[\left(\frac{5\varepsilon}{3\pi} \ln a_s\right) i\right] \tag{2.27}$$

Solving (2.25) with the condition of (2.20), we obtain

$$A_0 = \exp\left[\left(\theta_{||} - \frac{\pi}{2}\right) i\right] \exp\left(-\frac{5}{6}\varepsilon\right) \tag{2.28}$$

Higher order terms of A can be determined first by expressing it as

$$A = A_0 \left\{1 + \Delta^{(1)} \exp\left(-\frac{5}{6}\varepsilon\right) + \Delta^{(2)} \exp\left(-\frac{10}{6}\varepsilon\right) + O\left[\exp\left(-\frac{15}{6}\varepsilon\right)\right]\right\} \tag{2.29}$$

and then by equating the coefficients of powers of $\exp(-5\varepsilon/6)$ in the expanded form of (2.19), which is obtained by use of (2.23) and (2.29). The coefficients $\Delta^{(1)}$, $\Delta^{(2)}$,... are determined as

$$\Delta^{(1)} = -4 \sin\theta_{||} \sin\left(\theta_{||} + \frac{\pi}{3}\right) \sin\left(\theta_{||} - \frac{\pi}{3}\right) \tag{2.30a}$$

$$\Delta^{(2)} = \frac{1}{2} (\Delta^{(1)})^2 - 8i\Delta^{(1)} \cos\theta_{||} \cos\left(\theta_{||} + \frac{\pi}{3}\right) \cos\left(\theta_{||} - \frac{\pi}{3}\right) \tag{2.30b}$$

$$\vdots$$

In terms of these coefficients, a_s can be represented as

$$\ln |a_s| = \frac{3\pi}{5}\left(\theta_{||} - \frac{\pi}{2}\right)\frac{1}{\varepsilon} + \frac{3\pi}{5} \mathrm{Im}\,[\Delta^{(2)}]\,\frac{1}{\varepsilon} \exp\left(-\frac{10}{6}\varepsilon\right) + O\left[\frac{1}{\varepsilon}\exp\left(-\frac{20}{6}\varepsilon\right)\right] \tag{2.31a}$$

$$\operatorname{Arg}[a_s]=\frac{\pi}{2}-\frac{3\pi}{5}\Delta^{(1)}\frac{1}{\varepsilon}\exp\left(-\frac{5}{6}\varepsilon\right)+O\left[\frac{1}{\varepsilon}\exp\left(-\frac{15}{6}\varepsilon\right)\right] \tag{2.31b}$$

The results (2.30a) and (2.30b) can be used in (2.31a) and (2.31b) to find the relations, within the validity of this expansion,

$$a_s(\pi-\theta_{||})=[a_s^{-1}(\theta_{||})]^*, \qquad a_s(\theta_{||}+\pi/3)=[a_s(\theta_{||})\,x^{-1}]^* \tag{2.32}$$

Here we return to (2.19) to find some properties of (2.19) which support (2.32). It is trivial that if a pair $(a_0, \theta_{||})$ satisfies (2.19), then the pairs $(a_0^*, \theta_{||})$ and $(a_0^{-1}, \pi-\theta_{||})$ satisfy (2.19). After some calculations, it can be found that the pair $(a_0 x^{-1}, \theta_{||}+\pi/3)$ also satisfies (2.19). From these results, though we cannot prove it rigorously, we expect that (2.32) hold exactly. The relations (2.32) can be used in (2.21b) to obtain the relations

$$\xi(-\theta_{||})=\xi(\theta_{||}), \qquad \xi(\theta_{||}+\pi/3)=\xi(\theta_{||}) \tag{2.33}$$

Expanding (2.21b) and (2.21c) in the same way, we use (2.30a) and (2.30b) to get

$$\begin{aligned}&\langle\sigma_{00}\sigma_{lm}\rangle-\langle\sigma_{00}\rangle\langle\sigma_{lm}\rangle\\ &\quad\sim\alpha\exp\left(-\frac{r}{\xi}\right)\cos\left\{\frac{2\pi}{3}(l+m)\right.\\ &\qquad+r\left[-4\sqrt{3}\cos\theta_{||}\cos\left(\theta_{||}+\frac{\pi}{3}\right)\cos\left(\theta_{||}-\frac{\pi}{3}\right)\exp\left(-\frac{10}{6}\varepsilon\right)\right]\\ &\qquad\left.+O\left[\exp\left(-\frac{20}{6}\varepsilon\right)\right]+\delta\right\}\end{aligned} \tag{2.34a}$$

$$\begin{aligned}\xi&=\frac{1}{2\sqrt{3}}\exp\left(\frac{5}{6}\varepsilon\right)\left\{1-\left[1-8\sin^2\theta_{||}\sin^2\left(\theta_{||}+\frac{\pi}{3}\right)\sin^2\left(\theta_{||}-\frac{\pi}{3}\right)\right]\right.\\ &\quad\left.\times\exp\left(-\frac{10}{6}\varepsilon\right)+O\left[\exp\left(-\frac{20}{6}\varepsilon\right)\right]\right\}\end{aligned} \tag{2.34b}$$

Equation (2.34a) indicates that the angular dependence of the correlation function is $\cos[(2\pi/3)(l+m)]$ near the critical point. This reflect the ground-state configuration of this system. Equation (2.32b) shows that the anisotropy of ξ disappears as the system approaches the critical point. Further, we find that the critical exponent ν does not depend on the direction $\theta_{||}$:

$$\nu=5/6 \qquad \text{for all} \quad \theta_{||} \tag{2.35}$$

3. ORDERED STATE

3.1. Interfacial Tension 1

For $z > z_c$ we calculate the free energy of the system with a mismatched vertical seam to analyze the interfacial tension. The method by Baxter and Pearce[3] is summarized. Under the constraints $M = 1$ or 2 (mod 3), $N = 0$ (mod 3), the $M \times N$ lattice with the toroidal boundary condition is considered. In the M, $N \to \infty$ limit, reflecting the existence of a mismatched vertical seam, there is an excess free energy above the bulk free energy. From this excess free energy the interfacial tension σ along the vertical axis can be calculated. Using the notations in Section 2.1, we can represent the interfacial tension as

$$\begin{aligned} -\beta\sigma &= \lim_{N, M \to \infty} \frac{1}{N} \ln \left[\frac{1}{\kappa^{NM}} \operatorname{tr} \mathbf{V}^N \right] \\ &= \lim_{N, M \to \infty} \frac{1}{N} \ln \left[\frac{1}{\kappa^{NM}} \sum_p V(p)^N \right] \end{aligned} \tag{3.1}$$

where κ is the partition function per site,

$$\begin{aligned} \kappa &= \lim_{N, M \to \infty} [\operatorname{tr} \mathbf{V}^N]^{1/NM} \\ &= \lim_{N, M \to \infty} \left[\sum_p V(p)^N \right]^{1/NM} \end{aligned} \tag{3.2}$$

We introduce the shift operator to calculate the anisotropy of the interfacial tension. Inserting the shift operator can be regarded as tilting the interface by moving its endpoint and starting point along the horizontal direction (Fig. 3). The anisotropic interfacial tension is given by

$$\begin{aligned} -\beta\sigma &= \lim_{N, M \to \infty} \frac{1}{r} \ln \left[\frac{1}{\kappa^{NM}} \operatorname{tr}(\mathbf{V}\mathbf{T}^v)^N \right] \\ &= \lim_{N, M \to \infty} \frac{1}{r} \ln \left\{ \frac{1}{\kappa^{NM}} \sum_p [V(p)\, T(p)^v]^N \right\} \end{aligned} \tag{3.3}$$

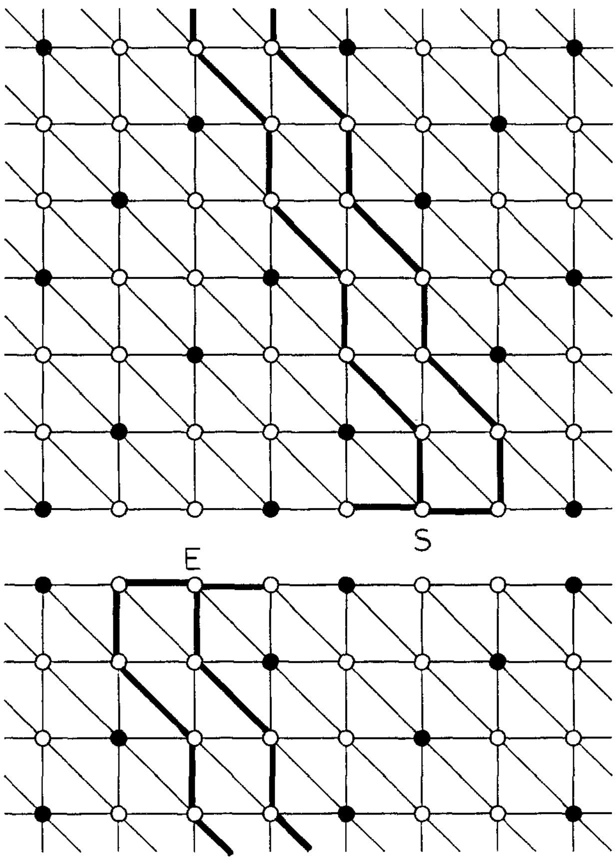
where

$$r = N(1 + v^2 - v)^{1/2} \tag{3.4}$$

and v is the parameter designating the direction of the interface. Instead of the above constraints, new constraints $M = 1$ or 2 (mod 3), $N(1 + v) = 0$ (mod 3), are imposed.

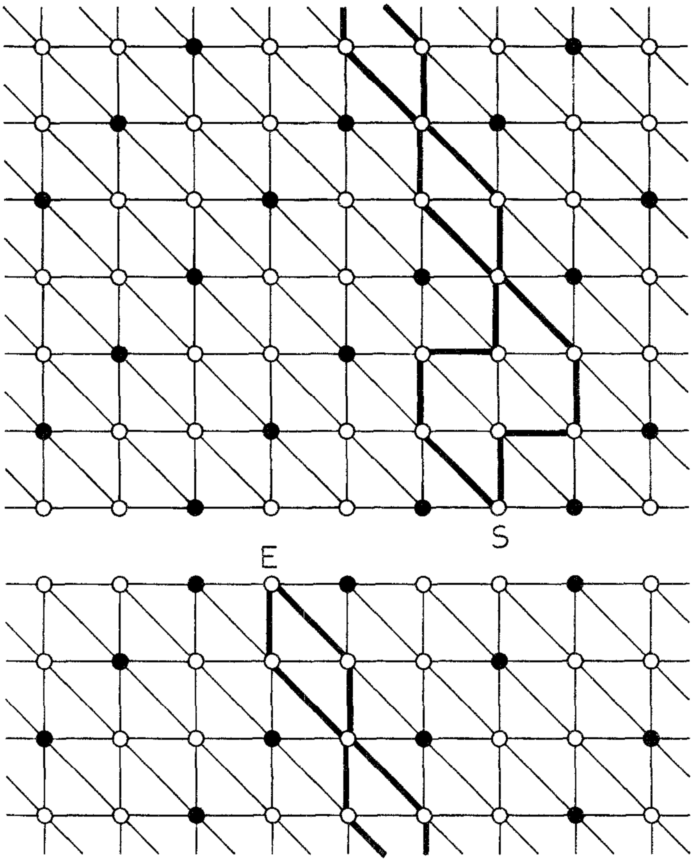
In contrast to the analysis by Baxter and Pearce, where the interfacial tension of $M=1$ (mod 3) and that of $M=2$ (mod 3) take the same value, it will be found that they are different in a general direction. To understand the physical meaning of this difference, we investigate what kinds of interface are considered in the case of $M=1$ (mod 3) and $M=2$ (mod 3).

For $z>z_c$ three phases in which every third site is preferentially occupied are degenerate. If $\rho_A>\rho_B=\rho_C$, this phase is called the A phase. The B phase and the C phase are defined in the same way. For a given direction six kinds of interface exist, corresponding to choosing any two phases for both sides of the interface from these three phases. The situation



(a)

Fig. 3. Typical configurations in the $z\to\infty$ limit when three shift operators are inserted between the fourth row and the fifth row of the lattice. (a) $M=1$ (mod 3), and (b) $M=2$ (mod 3). The starting point of the interface is denoted by S and the end point is denoted by E.



(b)

Fig. 3. (*Continued*)

where the lhs of the interface is A phase and the rhs is B phase is denoted by A/B. From the translational invariance of this system, it is found that three kinds of interface A/B, B/C, and C/A have the same interfacial tension, and that the interfacial tension of A/C, B/A, and C/B are also the same. With regard to the interfacial tension, we classify six kinds of interface into two types: the interfaces A/B, B/C, and C/A are of type 1, and the others are of type 2.

Pick a typical configuration of $M = 1 \pmod 3$). Restricting ourselves to the region near the interface, we divide the lattice into three sublattices. (Due to the toroidal boundary condition and the constraints for M and N, we cannot do this all over the lattice.) If the lhs of the interface is regarded as A phase, the rhs is B phase. This fact shows that the interface of $M=1$ (mod 3) is type 1. In the case $M=2$ (mod 3), fixing the lhs of the interface to be A phase, we find that the rhs is C phase, and that the interface of $M=2$ (mod 3) is type 2 (Fig. 3). The difference between the interfacial tension of $M=1$ (mod 3) and $M=2$ (mod 3) reflects the difference between the two types of interface.

In the following the problem is defined more precisely. The interfacial tension between the A phase and the B phase, denoted by $\sigma(A\to B)$, is considered. We regard $\sigma(A\to B)$ as a function of $\theta_\perp$, which is the angle between the normal vector of the interface drawn from the A phase toward the B phase and the horizontal axis in the triangular lattice; the horizontal axis corresponds to the direction connecting the nearest neighbor lattice site. The method is as follows. For $-\pi/2<\theta_\perp<\pi/2$, where the lhs of the interface is the A phase and the rhs is the B phase, with the type 1 interface, $\sigma(A\to B)$ can be calculated by using (3.3) with the constraints $M=1$ (mod 3), $N(1+v)=0$ (mod 3). For $-\pi<\theta_\perp<-\pi/2$ or $\pi/2<\theta_\perp<\pi$, where the lhs is the B phase and the rhs is the A phase, with the type 2 interface, $\sigma(A\to B)$ can be calculated by using (3.3) with the constraints $M=2$ (mod 3), $N(1+v)=0$ (mod 3).

The equilibrium crystal shape derived from $\sigma(A\to B)$ is the shape of the droplet of the A phase inside the sea of the B phase. Other kinds of interfacial tension can be simply related to $\sigma(A\to B)$. For example, the interfacial tension between the A phase and the C phase, $\sigma(A\to C)$, can be related to $\sigma(A\to B)$ by

$$\sigma(A\to C\mid\theta_\perp)=\sigma(A\to B\mid\pi+\theta_\perp) \tag{3.5}$$

3.2. Interfacial Tension 2

First the case of $-\pi/2<\theta_\perp<\pi/2$ is considered. Substituting the explicit forms of the eigenvalues of $\mathbf{V}$ and $\mathbf{T}$ into (3.3),[3] we get

$$-\beta\sigma=\lim_{N\to\infty}\frac{1}{N(1+v^2-v)^{1/2}}\ln\left\{\frac{1}{6\pi i}\oint_{|a|=1}\frac{da}{a}\,\rho(a)[\psi(ax)\,\psi(a)^v]^N\right\}$$
$$\text{for}\quad -\infty<v<\infty \tag{3.6a}$$

where $\sigma(A\to B)$ is abbreviated to σ, and

$$\psi(a)=-a^{1/3}\frac{f(a^{-1}x,x^3)}{f(ax,x^3)} \tag{3.6b}$$

$$v=\frac{\sqrt{3}}{2}\tan\theta_\perp+\frac{1}{2}\qquad\text{for}\quad -\frac{\pi}{2}<\theta_\perp<\frac{\pi}{2} \tag{3.6c}$$

The functions $\psi(ax)$ and $\psi(a)$ in (3.6a) correspond to $V(p)/\kappa^M$ and $T(p)$ in (3.3), respectively. The summation in (3.3) becomes an integral along unit circles on three sheets of the Riemann surface due to the continuous distribution of the eigenvalues denoted by $\rho(a)$. The parameter x is related to the one-particle activity z by

$$z = \frac{1}{x} \prod_{n=1}^{\infty} \left[\frac{(1-x^{5n-3})(1-x^{5n-2})}{(1-x^{5n-4})(1-x^{5n-1})} \right]^5 \qquad \text{for} \quad 0 < x < 1 \tag{3.7}$$

The integral in (3.6a) can be estimated by the method of steepest descent. It is convenient to rewrite (3.6a) as

$$-\beta\sigma = \lim_{N \to \infty} \frac{1}{N(1+v^2-v)^{1/2}} \times \ln \left(\frac{1}{6\pi i} \oint_{|a|=1} \frac{da}{a} \rho(a) \{ [\psi(ax)\, \psi(a)^{1/2}] [\psi(ax)\, \psi(a)^2]^{v'} \}^{N'} \right) \tag{3.8a}$$

where the new parameters v' and N' are related to the old ones by

$$v' = \frac{1/2 - v}{v-2} = \frac{\tan\theta_\perp}{\sqrt{3} - \tan\theta_\perp}, \qquad N = (1+v')\, N' \tag{3.8b}$$

and to use the derivative of $\ln[\psi(ax)\, \psi(a)^{1/2}]$,

$$\frac{d}{da} \ln[\psi(ax)\, \psi(a)^{1/2}] = -\frac{1}{2} f^2(x, x^3) \frac{1}{a} \frac{f(-a, x^3)\, f(a^{-1}x^{3/2}, x^3)\, f(-a^{-1}x^{3/2}, x^3)}{f(a, x^3)\, f(ax, x^3)\, f(a^{-1}x, x^3)} \tag{3.9}$$

For a given direction v three saddle points are found on the negative parts of the real axes, and the integral in (3.8a) can be estimated around them. The saddle point whose argument is π, denoted by a_s, is determined by

$$\frac{\sqrt{3} - \tan\theta_\perp}{\sqrt{3} + \tan\theta_\perp} = -a \frac{f(-ax, x^3)\, f(a^{-1}x^{1/2}, x^3)\, f(-a^{-1}x^{1/2}, x^3)}{f(-a^{-1}x, x^3)\, f(ax^{1/2}, x^3)\, f(-ax^{1/2}, x^3)}, \qquad a = a_s \tag{3.10}$$

and the condition

$$a_s = -1 \qquad \text{for} \quad \theta_\perp = 0 \tag{3.11}$$

The interfacial tension is represented as

$$-\beta\sigma=\frac{2}{\sqrt{3}}\left[\cos\theta_{\perp}\ \ln|\psi(a_s x)|+\cos\left(\theta_{\perp}-\frac{\pi}{3}\right)\ln|\psi(a_s)|\right]$$

$$\text{for}\quad -\pi/2<\theta_{\perp}<\pi/2 \tag{3.12}$$

Near the critical point, which is the $x\to 1$ limit, (3.12) can be solved in the form of the power series. Using the conjugate modulus transformation (2.22), we find

$$i\ln|a_s| = -i\frac{6\pi}{5\varepsilon}\theta_{\perp}+\Delta^{(1)}\frac{6\pi}{5\varepsilon}\exp\left(-\frac{5}{6}\varepsilon\right)+\left[\Delta^{(2)}-\frac{1}{2}(\Delta^{(1)})^2\right]\frac{6\pi}{5\varepsilon}$$

$$\times\exp\left(-\frac{10}{6}\varepsilon\right)+O\left[\frac{1}{\varepsilon}\exp\left(-\frac{15}{6}\varepsilon\right)\right] \tag{3.13a}$$

$$\operatorname{Arg}[a_s]=\pi \tag{3.13b}$$

where the new variable ε is related to x by

$$x=\exp(-4\pi^2/5\varepsilon) \tag{3.14}$$

and

$$\Delta^{(1)}=-4i\sin\theta_{\perp}\ \sin\left(\theta_{\perp}+\frac{\pi}{3}\right)\sin\left(\theta_{\perp}-\frac{\pi}{3}\right) \tag{3.15a}$$

$$\Delta^{(2)}=\frac{1}{2}[\Delta(1)]^2-8\Delta^{(1)}\cos\theta_{\perp}\ \cos\left(\theta_{\perp}+\frac{\pi}{3}\right)\cos\left(\theta_{\perp}-\frac{\pi}{3}\right) \tag{3.15b}$$

These results show the relations within the validity of this expansion,

$$a_s(-\theta_{\perp})=a_s^{-1}(\theta_{\perp}),\qquad a_s\left(\theta_{\perp}+\frac{2\pi}{3}\right)=a_s(\theta_{\perp})x \tag{3.16}$$

It is trivial to show that if a pair $(a_0, \theta_{\perp})$ satisfies (3.10), then the pair $(a_0^{-1}, -\theta_{\perp})$ satisfies (3.10). Further, after some calculations, it is found that the pair $(a_0 x, \theta_{\perp}+2\pi/3)$ also satisfies (3.10). From these we expect that the relations (3.16) hold exactly. After the rhs of (3.12) is expanded into power series of $\exp(-5\varepsilon/6)$, (3.15a) and (3.15b) can be used to get

$$\beta\sigma = 2\sqrt{3}\exp\left(-\frac{5}{6}\varepsilon\right) + 4\sqrt{3}\cos\theta_\perp \cos\left(\theta_\perp + \frac{\pi}{3}\right)$$
$$\times \cos\left(\theta_\perp - \frac{\pi}{3}\right)\exp\left(-\frac{10}{6}\varepsilon\right)$$
$$+ 2\sqrt{3}\left[1 + 8\sin^2\theta_\perp \sin^2\left(\theta_\perp + \frac{\pi}{3}\right)\sin^2\left(\theta_\perp - \frac{\pi}{3}\right)\right]\exp\left(-\frac{15}{6}\varepsilon\right)$$
$$+ O\left[\exp\left(-\frac{20}{6}\varepsilon\right)\right] \quad \text{for} \quad -\frac{\pi}{2} < \theta_\perp < \frac{\pi}{2} \tag{3.17}$$

Replacing the function $\psi(a)$ in (3.6a) by $\bar{\psi}(a)$, we get the representation of the interfacial tension for $-\pi < \theta_\perp < -\pi/2$, $\pi/2 < \theta_\perp < \pi$,

$$-\beta\sigma = \lim_{N\to\infty} \frac{1}{N(1+v^2-v)^{1/2}} \ln\left\{\frac{1}{6\pi i}\oint_{|b|=1} \frac{db}{b}\,[\bar{\psi}(bx)\,\bar{\psi}^v(b)]^N\right\}$$
$$\text{for} \quad -\infty < v < \infty \tag{3.18a}$$

where

$$\bar{\psi}(b) = b^{2/3}\frac{f(b^{-1}x^{1/2}, x^3)}{f(bx^{1/2}, x^3)} = \psi(b^{-1}x^{3/2}) \tag{3.18b}$$

and

$$v = \frac{\sqrt{3}}{2}\tan\theta_\perp + \frac{1}{2} \quad \text{for} \quad -\pi < \theta_\perp < -\frac{\pi}{2},\ \ \frac{\pi}{2} < \theta_\perp < \pi \tag{3.18c}$$

The integral in (3.18a) can be estimated by the method of steepest descent. The saddle point whose argument is π, denoted by b_s, is determined by the equation

$$\frac{\sqrt{3} - \tan\theta_\perp}{\sqrt{3} + \tan\theta_\perp} = \frac{f(-b^{-1}x^{1/2}, x^3)\, f(bx, x^3)\, f(-bx, x^3)}{f(-bx^{1/2}, x^3)\, f(b^{-1}x, x^3)\, f(-b^{-1}x, x^3)}, \quad b = b_s \tag{3.19}$$

and the condition

$$b_s = -1 \quad \text{for} \quad \theta_\perp = \pm\pi \tag{3.20}$$

The interfacial tension is given by

$$-\beta\sigma = -\frac{2}{\sqrt{3}}\left[\cos\theta_\perp \ln|\bar{\psi}(b_s x)| + \cos\left(\theta_\perp - \frac{\pi}{3}\right)\ln|\bar{\psi}(b_s)|\right]$$
$$\text{for} \quad -\pi < \theta_\perp < -\pi/2, \quad \pi/2 < \theta_\perp < \pi \tag{3.21}$$

Here we do not have to solve (3.19) and (3.20) actually. It is sufficient to find the relations between b_s and a_s, determined by (3.10) and (3.11). When b is transformed into a by

$$a = bx^{3/2} \qquad \text{for} \quad \pi/2 < \theta_\perp < \pi \tag{3.22a}$$

and

$$a = bx^{-3/2} \qquad \text{for} \quad -\pi < \theta_\perp < -\pi/2 \tag{3.22b}$$

(3.19) coincides with (3.10). If (3.11) is solved with the condition (3.10) in the extended region $-\pi < \theta_\perp < \pi$, because of the relations (3.16), the condition (3.20) is satisfied through (3.22a) and (3.22b). Thus, we find

$$a_s = b_s x^{3/2} \qquad \text{for} \quad \pi/2 < \theta_\perp < \pi \tag{3.23a}$$

and

$$a_s = b_s x^{-3/2} \qquad \text{for} \quad -\pi < \theta_\perp < -\pi/2 \tag{3.23b}$$

These relations can be used in (3.21) to get

$$-\beta\sigma = \frac{2}{\sqrt{3}}\left[\cos\theta_\perp \ln|\psi(a_s x)| + \cos\left(\theta_\perp - \frac{\pi}{3}\right)\ln|\psi(a_s)|\right]$$
$$\text{for} \quad -\pi < \theta_\perp < -\pi/2, \quad \pi/2 < \theta_\perp < \pi \tag{3.24}$$

The use of (3.16) in (3.12) and (3.24) shows the symmetry relations

$$\sigma(-\theta_\perp) = \sigma(\theta_\perp), \qquad \sigma(\theta_\perp + 2\pi/3) = \sigma(\theta_\perp) \tag{3.25}$$

From the expansion (3.17) we can see that the anisotropy of the interfacial tension disappears as the system approaches the critical point. The expansion (3.17) can be extended into the region $-\pi < \theta_\perp < \pi$. Thus, we find that the critical exponent μ does not depend on $\theta_\perp$:

$$\mu = 5/6 \qquad \text{for all} \quad \theta_\perp \tag{3.26}$$

The rotation of the interface between the A phase and the B phase around a site through $\pi/3$ is considered. Although, from the invariance of this system for this rotation, the rotated interface must have the same interfacial tension as the former one, it is not evident whether σ satisfies these conditions. If the center is on the C lattice, this rotation only causes the change of $\theta_\perp$ through $-2\pi/3$. The above condition is assured by the second relation of (3.25). If the center is on the A lattice, the relation

$$\sigma(A \to B \mid \theta_\perp) = \sigma(A \to C \mid \theta_\perp + \pi/3) \tag{3.27}$$

must be satisfied. The second relation (3.25) assures it through (3.5). Similarly, in the case that the center is on the B lattice, the above condition is satisfied.

3.3. Equilibrium Crystal Shape

Suppose an A phase whose volume (or area) is fixed to be V is embedded inside a sea of B phase. We consider the problem of finding the shape S of the minimum energy from the anisotropic interfacial tension. The answer to this problem is obtained by use of Wulff's theorem or Wulff's construction.[8–10] Wulff's theorem says that there is a special point O called the Wulff point inside S, and that if the position vector $\mathbf{R}(\mathbf{r})$ is drawn from O to each point on S in the direction designated by the unit vector $\mathbf{r}$, then $\mathbf{R}(\mathbf{r})$ satisfies the relation

$$\frac{\sigma[\mathbf{n}(\mathbf{r})]}{\mathbf{R}(\mathbf{r})\cdot\mathbf{n}(\mathbf{r})}=\lambda \qquad \text{for all} \quad \mathbf{r} \tag{3.28}$$

where $\mathbf{n}(\mathbf{r})$ is the normal vector of the interface at the point $\mathbf{R}(\mathbf{r})$, and the interfacial tension is represented as a function of the normal vector of the interface. The constant λ has a meaning of a scale factor adjusted to yield the volume V. The origin of this theorem goes back to Wulff's paper of 1901,[10] and later this theorem was proved for some special cases by the variational method.[11,12]

Using (3.28), we try to construct S. We start with the polar plot of σ around a fixed point O, which is denoted by Σ. Through each point on Σ designated by $\sigma(\mathbf{n})\mathbf{n}$ the line which is perpendicular to $\mathbf{n}$ is drawn. Proper sets of these lines construct infinite closed figures $\bar{S}_1, \bar{S}_2,..., \bar{S}_\alpha,...$ (Fig. 4). If the volume of $\bar{S}_\alpha$ is $\bar{V}_\alpha$, enlarging $\bar{S}_\alpha$ by $(V/\bar{V}_\alpha)^{1/2}$ times, we get the figure S_α whose volume is V and which satisfies (3.28), where the value of λ for S_α is

$$\lambda_\alpha=\left(\frac{\bar{V}_\alpha}{V}\right)^{1/2} \tag{3.29}$$

The remaining work is selecting S among the figures $S_1, S_2,..., S_\alpha,...$. To do this, a helpful relation[8,9] is derived by the use of (3.28). Denoting by E_α the total surface energy of S_α, we get

$$E_\alpha=2\lambda_\alpha V \tag{3.30}$$

With the relation (3.29), Eq. (3.30) shows that the minimum energy corresponds to the minimum value of $\bar{V}_\alpha$. From these results we can find

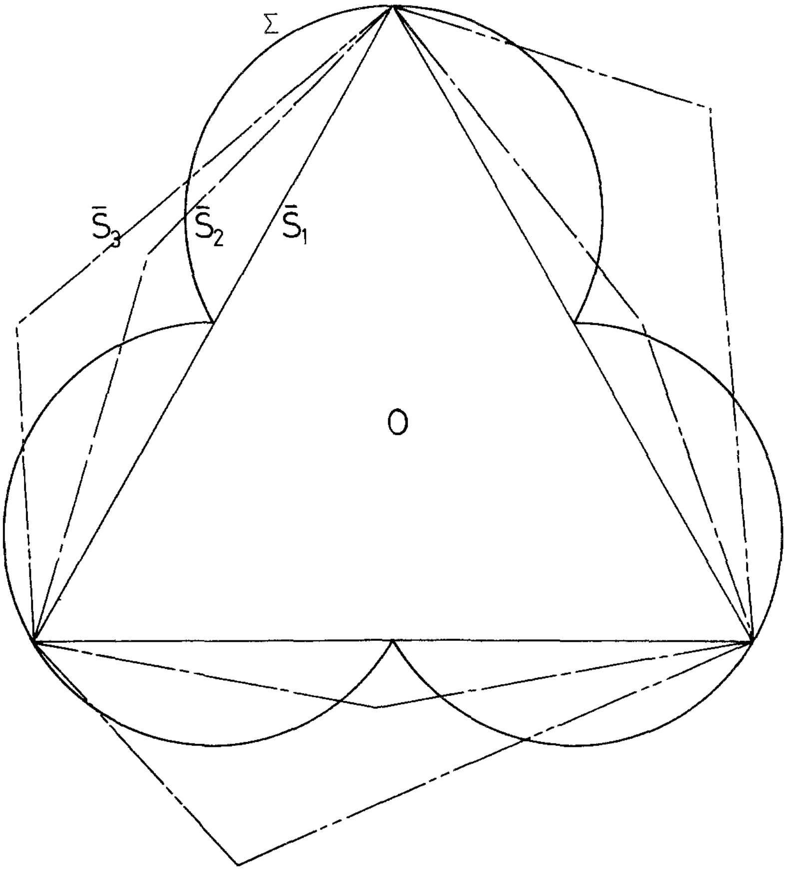


Fig. 4. The polar plot of σ/ζ denoted by Σ in the $z \to \infty$ limit. All the figures $\bar{S}_1$, $\bar{S}_2$, $\bar{S}_3$,... satisfy Wulff's theorem. The equilibrium shape is determined as the similar figure of the innermost figure $\bar{S}_1$.

that $\bar{S}$ corresponding to the minimum-energy S is determined as the inner envelope of the lines drawn on Σ. This method has long been known as Wulff's geometric construction.

Recently, some authors have succeeded in representing Wulff's construction analytically.[8,9,13] Zia represented it as

$$\lambda \mathbf{R}(\mathbf{r}) = \min_{\mathbf{n}} \frac{\sigma(\mathbf{n})}{(\mathbf{r} \cdot \mathbf{n})} \tag{3.31a}$$

where

$$R(\mathbf{r}) = |\mathbf{R}(\mathbf{r})| \tag{3.31b}$$

Assuming the differentiability of $\sigma(\mathbf{n})$, he also showed that if the global minimum in the rhs of (3.31a) can be replaced by local minimum, we get

$$\lambda \mathbf{R}(\mathbf{n}) = \mathbf{n}\sigma(\mathbf{n}) + \nabla'\sigma(\mathbf{n}) \tag{3.32a}$$

where ∇' is the surface gradient defined by

$$\delta\sigma(\mathbf{n}) = \delta\mathbf{n} \cdot \nabla'\sigma(\mathbf{n}) \qquad [\nabla'\sigma(\mathbf{n}) \cdot \mathbf{n} = 0] \tag{3.32b}$$

and $\mathbf{R}(\mathbf{n})$ is a position vector of the interface whose normal vector is $\mathbf{n}$.

We derive the equilibrium shape of the hard-hexagon crystal from the anisotropic interfacial tension $\sigma(A \to B \mid \theta_\perp)$ calculated in Section 3.2. The change in the equilibrium crystal shape upon varying one-particle activity z is interesting, and its volume is not important. Hereafter, we choose the chemical potential ζ related to z by

$$\beta\zeta = \ln z \tag{3.33}$$

as λ and deal with the interfacial tension normalized by ζ.

In the $z \to \infty$ limit, which is the $x \to 0$ limit, the behavior of a determined by (3.10) and (3.11) is

$$a_s(\theta_\perp) \sim \frac{\sin(\theta_\perp - \pi/3)}{\sin(\theta_\perp + \pi/3)} \qquad \text{for} \quad \theta_\perp - \frac{\pi}{3} < \theta_\perp < \frac{\pi}{3} \tag{3.34a}$$

$$a_s\left(\frac{\pi}{3}\right) = -x^{1/2} \tag{3.34b}$$

and we find

$$\frac{\sigma(\theta_\perp)}{\zeta} = \frac{2}{3\sqrt{3}} \cos\theta_\perp \qquad \text{for} \quad -\frac{\pi}{3} \leqslant \theta_\perp \leqslant \frac{\pi}{3} \tag{3.35}$$

(In this limit σ/ζ gives the number of particles per unit length which is removed from the ground state to construct a mismatched vertical seam.) Equation (3.35) shows that Σ has three cusps at $\theta_\perp = \pm\pi/3$, π (Fig. 4). Using Wulff's geometric construction, we draw the equilibrium crystal shape to find that it is a regular triangle consisting of three facets.

For $z < \infty$ we expect that there are no cusps on Σ, and use the analytic form of Wulff's construction (3.32a). The results of numerical calculation are shown in Fig. 5. We see how the equilibrium shape deforms into a regular triangle from a sphere near the critical point as z increases.

We can calculate the radius of curvature at $\theta_\perp = 0$, $\pi/3$, where a corner or a facet appears in $z \to \infty$ limit, respectively. Noting that Σ and the equilibrium shape coincide at $\theta_\perp = 0$, $\pi/3$, we get

$$\rho/R = 1 + \sigma^{-1}\, d^2\sigma/d\theta_\perp^2, \qquad \theta_\perp = 0, \quad \pi/3 \tag{3.36}$$

where ρ is the radius of curvature.[8,9,14] This calculation enables us to estimate the change in the equilibrium shape quantitatively, and will ensure the existence of the roughening transition in the $z \to \infty$ limit.

First, the radius of curvature at $\theta_\perp = 0$ is calculated. Fixing the parameter x, we expand a_s as

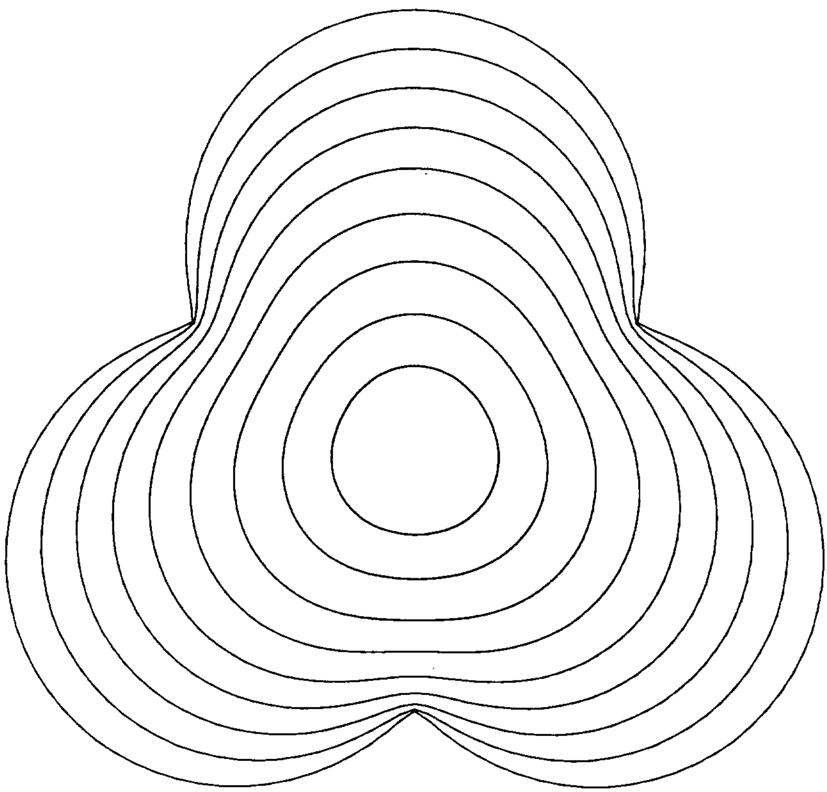
$$a_s = a_0(1 + \Delta^{(1)}\delta\theta_\perp + \Delta^{(2)}\delta\theta_\perp^2 + \cdots) \tag{3.37a}$$

where

$$a_0 = -1, \qquad \delta\theta_\perp = \theta_\perp - 0 \tag{3.37b}$$

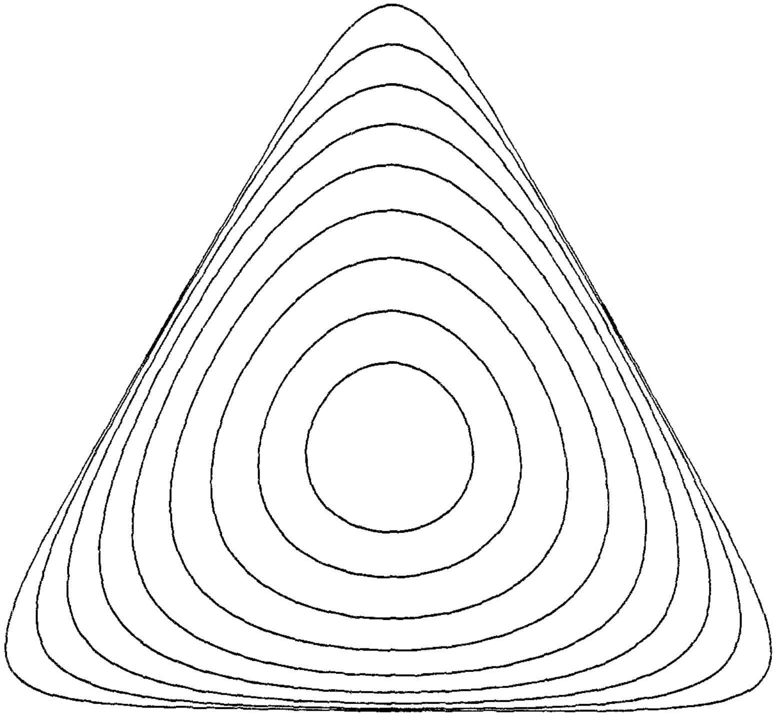
Expanding (3.10) into a power series of $\delta\theta_\perp$, we can determine the coefficients in (3.37a) as

$$\Delta^{(1)} = -\frac{2}{\sqrt{3}} \frac{Q^2(x^6)\, f(x, x^3)}{Q^4(x^3)\, f(-x, x^3)}, \qquad \Delta^{(2)} = \frac{1}{2}(\Delta^{(1)})^2, \ldots \tag{3.38}$$



(a)

Fig. 5. (a) The polar plot of σ/ζ, and (b) the equilibrium shape. From the outermost figure, $z = 1.0 \times 10^6$, 1.0×10^4, 1.0×10^3, 2.5×10^2, 1.0×10^2, 50, 30, 20, and 15, successively.



(b)

FIGURE 5 (*continued*)

where

$$Q(q) = \prod_{n=1}^{\infty} (1 - q^n) \tag{3.39}$$

In this calculation the second derivative,

$$\begin{aligned}
&\frac{d^2}{da^2} \ln[\psi(ax)\,\psi^{1/2}(a)] \\
&= \frac{1}{2a^2} f^2(x, x^3) \frac{f(-a, x^3)\, f(a^{-1}x^{3/2}, x^3)\, f(-a^{-1}x^{3/2}, x^3)}{f(a, x^3)\, f(ax, x^3)\, f(a^{-1}x, x^3)} \\
&\quad + \frac{1}{2a^2} f^2(x, x^3)\, f^2(-x, x^3) \frac{f^2(a^{-1}x^{3/2}, x^3)\, f^2(-a^{-1}x^{3/2}, x^3)}{f^2(ax, x^3)\, f^2(a^{-1}x, x^3)} \\
&\quad - \frac{1}{2a^2} f^2(x, x^3) \frac{Q^4(x^3)}{Q^2(x^6)} \frac{f(ia, x^3)\, f(-ia, x^3)\, f(iax^{3/2}, x^3)\, f(-iax^{3/2}, x^3)}{f^2(a, x^3)\, f(ax, x^3)\, f(a^{-1}x, x^3)}
\end{aligned} \tag{3.40}$$

is useful. The above results can be used in (3.12) to find

$$\beta\sigma = -\frac{2}{\sqrt{3}}\ln\left[x^{1/3}\frac{f(-1, x^3)}{f(-x, x^3)}\right] + \left\{\frac{1}{\sqrt{3}}\ln\left[x^{1/3}\frac{f(-1, x^3)}{f(-x, x^3)}\right] + \frac{1}{3\sqrt{3}}\frac{f^4(x, x^3)}{f^4(-x, x^3)}\right\}\delta\theta_\perp^2 + O(\delta\theta_\perp^4) \tag{3.41}$$

Using (3.41) in (3.36), we get

$$\frac{\rho}{R} = \frac{[1/(3\sqrt{3})][f^4(x, x^3)/f^4(-x, x^3)]}{-(2/\sqrt{3})\ln[x^{1/3}f(-1, x^3)/f(-x, x^3)]} \tag{3.42}$$

In the $z \to \infty$ limit, ρ/R behaves as

$$\frac{\rho}{R}\left(\sim -\frac{1}{\ln x}\right) \sim \frac{1}{\ln z} = \frac{1}{\beta\zeta} \tag{3.43}$$

and near the critical point, by the use of the conjugate modulus transformation (2.22), we find that

$$\frac{\rho}{R} = 1 - \frac{9}{2}\exp\left(-\frac{5}{6}\varepsilon\right) + O\left[\exp\left(-\frac{10}{6}\varepsilon\right)\right] \tag{3.44}$$

For $\theta_\perp = \pi/3$, similarly, a_s can be expanded as

$$a_s = a_0(1 + \Delta^{(1)}\delta\theta_\perp + \Delta^{(2)}\delta\theta_\perp^2 + \cdots) \tag{3.45a}$$

where

$$a_0 = -x^{1/2}, \qquad \delta\theta_\perp = \theta_\perp - \pi/3 \tag{3.45b}$$

and

$$\Delta^{(1)} = -\frac{1}{\sqrt{3}}x^{-1/2}\frac{f(x, x^3)\,f(-x^{3/2}, x^3)}{Q^3(x^3)\,f(-x^{1/2}, x^3)}, \qquad \Delta^{(2)} = \frac{1}{2}(\Delta^{(1)})^2, \ldots \tag{3.46}$$

From these results we obtain

$$\beta\sigma = -\frac{1}{\sqrt{3}}\ln\left[x^{1/3}\frac{f^2(-x^{1/2}, x^3)}{f^2(-x^{3/2}, x^3)}\right] + \left\{\frac{1}{2\sqrt{3}}\ln\left[x^{1/3}\frac{f^2(-x^{1/2}, x^3)}{f^2(-x^{3/2}, x^3)}\right] + \frac{1}{3\sqrt{3}}\frac{1}{x^{1/2}}\frac{f^4(x, x^3)}{f^4(-x^{1/2}, x^3)}\right\}\delta\theta_\perp^2 + O(\delta\theta_\perp^4) \tag{3.47}$$

and

$$\frac{\rho}{R}=\frac{(2/3\sqrt{3})(1/x^{1/2})[f^4(x,x^3)/f^4(-x^{1/2},x^3)]}{-(1/\sqrt{3})\ln[x^{1/3}f^2(-x^{1/2},x^3)/f^2(-x^{3/2},x^3)]} \tag{3.48}$$

The behavior of ρ/R in $z\to\infty$ is given by

$$\frac{\rho}{R}\left(\sim\frac{2x^{-1/2}}{-\ln x}\right)\sim\frac{2z^{1/2}}{\ln z}=2\frac{1}{\beta\zeta}\exp\left(\frac{\beta\zeta}{2}\right) \tag{3.49}$$

and near the critical point

$$\frac{\rho}{R}\sim 1+\frac{9}{2}\exp\left(-\frac{5}{6}\varepsilon\right)+O\left[\exp\left(-\frac{10}{6}\varepsilon\right)\right] \tag{3.50}$$

3.4. Correlation Length

The argument in Sections 2.1 and 2.2 is repeated. When v is fixed and l large, the correlation function is represented as

$$\begin{aligned}&\langle\sigma_{00}\sigma_{lm}\rangle-\langle\sigma_{00}\rangle\langle\sigma_{lm}\rangle\\ &\quad\sim\left(\frac{1}{6\pi i}\right)^2\oint_{|a|=1}\frac{da}{d}\oint_{|b|=1}\frac{db}{b}\,\rho(a,b)[\psi(ax)\,\psi^v(a)]^l\\ &\quad\times[\bar{\psi}(bx)\,\bar{\psi}^v(b)]^l\qquad\text{for}\quad \infty<v<\infty\end{aligned} \tag{3.51a}$$

where the parameter v is related to $\theta_{||}$ by

$$v=\frac{1}{2}-\frac{\sqrt{3}}{2\tan\theta_{||}} \tag{3.51b}$$

The integral in (3.51a) is estimated by the method of steepest descent. Noting that this calculation is the same as Section 3.2 except (3.51b), we find

$$\langle\sigma_{00}\sigma_{lm}\rangle-\langle\sigma_{00}\rangle\langle\sigma_{lm}\rangle\sim\exp\left(-\frac{r}{\xi}\right)\left\{\alpha+\alpha'\cos\left[\frac{2\pi}{3}(l+m)+\delta\right]\right\} \tag{3.52a}$$

$$\begin{aligned}-\frac{1}{\xi}&=\frac{2}{\sqrt{3}}\left[\sin\theta_{||}\ln|\gamma(a_s x)|+\sin\left(\theta_{||}-\frac{\pi}{3}\right)\ln|\psi(a_s)|\right]\\ &\quad+\frac{2}{\sqrt{3}}\left[\sin\theta_{||}\ln|\bar{\psi}(b_s x)|+\sin\left(\theta_{||}-\frac{\pi}{3}\right)\ln|\bar{\psi}(b_s)|\right]\end{aligned} \tag{3.52b}$$

where a_s is the saddle point of $|\psi(ax)\,\psi^v(a)|$ whose argument is π, and b_s is that of $|\bar{\psi}(bx)\,\bar{\psi}(b)|$ whose argument is π. Baxter and Pearce showed that a simple relation holds between the correlation length and the interfacial tension along the vertical axis.[3] This relation is extended here for all directions from (3.52b) as

$$1/\xi = \beta[\sigma(A \to B) + \sigma(A \to C)] \tag{3.53}$$

where $\sigma(A \to B)$ and $\sigma(A \to C)$ are the two types of interfacial tension defined in Section 3.1 in the direction of ξ.

The behavior of ξ near the critical point is given by

$$\xi = \frac{1}{4\sqrt{3}} \exp\left(\frac{5}{6}\varepsilon\right)\left\{1 - \left[1 + 8\cos^2\theta_{||}\cos^2\left(\theta_{||} + \frac{\pi}{3}\right)\cos^2\left(\theta_{||} - \frac{\pi}{3}\right)\right]\right.$$
$$\left. \times \exp\left(-\frac{10}{6}\varepsilon\right) + O\left[\exp\left(-\frac{20}{6}\varepsilon\right)\right]\right\} \tag{3.54}$$

We find that the critical exponent ν' does not depend on the direction:

$$\nu' = 5/6 \qquad \text{for all} \quad \theta_{||} \tag{3.55}$$

From (3.25) it is shown that ξ satisfies the relations

$$\xi(\theta_{||} + \pi/3) = \xi(\theta_{||}), \qquad \xi(-\theta_{||}) = \xi(\theta_{||}) \tag{3.56}$$

4. SUMMARY AND DISCUSSION

We have proposed a new method which enables us to calculate the anisotropy of the correlation length. In this method the shift operator and the transfer matrix are used simultaneously. Using this method, we have extended the analysis by Baxter and Pearce where the correlation length of the hard-hexagon model along the vertical axis has been calculated, and derived some equations which determine the anisotropic correlation length of this model. This method is expected to be applicable to other models. We will study this problem in a separate paper.

Similarly, for $z > z_c$, we have analyzed the anisotropic interfacial tension of the hard-hexagon model. In contrast to the Ising model, which is the only model whose anisotropic interfacial tension has been exactly calculated before, the hard-hexagon model has a feature that in the ordered state three phases degenerate. Noting this point, we have calculated the interfacial tension between the A phase and B phase. From this analysis the equilibrium shape of a droplet of A phase embedded inside the B phase has been found by the use of Wulff's construction. Further, considering the radius of curvature at some special points on the equilibrium shape, we have shown the roughening transition in the $z \to \infty$ limit quantitatively.

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