

Title	Anisotropic Interfacial Tension and Equilibrium Crystal Sha-pes of Exactly Solvable Models
Author(s)	藤本, 雅文
Citation	大阪大学, 1991, 博士論文
Version Type	VoR
URL	https://doi.org/10.11501/2964353
rights	
Note	

The University of Osaka Institutional Knowledge Archive : OUKA

https://ir.library.osaka-u.ac.jp/

The University of Osaka

Anisotropic Interfacial Tension and Equilibrium Crystal Shapes of Exactly Solvable Models

by

Masafumi Fujimoto

Department of Physics, Faculty of Science, Osaka University, Machikaneyama 1-1, Toyonaka 560, Japan.

March, 1991

Abstract

To find the anisotropic correlation length of the hard-hexagon model, the shift operator is introduced into the usual transfer matrix method; the shift operator has the effect of moving the particle configuration of a row to the right. The anisotropic correlation length is calculated from the largest and next-largest eigenvalues of the transfer matrix and those of the shift operator. This method is applied to the calculation of the interfacial tension of the hard-hexagon model in two ways. (A) An inhomogeneous system is defined on a square lattice with (1 + v)M columns as follows: the lhs of the (M + 1)th column is the hard-hexagon model; in the rhs of the (M + 1)th column the particle configuration of the (M + i + 1)th column is given by shifting that of the (M + i)th column by a lattice spacing downward, where $i = 1, 2, \dots, Mv$. It is found that a triplet of the largest eigenvalues of the transfer matrix are asymptotically degenerate as $M \to \infty$. The anisotropic interfacial tension is calculated from the finite size correction terms in this limit. (B) A system with a mismatched vertical seam is considered. The seam is tilted by the shift operator. Reflecting the existence of the seam, extra factors appear in the largest eigenvalues of the transfer matrix. The anisotropic interfacial tension is obtained from the extra factors. By the use of the anisotropic interfacial tension, the equilibrium crystal shape of the hard-hexagon model is derived via Wulff's construction.

ABSTRACT

The shift operator method is applicable to a wide class of solvable models other than the hard-hexagon model. The anisotropic interfacial tension of the eightvertex model is calculated by the method (A), and the equilibrium crystal shape is derived by the use of Wulff's construction. According to Baxter, the eight-vertex model is parametrized by three variables z, x, and q; z represents anisotropy of the interactions; x corresponds to the temperature; the eight-vertex model reduces to either the Ising model or the six-vertex model if we put q = 0 or x^4 , respectively. The anisotropic interfacial tension and the equilibrium crystal shape are shown to be independent of q, which is an extension of the fact that the equilibrium crystal shapes of the square lattice Ising model and the six-vertex model are essentially the same. It is pointed out that the equilibrium crystal shape of the eight-vertex model is represented as a symmetric biquadratic relation, and that the elliptic solution of the anisotropic interfacial tension can be regarded as a natural parametrization of this relation.

Contents

Abstractii
Chapter 1. Exactly Solvable Models:
Historical Background1
Chapter 2. Hard-Hexagon Model: Anisotropic
Correlation Length and Interfacial Tension
1. Introduction
2. Commuting transfer matrices argument
2.1 Star-triangle relation
2.2 Functional equations and eigenvalues
3. Disordered state
3.1 Anisotropic correlation length 1
3.2 Anisotropic correlation length 2
4. Ordered state
4.1 Anisotropic interfacial tension 1
4.2 Anisotropic interfacial tension 2
4.3 Anisotropic interfacial tension 3
4.4 Equilibrium crystal shape46
4.5 Anisotropic correlation length

CONTENTS

Chapter 3. Eight-vertex Model: Anisotropic Interfacial Tension and Equilibrium Crystal Shape

1. Introduction
2. Commuting transfer matrices argument
3. Shift operator method
4. Anisotropic interfacial tension
5. Equilibrium crystal shape
Appendix
Chapter 4. Summary and Discussion
Acknowledgments
References

Chapter 1. Exactly Solvable Models: Historical Background

In principle, averaged properties (like magnetization, pressure, etc.) of a mechanical system can be calculated from a microscopic Hamiltonian within the framework of the statistical mechanics. Practically, however, these kinds of calculations are very complicated. Generally, even the (zero-field) free energy is not susceptible to exact analysis! We call a model exactly solvable model if its free energy can be calculated without any approximations. In this paper our attentions are restricted to the two dimensional exactly solvable models.

The pioneering work in the two-dimensional exactly solvable models was done by Onsager (1944). He calculated the free energy of the square lattice (nearestneighbor) Ising model by diagonalizing the transfer matrix. After Onsager, many authors re-derived the free energy of this model by alternative techniques. Kasteleyn (1963) showed that the partition function of the square lattice Ising model can be expressed as a dimer problem on a decorated lattice, and wrote the partition function as a Pfaffian (Kasteleyn, 1961). This Pfaffian method is also useful for calculating other physical quantities than the partition function: the magnetization, the anisotropic correlation length, etc. (McCoy and Wu, 1973). It is known that all the planar Ising models without bond crossings can be solved by the Pfaffian method; for example, the triangular and honeycomb lattice Ising models (Stephenson, 1964), the free-fermion model (Fan and Wu, 1970), etc. were solved by this method.

The next example following the Ising model was the ice-type model (or the sixvertex model), which was solved by Lieb (1967a, b, c). There, he could use the same method that Bethe (1931) had used for the one-dimensional Heisenberg chain, since the eigenvectors of the transfer matrix of this model are those of the Hamiltonian of the Heisenberg chain (Sutherland, 1970). Lieb's solution became the starting point of discovering a wide class of exactly solvable models. Baxter (1982) reproduced Lieb's solution as follows: investigating the star-triangle relation among the local Boltzmann weights, he constructed a one-parameter family of commuting transfer matrices; then, by the use of an equation for the transfer matrix, their eigenvalues were determined. He solved the eight-vertex model by extending this alternative method (Baxter, 1971, 1972). After that, it was shown that, from the local Boltzmann weights, the free energy and the one-point function (or the magnetization) can be directly calculated by the matrix inversion method (Stroganov, 1979) and the corner transfer matrix method (Baxter, 1976), respectively. Baxter's method of solving a statistical model is summarized as follows:

- (i) Look for a model whose local Boltzmann weights satisfy the star-triangle relation.
- (ii) Calculate the free energy and the one-point function by the matrix inversion method and the corner transfer matrix method.

Using this method, Baxter (1980) solved the hard-hexagon model. Following Bax-

ter's program, many authors found hierarchies of infinite number of solvable models (Andrews et al., 1984; Kuniba et al., 1986).

Recently the interface and crystal shape problem has attracted much attention due to the roughening transition phenomena (Dobrushin, 1972; Gallavotti, 1972; Weeks et al., 1973; Abraham and Reed, 1974, 1976). Analysis of the anisotropic interfacial tension is very important there. For example, using Wulff's construction, we can find the equilibrium crystal shape from its anisotropy. Disappearance of facets in the equilibrium crystal shape is an indication of the roughening transition.

For the Ising models on the square, honeycomb, and triangular lattices, the equilibrium crystal shapes were derived (Rottman and Wortice, 1981; Avron et al., 1982; Zia, 1986). Before that time, it had been pointed out that the anisotropic correlation length and the anisotropic interfacial tension of these models are simply connected with each other (Zia, 1978; Fradkin et al., 1978). Furthermore, the anisotropic correlation length had been calculated by the Pfaffian method (Cheng and Wu, 1967; McCoy and Wu, 1973). By the use of these results, the equilibrium crystal shapes of the Ising models were found via Wulff's construction. On the other hand, Beijern (1977) and Jayaprakash et al. (1983) regarded the six-vertex model as a solid-on-solid model on a body centered cubic lattice (the BCSOS model), and discussed the roughening transition of the three dimensional crystal. There, the feature that the six-vertex model can be solved in external field was used (Yang, 1967; Sutherland et al., 1967).

It is clearly desirable to carry out such programs for the models solved by Baxter's method. In this paper we show how this is done for the hard-hexagon model

1. EXACTLY SOLVABLE MODELS

and the eight-vertex model. In Chapter 2 we calculate the anisotropic correlation length and the anisotropic interfacial tension of the hard-hexagon model (Fujimoto, 1990a, b). For the hard-hexagon model, the correlation length and the interfacial tension have been calculated along special directions by the usual transfer matrix method (Baxter and Pearce, 1982). This method, however, is not applicable to the analyses of the anisotropy. We propose a new method which introduces the shift operator into the usual transfer matrix method. By this method, the anisotropic correlation length and the anisotropic interfacial tension of the hard-hexagon model are calculated. From the anisotropic interfacial tension, the equilibrium shape of the hard-hexagon crystal is derived via Wulff's construction. We note that the shift operator method is applicable to a wide class of solvable models.

In Chapter 3 we calculated the anisotropic interfacial tension of the eight-vertex model by the method introduced in Chapter 2. Then, the equilibrium crystal shape of the eight-vertex model is derived. The eight-vertex model contains the square lattice Ising model and the six-vertex model as special limits. It is known that the equilibrium crystal shapes of these models are represented as a simple algebraic curve (Zia and Avron, 1982; Akutsu and Akutsu, 1990). We discuss a relation between the curve and the elliptic solutions of the interfacial tension. Chapter 4 is devoted to a summary and discussion.

Chapter 2. Hard-Hexagon Model: Anisotropic Correlation Length and Interfacial Tension

1. Introduction

The hard-hexagon model was originally introduced as a simplified model of atoms in real fluid with strongly repulsive cores (Runnels and Combs, 1966; Gaunt, 1967). In this model particles are placed on sites of a triangular lattice in such a way that no two particles occupy the same site or adjacent ones (Baxter, 1982). Because of this constraint, one particle excludes other particles from the hexagonal region around it (Fig. 2.1). Hence this model is called the hard-hexagon model. For a given value of one-particle activity z, we want to know the grand-partition function

$$Z = \sum_{n=0}^{N/3} z^n g(n, N)$$
(1.1)

where a lattice of N sites was assumed and g(n, N) is the number of allowed ways of placing n particles on the lattice. Since the particles can not occupy over 1/3 of the sites, n takes values from 0 to N/3. As z increases, this model undergoes a phase transition from a homogeneous phase to an inhomogeneous one, where every third site is preferentially occupied. This phase transition is represented by an order parameter, which is the difference between the sublattice densities ρ_A, ρ_B, ρ_C .

Baxter (1980) exactly calculated the free energy of this model and the order

-5 -

parameter. According to Baxter's exact calculation, the critical activity is

$$z_c = (11 + 5\sqrt{5})/2 \sim 11.09 \tag{1.2}$$

and the critical exponents are

$$\alpha = \alpha' = 1/3 \tag{1.3}$$

$$\beta = 1/9 \tag{1.4}$$

Later, Baxter and Pearce (1982) analyzed the correlation length and the interfacial tension using the transfer matrix method. They determined other critical exponents,

$$\nu = \nu' = 5/6, \qquad \mu = 5/6$$
 (1.5)

In this analysis, however, the anisotropy (or the directional dependence) of the correlation length and the interfacial tension was not taken into account: special directions of the line connecting two particles and the interface were assumed.

Naturally, the usual transfer matrix analyses of the correlation length and the interfacial tension have a fault that calculations of the anisotropy are not possible. Because of this difficulty, the calculations of the anisotropy have not been accomplished for other solvable models either. This chapter has three purposes. First, to improve the usual transfer matrix method, we introduce the shift operator. Secondly, by the use of the improved transfer matrix method, the anisotropy of the correlation length and the interfacial tension of the hard-hexagon model is calculated. Thirdly, from the calculated anisotropic interfacial tension, the equilibrium crystal shape of the hard-hexagon model is derived via Wulff's construction.

The outline of this chapter is as follows. To calculate the correlation length and the interfacial tension, we need eigenvalues of the transfer matrix is needed. In Section 2 diagonalization of the transfer matrix of the hard-hexagon model by Baxter and Pearce is summarized. My own work starts with Section 3, where the disordered state of the hard-hexagon model is considered. In Section 3.1 we propose a new method, which introduces the shift operator into the usual transfer matrix method (Fujimoto, 1990a). In Section 3.2 the anisotropic correlation length of the hard-hexagon model is calculated by the new method.

In Section 4 the ordered state of this model is considered. The hard-hexagon model has a feature that three phases are degenerate in the ordered state. Noting this point, we define two types of interfaces in Section 4.1. Baxter and Pearce found the interfacial tension for a special direction by two methods: (A) by analyzing asymptotic degeneracy of the largest eigenvalues of the transfer matrix; (B) by calculating extra factors in the largest eigenvalues of the transfer matrix. In Section 4.2 the method (B) is extended to the analysis of the anisotropic interfacial tension by the shift operator method given in Section 3.1. Extension of the method (A) is considered in Section 4.3, where an inhomogeneous system is studied (Fujimoto, 1990b). The results of Section 4.2 and 4.3 are used to derive the equilibrium shape of the hard-hexagon crystal in Section 4.4. In Section 4.5 the correlation length in the ordered state is discussed.

2. Commuting transfer matrices argument

2.1. Star-triangle relation

A heuristic method of finding a solvable model is to look for a one-parameter family of commuting transfer matrices (the commuting family). Generalizing the hard-hexagon model to the hard-square model, Baxter (1980, 1982) obtained the commuting family. Then, Baxter and Pearce (1982) derived a functional equation for eigenvalues of the commuting family. Using this equation, they determined explicit forms of the eigenvalues of all the commuting family. In Sections 2.1 and 2.2 we summarize their arguments.

The hard-hexagon model can be regarded as a special case of the hard-square model with diagonal interactions. In the hard-square model an occupation number σ_i is located at each site *i* on the square lattice; $\sigma_i = 0$ if the site *i* is empty, and $\sigma_i = 1$ if the site *i* is occupied by a particle. Owing to the hard-core condition, a constraint $\sigma_i \sigma_j = 0$ is imposed on every nearest neighbor pair *i*, *j*. If the occupation numbers around a face are *a*, *b*, *c*, and *d* counterclockwise starting from the southwest (SW) corner, the Boltzmann weight of the face is

$$W(a, b, c, d) = mz^{(a+b+c+d)/4} e^{Kac+Lbd} t^{-a+b-c+d}$$

if $ab = bc = cd = da = 0$ (2.1)

where z is the one-particle activity; K and L is the interaction energy (divided by the temperature) in the SW-NE and SE-NW diagonal, respectively (Fig. 2.2). For calculational convenience, two factors m and t are introduced; m is a trivial

otherwise

= 0

– 8 –

normalization factor of the partition function; t cancels out of the partition function from face to face; these factors are irrelevant to the statistical average. We denote the nonzero elements of W's as follows:

$$\omega_1 = W(0000) = m \tag{2.2a}$$

$$\omega_2 = W(1000) = W(0010) = mz^{1/4}t^{-1}$$
(2.2b)

$$\omega_3 = W(01000) = W(0001) = mz^{1/4}t \tag{2.2c}$$

$$\omega_4 = W(1010) = mz^{1/2}t^{-2}e^K \tag{2.2d}$$

$$\omega_5 = W(0101) = mz^{1/2} t^2 e^L \tag{2.2e}$$

These relations (2.2) give the one-one correspondence between five ω 's and (z, K, L, m, t). In the $K \to 0$ and $L \to -\infty$ limit, this model reduces to the hard-hexagon model. At this time, the square lattice is interpreted as a deformed triangular lattice where the hard-hexagon model is originally defined.

Let $\sigma = \{\sigma_1, \sigma_2, \dots, \sigma_M\}$ and $\sigma' = \{\sigma'_1, \sigma'_2, \dots, \sigma'_M\}$ be particle configurations of two successive rows of a square lattice wound a cylinder. The row-row transfer matrix has elements

$$\left[\mathbf{V}\right]_{\sigma,\sigma'} = \prod_{i=1}^{M} W\left(\sigma_i, \sigma_{i+1}, \sigma'_{i+1}, \sigma'_i\right)$$
(2.3)

where $\sigma_{M+1} = \sigma_1$ and $\sigma'_{M+1} = \sigma'_1$. We want to find a series of transfer matrices (with different values of z, K, L, m, and t) which commute with **V**.

Define another transfer matrix \mathbf{V}' in the same way, with (z, K, L, m, t) replaced by (z', K', L', m', t'). We denote the corresponding Boltzmann weight W (or ω) by

 $W'(\text{or }\omega')$. Consider the matrix products \mathbf{VV}' and $\mathbf{V'V}$. The elements of \mathbf{VV}' are represented as

$$\sum_{\sigma''} \left[\mathbf{V} \right]_{\sigma,\sigma''} \left[\mathbf{V}' \right]_{\sigma'',\sigma'} = \sum_{\sigma''} \prod_{i=1}^{M} W \left(\sigma_i, \sigma_{i+1}, \sigma_{i+1}', \sigma_i' \right) W' \left(\sigma_i'', \sigma_{i+1}', \sigma_{i+1}', \sigma_i' \right)$$
$$= \operatorname{Tr} \left\{ \mathbf{R} \left(\sigma_1, \sigma_2, \sigma_2', \sigma_1' \right) \mathbf{R} \left(\sigma_2, \sigma_3, \sigma_3', \sigma_2' \right) \cdots \cdots \mathbf{R} \left(\sigma_M, \sigma_1, \sigma_1', \sigma_M' \right) \right\}$$
(2.4)

where \mathbf{R} 's are two-by-two matrices with elements

$$[\mathbf{R}(a, b, c, d)]_{e,f} = W(a, b, f, e)W'(e, f, c, d)$$
(2.5)

Similarly

$$\sum_{\sigma''} \left[\mathbf{V}' \right]_{\sigma,\sigma''} \left[\mathbf{V} \right]_{\sigma'',\sigma'} = \operatorname{Tr} \left\{ \mathbf{R}' \left(\sigma_1, \sigma_2, \sigma'_2, \sigma'_1 \right) \mathbf{R}' \left(\sigma_2, \sigma_3, \sigma'_3, \sigma'_2 \right) \cdots \\ \cdots \mathbf{R}' \left(\sigma_M, \sigma_1, \sigma'_1, \sigma'_M \right) \right\}$$
(2.6)

where

$$[\mathbf{R}'(a, b, c, d)]_{e,f} = W'(a, b, f, e)W(e, f, c, d)$$
(2.7)

If there exist two-by-two nonsingular matrices \mathbf{M} 's such that

$$\mathbf{R}(a, b, c, d) = \mathbf{M}(d, a) \mathbf{R}'(a, b, c, d) \left[\mathbf{M}(b, c)\right]^{-1}$$
(2.8)

for all $a, b, c, d = \pm 1$, the transfer matrices **V** and **V'** commute with each other. Post-multiplying (2.8) by $\mathbf{M}(b, c)$, and rewriting the element of (a, c) of $\mathbf{M}(b, d)$ as W''(a, b, c, d), we obtain the star-triangle relation

$$\sum_{c} W(a, b, c, a'') W'(a'', c, b', a') W''(c, b, b'', b')$$

=
$$\sum_{c} W''(a'', a, c, a') W'(a, b, b'', c) W(c, b'', b', a') \qquad (2.9)$$

- 10 -

for all $a, a', a'', b, b', b'' = \pm 1$ (Fig. 2.3). It is also assumed that W'''s are given by (2.1), with z, K, L, m, and t replaced by z'', K'', L'', m'', and t''. Here, the problem is defined precisely:

"For given values of (z, K, L, m, t) and (z', K', L', m', t'), look for a third set (z'', K'', L'', m'', t'') which satisfies (2.9). If any, **V** and **V**' commute with each other." (2.10)

Since the normalization factors m, m', and m'' are canceled out of the both sides, (2.9) imposes seven conditions on the four unknowns z'', K'', L'', and t''. For general values of (z, K, L, t) and (z', K', L', t') this problem does not have a solution. Following Baxter, we return to (2.1) and restrict ourselves to the models which satisfy

$$z = (1 - e^{-K}) (1 - e^{-L}) / (e^{K+L} - e^{K} - e^{L})$$
(2.11)

We choose (z', K', L') from these models so that two sets (z, K, L) and (z', K', L')have the same value of Δ :

$$\Delta = z^{-1/2} \left(1 - z e^{K+L} \right)$$

= $z'^{-1/2} \left(1 - z' e^{K'+L'} \right)$ (2.12)

Because of (2.11) and (2.12), the number of independent conditions imposed on (z'', K'', L'', t'') is reduced to four. At this stage, we can find a solution.

To see this, it is convenient to parametrize (2.11) and (2.12) in terms of elliptic theta functions. Substituting (2.11) into (2.12), we get the symmetric biquadratic relation between e^{K} and e^{L}

$$\Delta^{-2} e^{K+L} = (e^{K} - 1) (e^{L} - 1) (e^{K+L} - e^{K} - e^{L})$$
(2.13)
- 11 -

This relation is naturally parametrized as follows:

$$e^{K} = \theta_{1}(\lambda)\theta_{1}(2\lambda + u)\theta_{1}(2\lambda - u) / \left[\theta_{1}(2\lambda)\theta_{1}^{2}(u)\right]$$
(2.14a)

$$e^{L} = \theta_{1}(\lambda)\theta_{1}(3\lambda - u)\theta_{1}(\lambda + u) / \left[\theta_{1}(2\lambda)\theta_{1}^{2}(\lambda - u)\right]$$
(2.14b)

$$\Delta^2 = \left[\theta_1(\lambda)/\theta_1(2\lambda)\right]^5 \tag{2.14c}$$

and

$$z = \theta_1^3(2\lambda)\theta_1^2(u)\theta_1^2(\lambda - u) / \left[\theta_1^3(2\lambda)\theta_1^4(2\lambda + u)\right]$$
(2.14d)

where $\lambda=\pi/5$ and the elliptic theta function defined by

$$\theta_1(u, q^2) = \sin u \prod_{n=1}^{\infty} \left(1 - q^{2n} e^{2iu} \right) \left(1 - q^{2n} e^{-2iu} \right) \left(1 - q^{2n} \right), \qquad -1 < q^2 < 1$$
(2.15)

is abbreviated to $\theta_1(u)$. After m and t are determined suitably, we get

$$\omega_1(u) = \theta_1(2\lambda + u)/\theta_1(2\lambda) \tag{2.16a}$$

$$\omega_2(u) = \pm \theta_1(u) / \left[\theta_1(\lambda)\theta(2\lambda)\right]^{1/2}$$
(2.16b)

$$\omega_3(u) = \theta_1(\lambda - u)/\theta_1(\lambda) \tag{2.16c}$$

$$\omega_4(u) = \theta_1(2\lambda - u)/\theta_1(2\lambda) \tag{2.16d}$$

$$\omega_5(u) = \theta_1(\lambda + u)/\theta_1(\lambda) \tag{2.16e}$$

The condition (2.12) requires the same value of q^2 for (z', K', L'). We use (2.16) for ω' 's, with u replaced by u'. The third set ω'' 's is also given by (2.16), ubeing replaced by u'-u. The fact that these three sets of Boltzmann weights satisfy the star-triangle relation (2.9) is directly verified by the use of addition formula

$$\theta_{1}(u+x)\theta_{1}(u-x)\theta_{1}(v+y)\theta_{1}(v-y) - \theta_{1}(u+y)\theta_{1}(u-y)\theta_{1}(v+x)\theta_{1}(v-x)$$

= $\theta_{1}(x+y)\theta_{1}(x-y)\theta_{1}(u+v)\theta_{1}(u-v)$ (2.17)

– 12 –

Thus, we get the one-parameter family of commuting transfer matrices

$$\left[\mathbf{V}(u)\right]_{\sigma,\sigma'} = \prod_{i=1}^{M} W\left(\sigma_i, \sigma_{i+1}, \sigma'_{i+1}, \sigma'_i \middle| u\right)$$
(2.18)

2.2. Functional equations and eigenvalues

To find a transfer matrix equation, we consider the matrix product $\mathbf{V}(u)\mathbf{V}(u + \lambda)$, which has elements

$$\sum_{\sigma''} \left[\mathbf{V}(u) \right]_{\sigma,\sigma''} \left[\mathbf{V}(u+\lambda) \right]_{\sigma'',\sigma'} = \operatorname{Tr} \left\{ \mathbf{R} \left(\sigma_1, \sigma_2, \sigma'_2, \sigma'_1 \middle| u \right) \mathbf{R} \left(\sigma_2, \sigma_3, \sigma'_3, \sigma'_2 \middle| u \right) \cdots \right. \\ \cdots \left. \mathbf{R} \left(\sigma_M, \sigma_1, \sigma'_1, \sigma'_M \middle| u \right) \right\}$$
(2.19)

where

$$\left[\mathbf{R}\left(a,b,c,d\big|u\right)\right]_{e,f} = W\left(a,b,f,e\big|u\right)W\left(e,f,c,d\big|u+\lambda\right)$$
(2.20)

It is found that **R**'s satisfy the relations

$$\mathbf{R}(1000|u)\,\mathbf{R}(0110|u') = 0 \tag{2.21a}$$

$$\mathbf{R}\left(0001|u\right)\mathbf{R}\left(0110|u'\right) = 0 \tag{2.21b}$$

$$\mathbf{R}\left(1000|u\right)\mathbf{R}\left(0000|u'\right) = \left[\theta_1^2(u')/\theta_1(\lambda)\theta_1(2\lambda)\right]\mathbf{R}\left(1000|u\right)$$
(2.21c)

$$\mathbf{R}\left(0001|u\right)\mathbf{R}\left(0000|u'\right) = \left[\theta_1^2(u')/\theta_1(\lambda)\theta_1(2\lambda)\right]\mathbf{R}\left(0001|u\right)$$
(2.21*d*)

$$\mathbf{R}\left(0000|u\right)\mathbf{R}\left(0110|u'\right) = \left[\theta_1(\lambda+u)\theta_1(\lambda-u)/\theta_1^2(\lambda)\right]\mathbf{R}\left(0110|u'\right) \quad (2.21e)$$

where, for later convenience, the generalized case was considered; here, we assume that u = u'. Because of the periodic boundary conditions, it follows from these

relations that the non-zero elements of $[V(u)V(u + \lambda)]_{\sigma,\sigma'}$ can be classified into two categories: $\sigma_j = \sigma'_j$ for all j, or $\sigma_j \sigma'_j = 0$ for all j. In the case $\sigma_j = \sigma'_j$, the matrix elements are all $[\theta_1(\lambda + u)\theta_1(\lambda - u)/\theta_1^2(u)]^M$. In the case $\sigma_j \sigma'_j = 0$, careful examination of the matrix elements shows that they give the matrix element of $[\theta_1(u)/\theta_1(\lambda)]^M \mathbf{V}(u - 2\lambda)$. Thus, we get the transfer matrix equation

$$\mathbf{V}(u)\mathbf{V}(u+\lambda) = \left[\frac{\theta_1(\lambda+u)\theta_1(\lambda-u)}{\theta_1^2(\lambda)}\right]^M \mathbf{I} + \left[\frac{\theta_1(u)}{\theta_1(\lambda)}\right]^M \mathbf{V}(u-2\lambda)$$
(2.22)

where **I** is the identity matrix.

As we showed in Section 2.1, $\mathbf{V}(u)$ is a one-parameter family of commuting transfer matrices, being simultaneously diagonalized for all u. The transfer matrix equation (2.22) gives the eigenvalue equation

$$T(u)T(u+\lambda) = 1 + T(u-2\lambda)$$
(2.23)

where we introduced the 'dimensionless' transfer matrix by

$$\mathbf{T}(u) = \left(-\frac{\omega_1(u)}{\omega_4(u)\omega_5(u)}\right)^M \mathbf{V}(u)$$
(2.24)

and T(u) is an eigenvalue of $\mathbf{T}(u)$. We also find the periodicity relation

$$T(u+5\lambda) = T(u) \tag{2.25}$$

By the use of (2.23) and (2.25), we can determine the explicit form of T(u). Such a calculation is not reproduced here, since it will be done for more general case in Section 4.3. Only the results needed in Sections 3.2 and 4.5 are listed in the following.

– 14 –

Hereafter, we restricted ourselves to the case $-\lambda < u < 0$. Two regimes are defined:

Regime
$$\mathbf{I}$$
 $-1 < q^2 < 0$, $-\lambda < u < 0$
Regime \mathbf{II} $0 < q^2 < 1$, $-\lambda < u < 0$

$$(2.26)$$

The regime **I** is the disordered regime, $q^2 = 0$ corresponds to the critical point, and the regime **II** is the triangular ordered regime, where every third site is occupied by a particle. The original hard-hexagon model corresponds to the $u \to -\lambda$ limit.

First, we consider the regime I. There, the eigenvalue T is labeled by r, which is a non-negative integer not greater than M/2. As $M \to \infty$, T behaves as (Baxter and Pearce, 1982)

$$T_r(w) = \phi^M(w) \prod_{i=1}^r \phi(a_i w^{-1}), \qquad x^4 < |w| < |x|^{-1}$$
(2.27)

where

$$\phi(w) = -\frac{1}{w} \frac{f(xw, x^6) f(x^2w, x^6)}{f(xw^{-1}, x^6) f(x^2w^{-1}, x^6)}$$
(2.28)

and

$$x = -e^{-\pi^2/5\varepsilon}, \qquad w = e^{2\pi u/\varepsilon}, \qquad q^2 = -e^{-\varepsilon}$$
 (2.29)

The function f(w, x) is defined by

$$f(w,x) = (1-w)\prod_{n=1}^{\infty} (1-wx^n)(1-w^{-1}x^n)(1-x^n)$$
(2.30)

The complex numbers a_i 's are determined by the equations

$$\phi^M(a_i) = -\prod_{j=1}^r \phi(a_i/a_j), \qquad i = 1, 2, \cdots, r$$
 (2.31)

with $|a_i| = 1$. For r = 0, (2.27) gives one real eigenvalue $T_0(w) = \phi^M(w)$, which is the largest in the regime **I**. When $r \neq 0$, there are many eigenvalues, corresponding

to the different solutions of (2.31). For r = 1, (2.27) and (2.31) give a band of the M next-largest eigenvalues. In the $M \to \infty$ limit, we shall assume a continuous distribution of a_i 's on the unit circle.

In the regime \mathbf{II} , the eigenvalue T is labeled by two integers p and r, which satisfy the relation

$$p + 2r \equiv M \pmod{3} \tag{2.32}$$

When $M \equiv 0 \pmod{3}$, a triplet of the largest eigenvalues are asymptotically degenerate as $M \to \infty$. These eigenvalues are given by $(p, r) = (0, 0) = \mathbf{0}$; for large M

$$T_{\mathbf{0};\tau}(w) = \tau \psi^M(w), \qquad x^{1/2} < |w| < x^{-2}$$
 (2.33)

where

$$\psi(w) = -w^{1/3} \frac{f(xw^{-1}, x^3)}{f(xw, x^3)}$$
(2.34)

and τ is a cube root of unity and

$$x = e^{-4\pi^2/5\varepsilon}, \qquad w = e^{-4\pi u/\varepsilon}, \qquad q^2 = e^{-\varepsilon}$$
 (2.35)

For $(p, r) \neq \mathbf{0}$

$$T_{p,r}(w) = \psi^M(w) \prod_{i=1}^p \psi(a_i w^{-1}) \prod_{j=1}^r \bar{\psi}(b_j w^{-1}), \qquad x^{1/2} < |w| < x^{-2}$$
(2.36)

where

$$\bar{\psi}(w) = \psi(x^{3/2}w^{-1}) = w^{2/3} \frac{f(x^{1/2}w^{-1}, x^3)}{f(x^{1/2}w, x^3)}$$
(2.37)

and a_i 's and b_j 's are solutions of the equations

$$\psi^{M}(a_{i}) = -\prod_{k=1}^{p} \psi(a_{i}/a_{k}) \prod_{l=1}^{r} \bar{\psi}(a_{i}/b_{l}), \qquad i = 1, 2, \cdots, p \qquad (2.38a)$$

$$\psi^{M}(b_{j}) = -\prod_{k=1}^{p} \bar{\psi}(b_{j}/a_{k}) \prod_{l=1}^{r} \psi(b_{j}/b_{l}), \qquad j = 1, 2, \cdots, r$$
(2.38b)

with $|a_i| = |b_j| = 1$. When $M \equiv 1 \pmod{3}$ [or $M \equiv 2 \pmod{3}$], there exists a band of the largest eigenvalues given by (p,r) = (1,0) [or (0,1)]. It will be shown that the interfacial tension can be calculated from the factors $\psi(a_i w^{-1})$ [or $\bar{\psi}(b_j w^{-1})$] in the largest eigenvalues. The next-largest eigenvalues are given by (2.36) and (2.38) with (p,r) = (1,1), (2,1), and (1,2) for $M \equiv 0, 1$, and 2 (mod 3), respectively.

3. Disordered state

3.1. Anisotropic correlation length 1

Letting $u \to -\lambda$ in the regime **I**, we consider the disordered state of the hardhexagon model. We start by reviewing the usual transfer matrix analysis of the correlation length (p.18 and p.114 of Baxter, 1982), and explain its difficulty of finding the anisotropy. Then, to avoid this difficulty, the shift operator is introduced (Fujimoto, 1990a).

A square lattice with M columns and N rows is assumed. We impose on it cyclic boundary conditions in both directions (toroidal boundary conditions). In the usual transfer matrix analysis, the correlation between the site (0,0) and the site (l,m) is represented as

$$<\sigma_{00}\sigma_{lm}>=\frac{\mathrm{Tr}[\mathbf{S}_{0}\mathbf{V}^{l}\mathbf{S}_{m}\mathbf{V}^{N-l}]}{\mathrm{tr}[\mathbf{V}^{N}]},\qquad N>l>0$$
(3.1)

where **V** is the transfer matrix given by (2.18), with $u = -\lambda$, and **S**_k's are matrices defined by

$$\begin{bmatrix} \mathbf{S}_k \end{bmatrix}_{\sigma,\sigma'} = \sigma_k \quad \text{if} \quad \sigma = \sigma' \\ = 0 \quad \text{otherwise}$$

$$(3.2)$$

for $k = 0, 1, 2, \dots, M-1$. Applying the similarity transformation which diagonalizes **V**, and letting $N, M \to \infty$, we get

$$<\sigma_{00}\sigma_{lm}> = \sum_{p} \tilde{S}_{0}(1,p)\tilde{S}_{m}(p,1) \left[\frac{V(p)}{V(1)}\right]^{l}, \qquad l>0$$
 (3.3)

where $\hat{\mathbf{S}}_k$ is the matrix transformed from \mathbf{S}_k by the matrix of eigenvectors of \mathbf{V} , and V(p) is the *p*th eigenvalue of \mathbf{V} in decreasing order of absolute value. For simplicity

– 18 –

we assumed that

$$|V(1)| > |V(2)| > \cdots$$
 (3.4)

Since

$$<\sigma_{00}><\sigma_{lm}>=\tilde{S}_0(1,1)^2=\tilde{S}_0(1,1)\tilde{S}_m(1,1)$$
 (3.5)

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

$$<\sigma_{00}\sigma_{lm}> - <\sigma_{00}><\sigma_{lm}> = \sum_{p\neq 1} \tilde{S}_0(1,p)\tilde{S}_m(p,1) \left[\frac{V(p)}{V(1)}\right]^l, \quad l>0 \quad (3.6)$$

When m is fixed and l becomes large, the rhs of (3.6) decays exponentially. Analyzing this decay rate, which can be calculated from the ratios between the largest and next-largest eigenvalues of \mathbf{V} , we can find the correlation length ξ along the vertical axis:

$$-1/\xi = \ln\left[\frac{V(2)}{V(1)}\right] \tag{3.7}$$

This is the usual method.

Now we find the anisotropy. The behavior of the correlation function, when the ratio m/l is fixed and l becomes large, comes into question. We expect that it also decays exponentially, and the correlation length along the direction designated by the ratio m/l can be calculated from the rate of this decay. In the rhs of (3.6), 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 complicated. Thus, the expression (3.7) is not suitable for finding the anisotropy of the correlation length.

To overcome this difficulty, we introduce the shift operator \mathbf{T} , which shifts the particle configuration of a row to the right:

$$[\mathbf{T}]_{\sigma,\sigma'} = \prod_{i=1}^{M} \delta(\sigma_i, \sigma'_{i+1})$$
(3.8)

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

$$\mathbf{S}_m = \mathbf{T}^m \mathbf{S}_0 \mathbf{T}^{-m} \tag{3.9}$$

The relation (3.9) can be used to rewrite (3.1) as

$$<\sigma_{00}\sigma_{lm}>=\frac{\mathrm{Tr}[\mathbf{S}_{0}\mathbf{V}^{l}\mathbf{T}^{m}\mathbf{S}_{0}\mathbf{T}^{-m}\mathbf{V}^{N-l}]}{\mathrm{tr}[\mathbf{V}^{N}]},\qquad N>l>0 \qquad (3.10)$$

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

$$<\sigma_{00}\sigma_{lm}> - <\sigma_{00}><\sigma_{lm}> = \sum_{p\neq 1}\tilde{S}_{0}(1,p)\tilde{S}_{0}(p,1)\left[\frac{V(p)}{V(1)}\left(\frac{T(p)}{T(1)}\right)^{v}\right]^{l} \quad (3.11)$$

for l > 0, where T(p) is the *p*th eigenvalue of **T**, and v = m/l.

Let v be fixed and l large. The rhs of (3.11) 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 those 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 \mathbf{T} practicable? As we mentioned in Section 2.1, finding a series of models whose transfer matrices commute with each other, the commuting family, has an important meaning in

– 20 –

Baxter's method of calculating the eigenvalues of the transfer matrix. The shift operator is always a member of the commuting family, being simultaneously diagonalized with the others. In the case of the hard-square model, the transfer matrix $\mathbf{V}(u)$ given by (2.18), with u = 0, corresponds to the shift operator. Thus, we can use the expression (2.27) with w = 1 for the eigenvalues of \mathbf{T} .

3.2. Anisotropic correlation length 2

Baxter and Pearce (1982) assumed the continuous distribution of the eigenvalues in (3.6), 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 l is large with v fixed, the correlation function is represented as

$$<\sigma_{00}\sigma_{lm}> - <\sigma_{00}> <\sigma_{lm}>$$

 $\sim \frac{1}{2\pi i} \oint_{|a|=1} \frac{da}{a} \rho(a) [\phi(ax^{-2})\phi(a)^{v}]^{l}, \qquad -\infty < v < \infty \qquad (3.12)$

where we used the expression (2.27) in (3.11), with $w = x^2$ and 1 for V(p)/V(1) and T(p)/T(1), respectively. In the $M \to \infty$ limit, the summation in (3.11) 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

$$z = -x \prod_{n=1}^{\infty} \left[\frac{(1 - x^{5n-4})(1 - x^{5n-1})}{(1 - x^{5n-3})(1 - x^{5n-2})} \right]^5, \qquad -1 < x < 0$$
(3.13)

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

$$v = \frac{1}{2} - \frac{\sqrt{3}}{2\tan\theta_{\parallel}}, \qquad 0 < \theta_{\parallel} < \pi$$
 (3.14)

We estimate the integral in the rhs of (3.12a) by the method of steepest descent. For example, when $\theta_{\parallel} = \pi/3$ (this is the case of Baxter and Pearce), from the derivative of $\ln \phi(a)$,

$$\frac{d}{da} \ln \phi(a) = -f(x^2, x^6) f(x^3, x^6)
\times \frac{1}{a} \frac{f(a^{-1}x^{3/2}, x^6) f(-a^{-1}x^{3/2}, x^6) f(ax^{3/2}, x^6) f(-ax^{3/2}, x^6)}{f(a^{-1}x, x^6) f(a^{-1}x^2, x^6) f(ax^2, x^6) f(ax, x^6)}$$
(3.15)

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, it follows that

$$<\sigma_{00}\sigma_{lm}> - <\sigma_{00}><\sigma_{lm}> \sim \alpha \exp(-l/\xi)\cos(l\eta+\delta)$$
(3.16a)

$$-1/\xi = \ln |\phi(x^{1/2})| \tag{3.16b}$$

$$\eta = \operatorname{Arg}[\phi(x^{1/2})] \tag{3.16c}$$

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

_

-22 -

For $\theta_{\parallel} \neq \pi/3$ the situation remains unchanged: two saddle points which are complex conjugate are found, and the rhs of (3.12a) can be estimated around them. The equation which determines the saddle points a_s is

$$\frac{d}{da}[\ln\phi(ax^{-2}) + v\ln\phi(a)] = 0, \qquad a = a_s$$
(3.17)

or from (3.14) and (3.15), after some calculations,

$$\frac{\sqrt{3} - \tan\theta_{\parallel}}{\sqrt{3} + \tan\theta_{\parallel}} = a \frac{f(ax, x^3) f(a^{-1}x^{1/2}, x^3) f(-a^{-1}x^{1/2}, x^3)}{f(a^{-1}x, x^3) f(ax^{1/2}, x^3) f(-ax^{1/2}, x^3)}, \quad a = a_s$$
(3.18)

Using (3.18) with the condition

_

$$a_s = x^{1/2}, \qquad \theta_{\parallel} = \pi/3$$
 (3.19)

we can uniquely determine the saddle point in the upper-half plane as an analytic function of θ_{\parallel} . (Hereafter we denote it by a_s .) For large l the correlation function can be represented as

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

$$-\frac{1}{\xi} = \frac{2}{\sqrt{3}} \left[\sin \theta_{\parallel} \ln |\phi(a_s x^{-2})| + \sin \left(\theta_{\parallel} - \frac{\pi}{3} \right) \ln |\phi(a_s)| \right]$$
(3.20b)

$$\eta = \{ \arg[\phi(a_s x^{-2})] + v \arg[\phi(a_s)] \} / (1+v)$$
(3.20c)

where

$$r = (l^2 + m^2 - lm)^{1/2} aga{3.20d}$$

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 useful

-23 –

to consider the conjugate modulus identities (p. 419 of Baxter, 1982; Baxter and Pearce, 1982)

$$\theta_{1} \left[u, \exp(-\varepsilon) \right] = \frac{1}{2} \left(\frac{2\pi}{\varepsilon} \right)^{1/2} \exp\left[\frac{\varepsilon}{8} - \frac{\pi^{2}}{2\varepsilon} + \frac{2u(\pi - u)}{\varepsilon} \right] \\ \times f \left[\exp\left(-\frac{4\pi u}{\varepsilon} \right), \exp\left(-\frac{4\pi^{2}}{\varepsilon} \right) \right]$$
(3.21)
$$\theta_{1} \left[u, -\exp(-\varepsilon) \right] = -\frac{1}{2} \left(\frac{\pi}{\varepsilon} \right)^{1/2} \exp\left[\frac{\varepsilon}{8} - \frac{\pi^{2}}{8\varepsilon} - \frac{u(2u + \pi)}{\varepsilon} \right] \\ \times f \left[\exp\left(\frac{2\pi u}{\varepsilon} \right), -\exp\left(-\frac{\pi^{2}}{\varepsilon} \right) \right]$$
(3.22)

These identities can be used in (3.18) to expand it into a power series of $\exp(-5\varepsilon/6)$ for large ε (or near the critical point), where the variable ε is related to x by (2.29). Keeping the dominant terms in the $\varepsilon \to \infty$ limit, and assuming the region of $0 < \operatorname{Arg}[a] < \pi$, we obtain

$$\frac{\sqrt{3} - \tan \theta_{\parallel}}{\sqrt{3} + \tan \theta_{\parallel}} = \exp\left(\frac{\pi}{3}i\right) \frac{A_0^2 - \exp(-5\varepsilon/3)\exp(-\pi i/3)}{A_0^2 - \exp(-5\varepsilon/3)\exp(\pi i/3)}$$
(3.23)

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

$$A = \exp\left[\left(\frac{5\varepsilon}{3\pi}\ln a_s\right)i\right] \tag{3.24}$$

From (3.23) and (3.19), it follows that

$$A_0 = \exp\left[\left(\theta_{\parallel} - \frac{\pi}{2}\right)i\right] \exp\left(-\frac{5}{6}\varepsilon\right)$$
(3.25)

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

$$A = A_0 \left\{ 1 + \Delta^{(1)} \exp\left(-\frac{5}{6}\varepsilon\right) + \Delta^{(2)} \exp\left(-\frac{10}{6}\varepsilon\right) + O\left[\exp\left(-\frac{15}{6}\varepsilon\right)\right] \right\} \quad (3.26)$$
$$-24 - C$$

and then by equating the coefficients of powers of $\exp(-5\varepsilon/6)$ in the expanded form of (3.18), which is obtained by the use of (3.22) and (3.26). The coefficients $\Delta^{(1)}, \Delta^{(2)}, \cdots$ are determined as

$$\Delta^{(1)} = -4\sin\theta_{\parallel}\sin\left(\theta_{\parallel} + \frac{\pi}{3}\right)\sin\left(\theta_{\parallel} - \frac{\pi}{3}\right)$$
(3.27*a*)

$$\Delta^{(2)} = \frac{1}{2} \left(\Delta^{(1)} \right)^2 - 8i\Delta^{(1)} \cos \theta_{\parallel} \cos \left(\theta_{\parallel} + \frac{\pi}{3} \right) \cos \left(\theta_{\parallel} - \frac{\pi}{3} \right)$$
(3.27b)
:

In terms of these coefficients, a_s can be represented as

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

$$\operatorname{Arg}[a_s] = \frac{\pi}{2} - \frac{3\pi}{5} \Delta^{(1)} \frac{1}{\varepsilon} \exp\left(-\frac{5}{6}\varepsilon\right) + \operatorname{O}\left[\frac{1}{\varepsilon} \exp\left(-\frac{15}{6}\varepsilon\right)\right]$$
(3.28b)

The results (3.27a) and (3.27b) can be used in (3.28a) and (3.28b) to find the relations, within the validity of this expansion,

$$a_s\left(\pi - \theta_{\parallel}\right) = \left[a_s^{-1}\left(\theta_{\parallel}\right)\right]^*, \qquad a_s\left(\theta_{\parallel} + \frac{\pi}{3}\right) = \left[a_s\left(\theta_{\parallel}\right)x^{-1}\right]^* \tag{3.29}$$

Here we return to (3.18) to find some properties which support (3.29). It is trivial that if a pair $(a_0, \theta_{\parallel})$ satisfies (3.18), then other pairs $(a_0^*, \theta_{\parallel})$ and $(a_0^{-1}, \pi - \theta_{\parallel})$ also satisfy (3.18). After some calculations, it is found that the pair $(a_0x^{-1}, \theta_{\parallel} + \pi/3)$ also satisfies (3.18). From these results, we expect that relations (3.29) hold exactly for all range of parameters, though we cannot prove it rigorously. Relations (3.29) can be used in (3.20b) to obtain the relations

$$\xi \left(-\theta_{\parallel}\right) = \xi \left(\theta_{\parallel}\right), \qquad \xi \left(\theta_{\parallel} + \pi/3\right) = \xi \left(\theta_{\parallel}\right) \tag{3.30}$$
$$-25 -$$

Expanding (3.20b) and (3.20c) in the same way, we use (3.27a) and (3.27b) to get

$$<\sigma_{00}\sigma_{lm} > - <\sigma_{00} > <\sigma_{lm} > \sim \alpha \exp\left(-\frac{r}{\xi}\right) \cos\left\{\frac{2\pi}{3}(l+m) + r\left[-4\sqrt{3}\cos\theta_{\parallel}\cos\left(\theta_{\parallel} + \frac{\pi}{3}\right)\cos\left(\theta_{\parallel} - \frac{\pi}{3}\right)\exp\left(-\frac{10}{6}\varepsilon\right) + O\left[\exp\left(-\frac{20}{6}\varepsilon\right)\right]\right] + \delta\right\}$$
(3.31*a*)
$$\xi = \frac{1}{2\sqrt{3}}\exp\left(\frac{5}{6}\varepsilon\right)\left\{1 - \left[1 - 8\sin^{2}\theta_{\parallel}\sin^{2}\left(\theta_{\parallel} + \frac{\pi}{3}\right)\sin^{2}\left(\theta_{\parallel} - \frac{\pi}{3}\right)\right]$$

$$\times \exp\left(-\frac{10}{6}\varepsilon\right) + O\left[\exp\left(-\frac{20}{6}\varepsilon\right)\right]\right\}$$
(3.31*b*)

Equation (3.31*a*) indicates that the angular dependence of the correlation function is $\cos [2\pi (l+m)/3]$ near the critical point. This reflects the ground-state configuration of this system. Equation (3.31b) 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 θ_{\parallel} :

$$\nu = 5/6$$
 for all θ_{\parallel} (3.32)

4. Ordered state

4.1. Anisotropic interfacial tension 1

The hard-hexagon model for $z > z_c$ is given by the $u \to -\lambda$ limit in the regime **II**. We assume a square lattice of M columns and N rows with toroidal boundary conditions. Baxter and Pearce (1982) calculated the interfacial tension for special directions by two methods. (A)When $M \equiv 0 \pmod{3}$, the triplet of the largest eigenvalues of the transfer matrix are asymptotically degenerate as $M \to \infty$ (see Section 2.2); they calculated the interfacial tension from the finite size correction terms at this time. (B)When $M \equiv 1$ or 2 (mod 3), extra factors $\psi(a_i w^{-1})$ and $\bar{\psi}(b_j w^{-1})$ appear in the largest eigenvalues of the transfer matrix; Baxter and Pearce pointed out that this fact reflects the existence of a mismatched vertical seam, and that these factors give the interfacial tension. In Sections 4.1 and 4.2, the method (B) is extended to the analysis of the anisotropic interfacial tension (Fujimoto, 1990a). In Section 4.3, we consider an extension of the method (A) (Fujimoto, 1990b).

The method (B) is explained in detail. When $M \equiv 1$ or 2 (mod 3) and $N \equiv 0$ (mod 3), there is a mismatched vertical seam (or an interface), since every third site is preferentially occupied by a particle for $z > z_c$. We expect that, in the $M, N \to \infty$ limit, an excess free energy above the bulk free energy proportional to N exists, and that this excess free energy gives the interfacial tension of the vertical direction. Using the notations in Section 3.1, we can represent the interfacial tension

– 27 –

as

$$-\beta\sigma = \lim_{N,M\to\infty} \frac{1}{N} \ln\left[\frac{1}{\kappa^{NM}} \operatorname{Tr} \mathbf{V}^{N}\right]$$
$$= \lim_{N,M\to\infty} \frac{1}{N} \ln\left[\sum_{p} \left(V(p)/\kappa^{M}\right)^{N}\right]$$
(4.1)

where β is the inverse temperature and κ is the partition function per site

$$\kappa = \lim_{N,M\to\infty} \left[\operatorname{Tr} \mathbf{V}^N \right]^{1/NM}$$
$$= \lim_{N,M\to\infty} \left[\sum_p V(p)^N \right]^{1/NM}$$
$$= \lim_{M\to\infty} \left[V(1) \right]^{1/M}$$
(4.2)

In the second line of (4.1), $V(p)/\kappa^M$ is the coefficient multiplied by the exponential divergence of V(p) as $M \to \infty$. From the fact that the summation is dominated by the largest eigenvalues in the $N \to \infty$ limit, $\beta\sigma$ can be calculated from these coefficients in the largest eigenvalues. They are factors $\psi(a_i w^{-1})$ and $\bar{\psi}(b_j w^{-1})$, which appear in (2.36) for (p, r) = (1, 0) or (0, 1).

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. 2.4). Similarly to (4.1), the anisotropic interfacial tension is given by

$$-\beta\sigma = \lim_{N,M\to\infty} \frac{1}{r} \ln\left[\frac{1}{\kappa^{NM}} \operatorname{Tr}\left(\mathbf{V}\mathbf{T}^{v}\right)^{N}\right]$$
$$= \lim_{N,M\to\infty} \frac{1}{r} \ln\left\{\frac{1}{\kappa^{NM}} \sum_{p} \left[V(p)T(p)^{v}\right]^{N}\right\}$$
(4.3)

where

$$r = N \left(1 + v^2 - v \right)^{1/2}$$
(4.4)
- 28 -

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

In contrast to the analysis by Baxter and Pearce, where the interfacial tension of $M \equiv 1 \pmod{3}$ and that of $M \equiv 2 \pmod{3}$ take the same value, it will be found that the interfacial tension for $M \equiv 1 \pmod{3}$ and $M \equiv 2 \pmod{3}$ are different in a general direction. To understand the physical meaning of this difference, we investigate what kinds of interfaces are considered in the cases of $M \equiv 1 \pmod{3}$ and $M \equiv 2 \pmod{3}$.

As we mentioned in the beginning of this section, 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 interfaces exist, corresponding to choosing any two phases for both sides of the interface from these three phases. The situation 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 interfaces 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 interfaces 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 $M \equiv 1 \pmod{3}$. 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 can not do this

-29 –

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 $M \equiv 1 \pmod{3}$ is type 1. In the case $M \equiv 2 \pmod{3}$, fixing the lhs of the interface to be A-phase, we find that the rhs is *C*-phase, and that the interface of $M \equiv 2 \pmod{3}$ is type 2 (Fig. 2.4). The difference between the interfacial tension of $M \equiv 1 \pmod{3}$ and $M \equiv 2 \pmod{3}$ reflects the difference between the two types of interfaces.

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 θ_{\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 sites. 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 (4.3) with the constraints $M \equiv 1 \pmod{3}$, $N(1+v)M \equiv 0 \pmod{3}$. 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 (4.3) with the type 2 interface, $\sigma(A \to B)$ can be calculated by using (4.3) with the type 2 interface, $\sigma(A \to B)$ can be calculated by using (4.3) with the type 2 interface, $N(1+v) \equiv 0 \pmod{3}$.

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

$$\sigma \left(A \to C \big| \theta_{\perp} \right) = \sigma \left(A \to B \big| \pi + \theta_{\perp} \right) \tag{4.5}$$

4.2. Anisotropic interfacial tension 2

The explicit forms of the eigenvalues of **V** and **T** are given by (2.36) with $w = x^{-1}$ and 1, respectively. For $-\pi/2 < \theta_{\perp} < \pi/2$, the eigenvalues of (p, r) = (1, 0) are the largest. Substituting their explicit forms into (4.3), we get

$$-\beta\sigma = \lim_{N \to \infty} \frac{1}{N \left(1 + v^2 - v\right)^{1/2}} \ln \left\{ \frac{1}{6\pi i} \oint_{|a|=1} \frac{da}{a} \rho(a) \left[\psi(ax)\psi(a)^v\right]^N \right\}, \\ -\infty < v < \infty$$
(4.6a)

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

$$v = \frac{\sqrt{3}}{2} \tan \theta_{\perp} + \frac{1}{2}, \qquad -\frac{\pi}{2} < \theta_{\perp} < \frac{\pi}{2}$$
 (4.6b)

The functions $\psi(ax)$ and $\psi(a)$ in (4.6*a*) correspond to $V(p)/\kappa^M$ and T(p) in (4.3), respectively. The summation in (4.3) 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

$$z = \frac{1}{x} \prod_{n=1}^{\infty} \left[\frac{\left(1 - x^{5n-3}\right) \left(1 - x^{5n-2}\right)}{\left(1 - x^{5n-4}\right) \left(1 - x^{5n-1}\right)} \right]^5, \qquad 0 < x < 1 \qquad (4.7)$$

The integral in (4.6a) can be estimated by the method of steepest descent. It is convenient to rewrite (4.6a) as

$$-\beta\sigma = \lim_{N \to \infty} \frac{1}{N(1+v^2-v)^{1/2}} \\ \times \ln\left(\frac{1}{6\pi i} \oint_{|a|=1} \frac{da}{a} \rho(a) \left\{ \left[\psi(ax)\psi(a)^{1/2}\right] \left[\psi(ax)\psi(a)^2\right]^{v'}\right\}^{N'} \right\} (4.8a)$$

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

$$v' = -\frac{v - 1/2}{v - 2} = \frac{\tan \theta_{\perp}}{\sqrt{3} - \tan \theta_{\perp}}, \qquad N = (1 + v')N'$$
(4.8b)

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

$$\frac{d}{da} \ln \left[\psi(ax)\psi(a)^{1/2} \right] = -\frac{1}{2} f^2(x, x^3) \frac{1}{a} \frac{f(-a, x^3)f(a^{-1}x^{3/2}, x^3)f(-a^{-1}x^{3/2}, x^3)}{f(a, x^3)f(ax, x^3)f(a^{-1}x, x^3)}$$
(4.9)

For a given direction v three saddle points are found on the negative parts of the real axes, and the integral in (4.8*a*) can be estimated around them. The saddle point whose argument is π , denoted by a_s , is determined by

$$\frac{\sqrt{3} - \tan \theta_{\perp}}{\sqrt{3} + \tan \theta_{\perp}} = -a \frac{f(-ax, x^3) f(a^{-1}x^{1/2}, x^3) f(-a^{-1}x^{1/2}, x^3)}{f(-a^{-1}x, x^3) f(ax^{1/2}, x^3) f(-ax^{1/2}, x^3)}, \quad a = a_s \quad (4.10)$$

and the condition

$$a_s = -1, \qquad \qquad \theta_\perp = 0 \tag{4.11}$$

The interfacial tension is represented as

$$-\beta\sigma = \frac{2}{\sqrt{3}} \left[\cos\theta_{\perp} \ln|\psi(a_s x)| + \cos\left(\theta_{\perp} - \frac{\pi}{3}\right) \ln|\psi(a_s)| \right],$$
$$-\pi/2 < \theta_{\perp} < \pi/2$$
(4.12)

-32 –

Near the critical point, which is the $x \to 1$ limit, (4.12) can be solved in the form of the power series. Using the conjugate modulus identities (3.21), we find

$$\begin{split} i\ln|a_s| &= -i\frac{6\pi}{5\varepsilon}\theta_{\perp} + \Delta^{(1)}\frac{6\pi}{5\varepsilon}\exp\left(-\frac{5}{6}\varepsilon\right) + \left[\Delta^{(2)} - \frac{1}{2}\left(\Delta^{(1)}\right)^2\right]\frac{6\pi}{5\varepsilon}\exp\left(-\frac{10}{6}\varepsilon\right) \\ &+ O\left[\frac{1}{\varepsilon}\exp\left(-\frac{15}{6}\varepsilon\right)\right] \end{split}$$
(4.13a)

$$\operatorname{Arg}[a_s] = \pi \tag{4.13b}$$

where the variable ε is related to x by (2.35) and

$$\Delta^{(1)} = -4i\sin\theta_{\perp}\sin\left(\theta_{\perp} + \frac{\pi}{3}\right)\sin\left(\theta_{\perp} - \frac{\pi}{3}\right)$$
(4.14a)

$$\Delta^{(2)} = \frac{1}{2} \left[\Delta(1) \right]^2 - 8\Delta^{(1)} \cos \theta_{\perp} \cos \left(\theta_{\perp} + \frac{\pi}{3} \right) \cos \left(\theta_{\perp} - \frac{\pi}{3} \right)$$
(4.14b)

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

$$a_s\left(-\theta_{\perp}\right) = a_s^{-1}\left(\theta_{\perp}\right), \qquad a_s\left(\theta_{\perp} + \frac{2\pi}{3}\right) = a_s\left(\theta_{\perp}\right)x \tag{4.15}$$

It is trivial to show that if a pair (a_0, θ_{\perp}) satisfies (4.10), then the pair $(a_0^{-1}, -\theta_{\perp})$ satisfies (4.10). Further, after some calculations, it is found that the pair $(a_0x, \theta_{\perp} + 2\pi/3)$ also satisfies (4.10). From these we expect that the relations (4.15) hold exactly. After the rhs of (4.12) is expanded into power series of exp $(-5\varepsilon/6)$, (4.14*a*) and (4.14b) can be used to get

$$\beta \sigma = 2\sqrt{3} \exp\left(-\frac{5}{6}\varepsilon\right) + 4\sqrt{3} \cos\theta_{\perp} \cos\left(\theta_{\perp} + \frac{\pi}{3}\right) \cos\left(\theta_{\perp} - \frac{\pi}{3}\right) \exp\left(-\frac{10}{6}\varepsilon\right) + 2\sqrt{3} \left[1 + 8\sin^{2}\theta_{\perp} \sin^{2}\left(\theta_{\perp} + \frac{\pi}{3}\right)\sin^{2}\left(\theta_{\perp} - \frac{\pi}{3}\right)\right] \exp\left(-\frac{15}{6}\varepsilon\right) + O\left[\exp\left(-\frac{20}{6}\varepsilon\right)\right], \qquad -\frac{\pi}{2} < \theta_{\perp} < \frac{\pi}{2}$$
(4.16)
$$- 33 -$$

Replacing the function $\psi(a)$ in (4.6*a*) by $\overline{\psi}(a)$, we get the representation of the interfacial tension for $-\pi < \theta_{\perp} < -\pi/2$, $\pi/2 < \theta_{\perp} < \pi$,

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

where the function $\bar{\psi}(b)$ is defined by (2.37) and

$$v = \frac{\sqrt{3}}{2} \tan \theta_{\perp} + \frac{1}{2}, \qquad -\pi < \theta_{\perp} < -\frac{\pi}{2}, \quad \frac{\pi}{2} < \theta_{\perp} < \pi \qquad (4.17b)$$

The integral in (4.17*a*) 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

$$\frac{\sqrt{3} - \tan \theta_{\perp}}{\sqrt{3} + \tan \theta_{\perp}} = \frac{f\left(-b^{-1}x^{1/2}, x^3\right)f\left(bx, x^3\right)f\left(-bx, x^3\right)}{f\left(-bx^{1/2}, x^3\right)f\left(b^{-1}x, x^3\right)f\left(-b^{-1}x, x^3\right)}, \quad b = b_s$$
(4.18)

and the condition

$$b_s = -1, \qquad \qquad \theta_\perp = \pm \pi \tag{4.19}$$

The interfacial tension is given by

$$-\beta\sigma = -\frac{2}{\sqrt{3}} \left[\cos\theta_{\perp} \ln|\bar{\psi}(b_s x)| + \cos\left(\theta_{\perp} - \frac{\pi}{3}\right) \ln|\bar{\psi}(b_s)| \right],$$
$$-\pi < \theta_{\perp} < -\pi/2, \quad \pi/2 < \theta_{\perp} < \pi$$
(4.20)

Here we do not have to solve (4.18) and (4.19) actually. It is sufficient to find the relations between b_s and a_s , determined by (4.10) and (4.11). When b is transformed into a by

$$a = bx^{3/2}, \qquad \pi/2 < \theta_{\perp} < \pi$$
 (4.22a)

$$a = bx^{-3/2}, \qquad -\pi < \theta_{\perp} < -\pi/2$$
(4.22b)

-34 –

Eq. (4.18) coincides with (4.10). If (4.11) is solved with the condition (4.10) in the extended region $-\pi < \theta_{\perp} < \pi$, because of the relations (4.15), the condition (4.19) is satisfied through (4.21*a*) and (4.21*b*). Thus, we find

$$a_s = b_s x^{3/2}, \qquad \pi/2 < \theta_\perp < \pi$$
 (4.22*a*)

$$a_s = b_s x^{-3/2}, \qquad -\pi < \theta_\perp < -\pi/2$$
 (4.22b)

These relation can be used in (4.20) to get

$$-\beta\sigma = \frac{2}{\sqrt{3}} \left[\cos\theta_{\perp} \ln|\psi(a_s x)| + \cos\left(\theta_{\perp} - \frac{\pi}{3}\right) \ln|\psi(a_s)| \right],$$
$$-\pi < \theta_{\perp} < -\pi/2, \quad \pi/2 < \theta_{\perp} < \pi$$
(4.23)

The use of (4.15) in (4.12) and (4.23) shows the symmetry relations

$$\sigma(-\theta_{\perp}) = \sigma(\theta_{\perp}), \qquad \sigma(\theta_{\perp} + 2\pi/3) = \sigma(\theta_{\perp})$$
(4.24)

From the expansion (4.16) we can see that the anisotropy of the interfacial tension disappears as the system approaches the critical point. The expansion (4.16) can be extended into the region $-\pi < \theta_{\perp} < \pi$. Thus, we find that the critical exponent μ does not depend on θ_{\perp} :

$$\mu = 5/6$$
 for all θ_{\perp} (4.25)

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

-35-

on the C-lattice, this rotation only causes the change of θ_{\perp} through $-2\pi/3$. The above condition is assured by the second relation of (4.24). If the center is on the A-lattice, the relation

$$\sigma \left(A \to B | \theta_{\perp} \right) = \sigma \left(A \to C | \theta_{\perp} + \pi/3 \right) \tag{4.26}$$

must be satisfied. The second relation (4.24) assures it through (4.5). Similarly, in the case that the center is on the *B*-lattice, the above condition is satisfied.

4.3. Anisotropic interfacial tension 3

We consider an expansion of the method (A). In the first place, an inhomogeneous system is introduced (Fujimoto, 1990b). Next, the eigenvalues of the transfer matrix are calculated by the commuting transfer matrices method given in Section 2. It is shown that a triplet of the largest eigenvalues are asymptotically degenerate as the width of the system becomes large. The anisotropic interfacial tension of the hard-hexagon model is calculated from the finite size correction terms in this limit.

Until now in this chapter, the parameter u is common to all the faces. This condition is relaxed: u can vary from column to column (Baxter, 1972, 1982). The value of u between the *i*th column and the (i + 1)th column is denoted by u_i . Consider a lattice of (1 + v)M ($0 < v < \infty$) columns and N rows with toroidal boundary conditions, and set $u_1 = u_2 = \cdots = u_M = -\lambda$, $u_{M+1} = u_{M+2} \cdots =$ $u_{(1+v)M} = \lambda$. The region $u = \lambda$ has the effect of shifting the particle configuration

of a column downward: if the particle configuration of the (M + 1)th column is shifted downward by Mv lattice spacings, it is identical with that of the first column. When M and N become large under the conditions that $(1 - v)M \equiv 0 \pmod{3}$ with v being fixed to be constant and $N \equiv 1$ or 2 (mod 3), there is a mismatched horizontal seam in the hard-hexagon region where $u = -\lambda$ (Fig. 2.5). This seam is tilted due to the region $u = \lambda$. The tilt angle is determined by v.

Restricting ourselves to near the interface (or the seam), we divide the lattice into three sublattices A, B, and C so that, on both sides of the interface, either the A-lattice or the B-lattice is preferentially occupied by particles. It is found that the positions of the A-phase and the B-phase are interchanged according as $N \equiv 1 \pmod{3}$ or $N \equiv 2 \pmod{3}$. In Sections 4.1 and 4.2, it was shown that the interfacial tension of these two types of interfaces are different. Taking account of this fact, we introduce a parameter θ_{\perp} by

$$-\frac{1}{v} = \frac{\sqrt{3}}{2} \tan \theta_{\perp} + \frac{1}{2}, \qquad \begin{cases} -\frac{\pi}{2} < \theta_{\perp} < -\frac{\pi}{6} & \text{for} \quad N \equiv 1 \pmod{3} \\ \frac{\pi}{2} < \theta_{\perp} < \frac{5\pi}{6} & \text{for} \quad N \equiv 2 \pmod{3} \end{cases}$$
(4.27)

and calculate the interfacial tension as a function of θ_{\perp} . Considering the case $u_1 = u_2 = \cdots = u_M = -\lambda$, $u_{M+1} = u_{M+2} = \cdots = u_{(1+v)M} = 0$, we find the interfacial tension for $-\pi/6 < \theta_{\perp} < \pi/2$, $5\pi/6 < \theta_{\perp} < 3\pi/2$. Since the calculational methods are almost the same, only the calculation for $u_1 = u_2 = \cdots = u_M = -\lambda$, $u_{M+1} = u_{M+2} = \cdots = u_{(1+v)M} = \lambda$ is explained, and that for $u_1 = u_2 = \cdots = u_M = -\lambda$, $u_M = -\lambda$, $u_{M+1} = u_{M+2} = \cdots = u_{(1+v)M} = 0$ is omitted in the following.

We consider a generalized problem where the values of u_i are given by a parame-

ter $u_0: u_1 = u_2 = \cdots = u_M = u_0, u_{M+1} = u_{M+2} = \cdots = u_{(1+v)M} = u_0 + 2\lambda$. Hereafter, the new parameter u_0 is abbreviated to u. A one-parameter family of transfer matrices is introduced. If $\sigma = \{\sigma_1, \sigma_2, \cdots, \sigma_{(1+v)M}\}$ and $\sigma' = \{\sigma'_1, \sigma'_2, \cdots, \sigma'_{(1+v)M}\}$ are the configurations of two successive rows, the row-row transfer matrix is defined by

$$[\mathbf{V}_{IH}(u)]_{\sigma,\sigma'} = \prod_{i=1}^{M} W\left(\sigma_{i}, \sigma_{i+1}, \sigma_{i+1}', \sigma_{i}' \middle| u\right) \prod_{j=M+1}^{(1+\nu)M} W\left(\sigma_{j}, \sigma_{j+1}, \sigma_{j+1}', \sigma_{j}' \middle| u + 2\lambda\right)$$
(4.28)

where $\sigma_{(1+v)M+1} = \sigma_1$, $\sigma'_{(1+v)M+1} = \sigma'_1$. We also define the 'dimensionless' transfer matrix by

$$\mathbf{T}_{IH}(u) = \left(-\frac{\omega_1(u)}{\omega_4(u)\omega_5(u)}\right)^M \left(-\frac{\omega_1(u+2\lambda)}{\omega_4(u+2\lambda)\omega_5(u+2\lambda)}\right)^{Mv} \mathbf{V}_{IH}(u)$$
(4.29)

The argument in Section 2.1 also assures that the family of $\mathbf{T}_{IH}(u)$ (or $\mathbf{V}_{IH}(u)$) commute with each other, being simultaneously diagonalized. (The essential point is that W'''s depend on the difference between u and u' in the star-triangle relation (2.9).) The eigenvalues of $\mathbf{T}_{IH}(u)$ (or $\mathbf{V}_{IH}(u)$) are denoted by $T_{IH}(u)$ (or $V_{IH}(u)$). It follows from the same derivation of (2.33) that each eigenvalue $T_{IH}(u)$ satisfies the equation

$$T_{IH}(u)T_{IH}(u+\lambda) = 1 + T_{IH}(u-2\lambda)$$
 (4.30)

where the relations (2.21) were fully used. We also find that

$$T_{IH}(u+5\lambda) = T_{IH}(u) \tag{4.31}$$

For calculational convenience, we transform the parametrization (2.16) into the conjugate modulus form by the use of (2.35) and (3.21):

$$\omega_1(w) = f(x^2 w, x^5) / f(x^2, x^5)$$

$$- 38 -$$
(4.32a)

$$\omega_2(w) = -x^{1/2} f(w, x^5) / \left[f(x, x^5) f(x^2, x^5) \right]^{1/2}$$
(4.32b)

$$\omega_3(w) = f(xw^{-1}, x^5) / f(x, x^5)$$
(4.32c)

$$\omega_4(w) = f(x^2 w^{-1}, x^5) / f(x^2, x^5)$$
(4.32d)

$$\omega_5(w) = w^{-1} f(xw, x^5) / f(x, x^5)$$
(4.32e)

The transfer matrix \mathbf{V}_{IH} (or \mathbf{T}_{IH}) is re-defined as a function of w and x by (4.28) (or (4.29)), with the alternative parametrization (4.32):

$$[\mathbf{V}_{IH}(w)]_{\sigma,\sigma'} = \prod_{i=1}^{M} W\left(\sigma_{i}, \sigma_{i+1}, \sigma_{i+1}', \sigma_{i}' \middle| w\right) \prod_{j=M+1}^{(1+v)M} W\left(\sigma_{j}, \sigma_{j+1}, \sigma_{j+1}', \sigma_{j}' \middle| x^{2} w\right)$$
(4.33)

or

$$\mathbf{T}_{IH}(w) = \left(-\frac{\omega_1(w)}{\omega_4(w)\omega_5(w)}\right)^M \left(-\frac{\omega_1(x^2w)}{\omega_4(x^2w)\omega_5(x^2w)}\right)^{Mv} \mathbf{V}_{IH}(w)$$
(4.34)

The functional equations (4.30) and (4.31) become

$$T_{IH}(w)T_{IH}(xw) = 1 + T_{IH}(x^3w)$$
(4.35)

$$T_{IH}(x^5w) = T_{IH}(w)$$
 (4.36)

Unless otherwise mentioned, x and v are regarded as constants; w is regarded as a complex variable. Assuming some analytic properties of $T_{IH}(w)$, and using (4.35) and (4.36), we can determine its asymptotic form as $M \to \infty$ (Baxter and Pearce, 1982).

We want to calculate the largest eigenvalues at the point $w = x^{-1}$. Hereafter, we confine ourselves to the eigenvalues which are the largest in the regime $1 \leq$

-39-

 $|w| \leq x^{-1}$. First, the leading term of $T_{IH}(w)$ as $M \to \infty$ is considered. We always keep only the dominant term in the rhs of (4.35) In the $x \to +0$ limit, there is complete triangular order in the regimes $1 \leq |w| \leq x^{-1}$, $x^{5/2} \leq |w| \leq x^{3/2}$. This fact suggests that, in the $M \to \infty$ and the $x \to 0$ limit, the eigenvalues we consider behave as

$$V_{IH}(w) \sim w^{M/3} \left(\frac{1}{xw}\right)_{,}^{Mv/3} \qquad 1 \le |w| \le x^{-1}$$
(4.37a)

It is also found that these eigenvalues are the largest in the regime $x^{5/2} \leq |w| \leq x^{3/2}$, and that, in the $M \to \infty$ and the $x \to \infty$ limit, they behave as

$$V_{IH}(w) \sim \left(\frac{x}{w}\right)^{M/3} \left(-\frac{1}{w^2}\right)_{,}^{Mv/3} \qquad x^{5/2} \le |w| \le x^{3/2} \tag{4.37b}$$

In (4.37*a*) and (4.37b), the factors $w^{M/3}$, $(-1/w^2)^{Mv/3}$ correspond to the complete triangular order where the faces ω_3 , ω_4 are dominant, and the factors $(1/xw)^{Mv/3}$, $(x/w)^{M/3}$ are related to the complete triangular order dominated by the faces ω_2 , ω_5 . We expect from (4.35) (4.37*a*), and (4.37b) that there exists a positive real number δ such that, for $0 < x < \delta$ and as $M \to \infty$,

$$|T_{IH}(w)| = O(x^{-\varepsilon M}) \gg 1, \qquad x^{5/2} \le |w| \le x^{3/2}, \quad 1 \le |w| \le x^{-1}$$

$$|T_{IH}(w)| = O(x^{\varepsilon M}) \ll 1, \qquad x^{7/2} \le |w| \le x^3, \quad x \le |w| \le x^{1/2}$$
(4.38)

with $\varepsilon > 0$.

It is assumed that, except for exponential divergence as $M \to \infty$, $V_{IH}(w)$ has no infinity for $0 < |w| < \infty$. We also assume that the leading term of $V_{IH}(w)$ as $M \to \infty$ is analytic in the annuli a < |w| < b containing the points $w = 1, x^{-1}$ and a' < |w| < b' containing the points $w = x^{5/2}, x^{3/2}$. In the limit $M \to \infty$, and for $0 < x < \delta$, it follows from (4.35)and (4.38) that the zeros of $V_{IH}(w)$ exist in the

six annuli $x^{-1/2} < |w| < x^{-1}, x^{5/2} < |w| < x^2, 1 < |w| < x^{-1/2}, x^2 < |w| < x^{3/2}, x^{-3/2} < |w| < x^{-2}, x < |w| < x^{1/2}, and that the zeros <math>w = ax^{-1}, ax^2 (x^{1/2} < |a| < 1)$ and $w = bx^{-1/2}, bx^{3/2} (x^{1/2} < |b| < 1)$ appear in pairs. It is found that , for $0 < x < \delta$ and M large, $T_{IH}(w)$ can be written in the form

$$T_{IH}(w) = L(w)w^{\bar{m}} \frac{\prod_{i=1}^{p} \left(1 - \frac{xw}{a_i}\right) \prod_{j=1}^{r} \left(1 - \frac{x^{1/2}w}{b_j}\right)}{(1 - xw)^M (1 - w^{-1})^{Mv}}, \qquad 1 \le |w| \le x^{-3/2}$$

$$T_{IH}(w) = \bar{L}(w)w^{\bar{m}} \frac{\prod_{i=1}^{p} \left(1 - \frac{x^2a_i}{w}\right) \prod_{j=1}^{r} \left(1 - \frac{x^{3/2}b_j}{w}\right)}{\left(1 - \frac{x^2}{w}\right)^{(1+v)M}}, \qquad x^{5/2} \le |w| \le x$$
(4.39)

where L(w) is analytic and nonzero for $1 < |w| < x^{-3/2}$ and $\overline{L}(w)$ is analytic and non-zero for $x^{5/2} < |w| < x$.

For the moment, we regard the a_i and b_j as known. Consider Eq. (4.35) in the annuli $x^{3/2} < |w| < x, x^{-1} < |w| < x^{-3/2}$, where the second terms in the rhs of (4.35) are dominant. Taking logarithms of both sides of (4.35), using (4.39), Laurent expanding, and equating coefficients, we can determine the explicit forms of L(w)and $\bar{L}(w)$. It follows that p and r must satisfy the condition that $p + 2r \equiv (1-v)M$ (mod 3). We find that for $(p, r) = \mathbf{0} = (0, 0)$

with $\tau^3 = 1$, and that for $(p, r) \neq \mathbf{0}$

$$T_{IH;p,r}(w) = \psi(w)^{M} \psi(1/xw)^{Mv} \prod_{i=1}^{p} \psi(a_i/w) \prod_{j=1}^{r} \bar{\psi}(b_j/w), \quad 1 \le |w| \le x^{-3/2}$$
$$= \psi(x/w)^{M} \psi(w)^{Mv} \prod_{i=1}^{p} \psi(w/xa_i) \prod_{j=1}^{r} \bar{\psi}(w/xb_j), \quad x^{5/2} \le |w| \le x$$
(4.40b)

where the a_i and b_j are defined on the three sheets of the Riemann surface. The definitions of $\psi(w)$ and $\bar{\psi}(w)$ are given by (2.34) and (2.37), respectively. The facts that $|\psi(w)| > 1$ for $1 < |w| < x^{-3/2}$, $|\psi(w)| < 1$ for $x^{3/2} < |w| < 1$, and $\psi(x^3w) = \psi(w)$ show that the conditions (4.38) are satisfied for 0 < x < 1. Therefore, the argument from (4.38)-(4.40) makes sense for 0 < x < 1. The leading term of $T_{IH}(w)$ for x < |w| < 1, $x^{7/2} < |w| < x^{5/2}$ can be determined by the use of (4.40) and (4.35).

The a_i and b_j are solutions of the equations

$$\psi(a_i)^M \psi(1/a_i x)^{Mv} = -\prod_{k=1}^p \psi(a_i/a_k) \prod_{l=1}^r \bar{\psi}(a_i/b_l), \quad i = 1, 2, \cdots, p$$

$$\bar{\psi}(b_j)^M \bar{\psi}(1/b_j x)^{Mv} = -\prod_{k=1}^p \bar{\psi}(b_j/a_k) \prod_{l=1}^r \psi(b_j/b_l), \quad j = 1, 2, \cdots, r$$
(4.41)

Equations (4.41) shows that as $M \to \infty$, the a_i and b_j approach the contours $|\psi(a) \ \psi(1/ax)^v| = 1$ and $|\bar{\psi}(b)\bar{\psi}(1/bx)^v| = 1$, respectively. This fact is consistent with the requirements that $x^{1/2} < |a_i| < 1$, $x^{1/2} < |b_j| < 1$. We find that, when $(1-v)M \equiv 0 \pmod{3}$, the triplet of eigenvalues $T_{IH;\mathbf{0},\tau}(w)$ are the largest in the regimes $1 \le |w| \le x^{-1}$, $x^{5/2} \le |w| \le x^{3/2}$.

Next, for the triplet of the largest eigenvalues $T_{IH;\mathbf{0},\tau}(w)$, an integral equation determining the finite size correction terms as $M \to \infty$ is derived. In this

calculation, we keep both terms in the rhs of (4.35). We define $K_{\tau}(w)$, $\bar{K}_{\tau}(w)$ by

$$T_{IH;\mathbf{0},\tau}(w) = \tau \psi(w)^{M} \psi(1/xw)^{Mv} K_{\tau}(w), \quad 1 \le |w| \le x^{-3/2}$$

$$= \frac{1}{\tau} \psi(x/w)^{M} \psi(w)^{Mv} \bar{K}_{\tau}(w), \quad x^{5/2} \le |w| \le x$$
(4.42)

It follows from (4.35) that

$$\frac{K_{\tau}(w)K_{\tau}(xw)}{\bar{K}_{\tau}(x^{3}w)} = 1 + 1/T_{IH;\mathbf{0},\tau}(x^{3}w), \quad x^{-1} < |w| < x^{-3/2}
\frac{\bar{K}_{\tau}(w)\bar{K}_{\tau}(xw)}{K_{\tau}(x^{-2}w)} = 1 + 1/T_{IH;\mathbf{0},\tau}(x^{-2}w), \quad x^{3/2} < |w| < x$$
(4.43)

For sufficiently large M, the second terms in the rhs of (4.43) are exponentially smaller than 1. Taking logarithms of the both sides of (4.43), Laurent expanding, and equating coefficients, we get the integral equation,

$$\ln K_{\tau}(w) = -\frac{1}{2\pi i} \oint_{C_1} \frac{dw'}{w'} \ln \left[1 + 1/T_{IH;\mathbf{0},\tau}(x^3w') \right] J(xw/w') + \frac{1}{2\pi i} \oint_{C_2} \frac{dw'}{w'} \ln \left[1 + 1/T_{IH;\mathbf{0},\tau}(x^{-2}w') \right] J(x^2w/w')$$
(4.44)

where C_1 is a circle in $x^{-1} < |w'| < x^{-3/2}$, C_2 is a circle in $x^{3/2} < |w'| < x$, and

$$J(w) = w\psi'(w)/\psi(w) \tag{4.45}$$

For $1 \leq |w| \leq x^{-3/2}$, Eqs. (4.42) and (4.44) determine the asymptotic form of $T_{IH;\mathbf{0},\tau}(w)$ as $M \to \infty$.

For large M, using (4.40*a*), we estimate the logarithms in the integrands of (4.44) by

$$\ln \left[1 + 1/T_{IH;\mathbf{0},\tau}(x^3w') \right] \sim \tau \left[\psi(w'/x)\psi(1/w')^v \right]^M$$

$$\ln \left[1 + 1/T_{IH;\mathbf{0},\tau}(x^{-2}w') \right] \sim \frac{1}{\tau} \left[\psi(x^2/w')\psi(w'/x)^v \right]^M$$

$$-43 -$$
(4.46)

and integrate (4.44) by steepest descent. It follows that

$$K_{\tau}(w) = 1 + \alpha(w)\tau\psi(w_s/x)^M\psi(1/w_s)^{Mv} + \bar{\alpha}(w)\frac{1}{\tau}\psi(x^2/\bar{w}_s)^M\psi(\bar{w}_s/x)^{Mv} + \cdots$$
(4.47)

where w_s and \bar{w}_s are the saddle point of $|\psi(w'/x)\psi(1/w')^v|$ and $|\psi(x^2/w')\psi(w'/x)^v|$, respectively. When w_s and \bar{w}_s are regarded as functions of v, they satisfy the conditions that $w_s = -x^{-1}$, $\bar{w}_s = -x^{3/2}$ for v = 1. The functions $\alpha(w)$, $\bar{\alpha}(w)$ are represented by J(w) and the derivatives of $\psi(w)$, and their explicit forms are not important here. For $(1 - v)M \equiv 0 \pmod{3}$ and $1 \leq |w| \leq x^{-1}$, Eqs. (4.42) and (4.47) show that the triplet of the largest eigenvalues $T_{IH;\mathbf{0},\tau}(w)$ are asymptotically degenerate as $M \to \infty$.

Now, setting $w = x^{-1}$ in (4.42) and (4.47), we calculate the anisotropic interfacial tension of the hard-hexagon model. When $(1 - v)M \equiv 0 \pmod{3}$ and M, N become large, the partition function can be represented by the use of (4.42) and (4.47) as

$$Z \sim \left[\left(1 + \tau_0^N + \frac{1}{\tau_0^N} \right) + \alpha(x^{-1})N \left(1 + \tau_0^{N+1} + \frac{1}{\tau_0^{N+1}} \right) \psi(w_s/x)^M \psi(1/w_s)^{Mv} + \bar{\alpha}(x^{-1})N \left(1 + \tau_0^{N-1} + \frac{1}{\tau_0^{N-1}} \right) \psi(x^2/\bar{w}_s)^M \psi(\bar{w}_s/x)^{Mv} \right] \kappa^{MN}$$
(4.48)

where $\tau_0 = (-1 + \sqrt{3}i)/2$ and

$$\kappa = \left(-\frac{\omega_4(w)\omega_5(w)}{\omega_1(w)}\right)\psi(w), \qquad w = x^{-1}$$
(4.49)

The second and the third terms in the square brackets of (4.48), which come from the finite size correction terms in (4.47), give the excess free energy for $N \equiv 2$ and

1 (mod 3), respectively. From (4.47) and (4.48), after some calculations, we find that

$$-\beta\sigma = \frac{2}{\sqrt{3}} \left[\cos\theta_{\perp} \ln|\psi(a_s x)| + \cos\left(\theta_{\perp} - \frac{\pi}{3}\right) \ln|\psi(a_s)| \right],$$
$$-\frac{\pi}{2} < \theta_{\perp} < -\frac{\pi}{6}, \quad \frac{\pi}{2} < \theta_{\perp} < \frac{5\pi}{6}$$
(4.50)

where β is the inverse temperature and σ is the interfacial tension defined on the triangular lattice. The saddle point a_s is determined by

$$\frac{\sqrt{3} - \tan\theta_{\perp}}{\sqrt{3} + \tan\theta_{\perp}} = -a \frac{f(-ax, x^3) f(a^{-1}x^{1/2}, x^3) f(-a^{-1}x^{1/2}, x^3)}{f(-a^{-1}x, x^3) f(ax^{1/2}, x^3) f(-ax^{1/2}, x^3)}, \quad a = a_s \quad (4.51a)$$

and the conditions

$$a_s = -x^{1/2}, \quad \theta_{\perp} = -\frac{\pi}{3}$$

 $a_s = -x, \qquad \theta_{\perp} = \frac{2\pi}{3}$ (4.51b)

Combining the result of the case $w_1 = w_2 = \cdots = w_M = x^{-1}$, $w_{M+1} = w_{M+2} = \cdots = w_{(1+v)M} = 1$ with (4.50) and (4.51), we obtain the expression of the interfacial tension for all directions which is the same result that was given in Section 4.2.

4.4. 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 from the anisotropic interfacial tension. The answer to this problem is obtained by the use of Wulff's theorem or Wulff's construction. Wulff's theorem says that there is a special point O called the Wulff point inside S, and that the position vector \mathbf{R} drawn from O to each point on S satisfies the relation

$$\frac{\sigma \left[\mathbf{n}(\mathbf{R}) \right]}{\mathbf{R} \cdot \mathbf{n}(\mathbf{R})} = \Lambda \qquad \text{for all } \mathbf{R} \qquad (4.52)$$

where $\mathbf{n}(\mathbf{R})$ is the normal vector of the interface at the point \mathbf{R} ; the interfacial tension is represented as a function of the normal vector of the interface; Λ is a constant independent of \mathbf{R} , which plays a scale factor adjusted to yield the volume V in the following argument. The origin of this theorem goes back to Wulff's paper of 1901, where the relation (4.52) was found experimentally. After that, this theorem was proved for some special cases (von Laue, 1944; Burton et al., 1951).

Using (4.52), 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 $\sigma(\mathbf{n})\mathbf{n}$ a line which is perpendicular to \mathbf{n} is drawn. Proper sets of these lines construct closed figures $\bar{S}_1, \bar{S}_2, \dots, \bar{S}_{\alpha}, \dots$ (Fig. 2.6). If the volume of \bar{S}_{α} is \bar{V}_{α} , enlarging \bar{S}_{α} by $(V/\bar{V}_{\alpha})^{1/2}$ times, we get all the figure S_{α} whose volume is V and which satisfies (3.28), where the value of Λ for S_{α} is

$$\Lambda_{\alpha} = \left(\frac{\bar{V}_{\alpha}}{V}\right)^{1/2} \tag{4.53}$$
$$-46 -$$

The remaining work is selecting S among the figures $S_1, S_2, \dots, S_{\alpha}, \dots$. To do this, a helpful relation is derived by the use of (4.52). Denoting by E_{α} the total surface energy of S_{α} , we get

$$E_{\alpha} = 2\Lambda_{\alpha}V \tag{4.54}$$

With the relation (4.53), Eq. (4.54) shows that the minimum energy corresponds to the minimum value of \bar{V}_{α} . From these results we can find that \bar{S} corresponding to the minimum energy S is determined as the inner envelope of the lines drawn on Σ : for a given direction designated by a unit vector \mathbf{r} ,

$$\Lambda R(\mathbf{r}) = \min_{\mathbf{n}} \frac{\sigma(\mathbf{n})}{(\mathbf{r} \cdot \mathbf{n})}$$
(4.55*a*)

where \mathbf{R} is represented as a function of \mathbf{r} and

$$R(\mathbf{r}) = |\mathbf{R}(\mathbf{r})| \tag{4.55b}$$

This method has long been known as Wulff's geometric construction.

Assuming the differentiability of $\sigma(\mathbf{n})$, and that the global minimum in the rhs of (4.55*a*) can be replaced by local minimum, we can rewrite Eq. (4.55*a*) into analytic form

$$\Lambda \mathbf{R}(\mathbf{n}) = \mathbf{n}\sigma(\mathbf{n}) + \nabla_{\mathbf{n}}\sigma(\mathbf{n}) \tag{4.56a}$$

where $\nabla_{\mathbf{n}}$ is the surface gradient defined by

$$\delta\sigma(\mathbf{n}) = \delta\mathbf{n} \cdot \nabla_{\mathbf{n}}\sigma(\mathbf{n}), \qquad \nabla_{\mathbf{n}}\sigma(\mathbf{n}) \cdot \mathbf{n} = 0 \tag{4.56b}$$

and, noting the one-one correspondence between \mathbf{r} and \mathbf{n} , we represent the position vector \mathbf{R} as a function of the normal vector \mathbf{n} : $\mathbf{R}(\mathbf{n})$ is the position vector of

-47 –

the interface whose normal vector is **n** (Avron et al., 1982; Zia and Avron, 1982; Hoffman and Cahn, 1972; Cahn and Hoffman, 1974).

Now we draw the equilibrium shape in the X - Y plane from the result of Sections 4.2 and 4.3. The change in the equilibrium 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

$$\beta \zeta = \ln z \tag{4.57}$$

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

For $z_c < z < \infty$, where σ is an analytic function of θ_{\perp} , we get by the use of (4.56*a*)

$$\Lambda X = -\frac{2}{\sqrt{3}} \ln |\psi(a_s x)| - \frac{1}{\sqrt{3}} \ln |\psi(a_s)|$$

$$\Lambda Y = -\ln |\psi(a_s)|$$
(4.58)

where and a_s is a parameter determined as a function of θ_{\perp} by (4.10) and (4.11). The results (4.58) can be reduced into more compact form,

$$\exp\left[\sqrt{3}\Lambda\left(X+\sqrt{3}Y\right)/2\right] + \exp\left[\sqrt{3}\Lambda\left(X-\sqrt{3}Y\right)/2\right] + \exp\left[-\sqrt{3}\Lambda X\right] = C$$
$$C = 2x^{-1/3}\frac{f(-x,x^3)}{f(-1,x^3)} + x^{2/3}\frac{f^2(-1,x^3)}{f^2(-x,x^3)}$$
(4.59)

In the $z \to \infty$ limit, which is the $x \to 0$ limit, the behavior of *a* determined by (4.10) and (4.11) is

$$a_s(\theta_{\perp}) \sim \sin(\theta_{\perp} - \pi/3) / \sin(\theta_{\perp} + \pi/3), \qquad -\frac{\pi}{3} < \theta_{\perp} < \frac{\pi}{3} \qquad (4.60a)$$

$$a_s \left(\pi/3 \right) = -x^{1/2} \tag{4.60b}$$

– 48 –

and we find

$$\frac{\sigma\left(\theta_{\perp}\right)}{\zeta} = \frac{2}{3\sqrt{3}}\cos\theta_{\perp}, \qquad -\frac{\pi}{3} \le \theta_{\perp} \le \frac{\pi}{3} \tag{4.61}$$

Equation (4.61) shows that Σ has three cusps at $\theta_{\perp} = \pm \pi/3, \pi$ (Fig. 2.6). From Wulff's geometric construction, it is found that the equilibrium shape is a regular triangle consisting of three facets. In Figure 2.7, it is shown how the equilibrium shape deforms into a regular triangle from a sphere near the critical point as zincreases.

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

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

$$(4.62)$$

where ρ is the radius of curvature (Avron et al., 1982; Zia and Avron, 1982; Zia, 1986; Akutsu and Akutsu, 1986). This calculation enable us to estimate the change in the equilibrium shape quantitatively, and will ensure us 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

$$a_s = a_0 \left(1 + \Delta^{(1)} \delta \theta_\perp + \Delta^{(2)} \delta \theta_\perp^2 + \cdots \right)$$
(4.63a)

where

$$a_0 = -1, \qquad \qquad \delta\theta_\perp = \theta_\perp - 0 \qquad (4.63b)$$

Expanding (4.10) into a power series of $\delta \theta_{\perp}$, we can determine the coefficients in

– 49 –

(4.63a) as

$$\Delta^{(1)} = -\frac{2}{\sqrt{3}} \frac{Q^2(x^6) f(x, x^3)}{Q^4(x^3) f(-x, x^3)}, \qquad \Delta^{(2)} = \frac{1}{2} \left(\Delta^{(1)}\right)^2, \quad \cdots \tag{4.64}$$

where

$$Q(q) = \prod_{n=1}^{\infty} (1 - q^n)$$
(4.65)

In this calculation the second derivative,

$$\frac{d^{2}}{da^{2}} \ln \left[\psi(ax)\psi^{1/2}(a) \right] = \frac{1}{2a^{2}} f^{2}(x,x^{3}) \frac{f(-a,x^{3})f\left(a^{-1}x^{3/2},x^{3}\right)f\left(-a^{-1}x^{3/2},x^{3}\right)}{f(a,x^{3})f(ax,x^{3})f\left(a^{-1}x,x^{3}\right)} + \frac{1}{2a^{2}} f^{2}(x,x^{3})f^{2}(-x,x^{3}) \frac{f^{2}\left(a^{-1}x^{3/2},x^{3}\right)f^{2}\left(-a^{-1}x^{3/2},x^{3}\right)}{f^{2}(ax,x^{3})f^{2}\left(a^{-1}x,x^{3}\right)} - \frac{1}{2a^{2}} f^{2}(x,x^{3}) \frac{Q^{4}(x^{3})}{Q^{2}(x^{6})} \frac{f(ia,x^{3})f(-ia,x^{3})f\left(iax^{3/2},x^{3}\right)f\left(-iax^{3/2},x^{3}\right)}{f^{2}(a,x^{3})f(ax,x^{3})f\left(a^{-1}x,x^{3}\right)} - \frac{1}{2a^{2}} f^{2}(x,x^{3}) \frac{Q^{4}(x^{3})}{Q^{2}(x^{6})} \frac{f(ia,x^{3})f(-ia,x^{3})f\left(iax,x^{3})f\left(a^{-1}x,x^{3}\right)}{f^{2}(a,x^{3})f(ax,x^{3})f\left(a^{-1}x,x^{3}\right)}$$

$$(4.66)$$

is useful. The above results can be used in (4.12) to find

$$\beta \sigma = -\frac{2}{\sqrt{3}} \ln \left[x^{1/3} \frac{f(-1, x^3)}{f(-x, x^3)} \right] \\ + \left\{ \frac{1}{\sqrt{3}} \ln \left[x^{1/3} \frac{f(-1, x^3)}{f(-x, x^3)} \right] + \frac{1}{3\sqrt{3}} \frac{f^4(x, x^3)}{f^4(-x, x^3)} \right\} \delta \theta_{\perp}^2 + \mathcal{O}\left(\delta \theta_{\perp}^4\right)$$
(4.67)

Using (4.67) in (4.62), we get

$$\frac{\rho}{R} = \frac{(2/3\sqrt{3}) \left[f^4(x, x^3) / f^4(-x, x^3) \right]}{-(2/\sqrt{3}) \ln \left[x^{1/3} f(-1, x^3) / f(-x, x^3) \right]}$$
(4.68)

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

$$\frac{\rho}{R} \left(\sim -\frac{1}{\ln x} \right) \sim \frac{1}{\ln z} = \frac{1}{\beta \zeta}$$
(4.69)

and near the critical point, by the use of the conjugate modulus transformation (3.21), we find that

$$\frac{\rho}{R} = 1 - \frac{9}{2} \exp\left(-\frac{5}{6}\varepsilon\right) + O\left[\exp\left(-\frac{10}{6}\varepsilon\right)\right]$$
(4.70)

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

$$a_s = a_0 \left(1 + \Delta^{(1)} \delta \theta_\perp + \Delta^{(2)} \delta \theta_\perp^2 + \cdots \right)$$
(4.71a)

where

$$a_0 = -x^{1/2}, \qquad \delta\theta_{\perp} = \theta_{\perp} - \pi/3$$
 (4.71b)

and

$$\Delta^{(1)} = -\frac{1}{\sqrt{3}} x^{-1/2} \frac{f(x, x^3) f\left(-x^{3/2}, x^3\right)}{Q^3(x^3) f\left(-x^{1/2}, x^3\right)}, \qquad \Delta^{(2)} = \frac{1}{2} \left(\Delta^{(1)}\right)^2, \quad \cdots \quad (4.72)$$

From these results we obtain

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

$$(4.73)$$

and

$$\frac{\rho}{R} = \frac{(2/3\sqrt{3})(1/x^{1/2}) \left[f^4(x, x^3)/f^4\left(-x^{1/2}, x^3\right)\right]}{-(1/\sqrt{3}) \ln \left[x^{1/3}f^2\left(-x^{1/2}, x^3\right)/f^2\left(-x^{3/2}, x^3\right)\right]}$$
(4.74)

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

$$\frac{\rho}{R} \left(\sim \frac{2x^{-1/2}}{-\ln x} \right) \sim \frac{2z^{1/2}}{\ln z} = 2\frac{1}{\beta\zeta} \exp\left(\frac{\beta\zeta}{2}\right) \tag{4.75}$$

and near the critical point

$$\frac{\rho}{R} \sim 1 + \frac{9}{2} \exp\left(-\frac{5}{6}\varepsilon\right) + O\left[\exp\left(-\frac{10}{6}\varepsilon\right)\right]$$
(4.76)

– 51 –

4.5. Anisotropic correlation length

The argument in Sections 3.1 and 3.2 is repeated (Fujimoto, 1990a). When v is fixed and l large, the correlation function is represented as

$$<\sigma_{00}\sigma_{lm}> - <\sigma_{00}> <\sigma_{lm}>$$

$$\sim \left(\frac{1}{6\pi i}\right)^{2} \oint_{|a|=1} \frac{da}{a} \oint_{|b|=1} \frac{db}{b} \rho(a,b) \left[\psi(ax)\psi^{v}(a)\right]^{l} \left[\bar{\psi}(bx)\bar{\psi}^{v}(b)\right]^{l},$$

$$\infty < v < \infty$$
(4.77a)

where we used the expression (2.36) with $w = x^{-1}$ and 1 for V(p)/V(1) and T(p)/T(1) in (3.11), respectively. The parameter v is related to θ_{\parallel} by

$$v = \frac{1}{2} - \frac{\sqrt{3}}{2\tan\theta_{\parallel}} \tag{4.77b}$$

The integral in (4.77a) is estimated by the method of steepest descent. Noting that this calculation is the same as Sections 4.2 and 4.3 except (4.75b), we find

$$<\sigma_{00}\sigma_{lm}> - <\sigma_{00}><\sigma_{lm}> \sim \exp\left(-\frac{r}{\xi}\right)\left\{\alpha + \alpha'\cos\left[\frac{2\pi}{3}(l+m) + \delta\right]\right\}$$
(4.78*a*)

$$-\frac{1}{\xi} = \frac{2}{\sqrt{3}} \left[\sin \theta_{\parallel} \ln |\psi(a_s x)| + \sin \left(\theta_{\parallel} - \frac{\pi}{3}\right) \ln |\psi(a_s)| \right] + \frac{2}{\sqrt{3}} \left[\sin \theta_{\parallel} \ln |\bar{\psi}(b_s x)| + \sin \left(\theta_{\parallel} - \frac{\pi}{3}\right) \ln |\bar{\psi}(b_s)| \right]$$
(4.78b)

where a_s is the saddle point of $|\psi(a_x)\psi^v(a)|$ whose argument is π , and b_s is that of $|\bar{\psi}(bx)\bar{\psi}(b)|$ whose argument is π . Baxter and Pearce (1982) showed that a simple relation holds between the correlation length and the interfacial tension along the vertical axis. This relation is extended here for all directions as

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

$$-52 -$$

$$(4.79)$$

where $\sigma(A \to B)$ and $\sigma(A \to C)$ are the two types of interfacial tension defined in Section 4.1 in the direction of ξ .

The behavior of ξ near the critical point is given by

$$\xi = \frac{1}{4\sqrt{3}} \exp\left(\frac{5}{6}\varepsilon\right) \left\{ 1 - \left[1 + 8\cos^2\theta_{\parallel}\cos^2\left(\theta_{\parallel} + \frac{\pi}{3}\right)\cos^2\left(\theta_{\parallel} - \frac{\pi}{3}\right)\right] \times \exp\left(-\frac{10}{6}\varepsilon\right) + O\left[\exp\left(-\frac{20}{6}\varepsilon\right)\right] \right\}$$
(4.80)

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

$$\nu' = 5/6$$
 for all θ_{\parallel} (4.81)

From the relation (4.15), it follows that

$$\xi(\theta_{\parallel} + \pi/3) = \xi(\theta_{\parallel}), \qquad \xi(-\theta_{\parallel}) = \xi(\theta_{\parallel}) \tag{4.82}$$

Chapter 3. Eight-Vertex Model: Anisotropic Interfacial Tension and Equilibrium Crystal Shape

1. Introduction

In the eight-vertex model an arrow is placed on every edge of the square lattice so that even number of arrows point into (and out of) each site (or vertex) (Baxter, 1982). There are eight such configurations around a vertex (Fig. 3.1). We represent the arrow configuration by associating an arrow-spin α_i with each edge i; $\alpha_i = +1$ if the corresponding arrow points up or to the right, and $\alpha_i = -1$ otherwise. When arrow-spins around a vertex are ν , α , β , and μ counterclockwise starting from the west bond, a Boltzmann weight $W(\nu, \alpha | \beta, \mu)$ is assigned on this vertex, where

$$W(++|++) = W(--|--) = a = \exp(-\varepsilon_1/k_B T)$$

$$W(+-|+-) = W(-+|+-) = b = \exp(-\varepsilon_2/k_B T)$$

$$W(+-|+-) = W(-+|-+) = c = \exp(-\varepsilon_3/k_B T)$$

$$W(++|--) = W(--|++) = d = \exp(-\varepsilon_4/k_B T)$$
(1.1a)

and

$$W(\nu, \alpha | \beta, \mu) = 0, \qquad \nu \alpha \beta \mu = -1 \tag{1.1b}$$

This model was introduced as a generalization of the ice-type (or six-vertex) model. The situation of the ice-type model is as follows. For example, imagine a square ice. There, oxygen ions form a square lattice. A hydrogen ion (or a proton)

is located near or other end of each bond connecting the adjacent pair of oxygen ions. Because of the charge neutrality condition around each site, four protons surrounding it should satisfy the ice-rule: two of them are close to it, and the others are away from it, on their respective bonds. By drawing an arrow on every edge, we represent which end of the bond is occupied by a proton. The ice-rule allows six local arrow configurations, which correspond to the vertices $1\sim6$ in the eight-vertex model (Fig. 3.1). The ice-type model has some unusual features: the antiferroelectric phase transition is infinite order, i.e., the free energy and all its derivatives are finite at the critical temperature; in the ferroelectric ordered state, the ordering is complete even at nonzero temperatures, etc. (Lieb, 1967a, b, c). It is naturally thought that these features come from the ice-rule. To understand the effects of the ice-rule, Sutherland (1970) introduced the vertices 7 and 8.

The eight-vertex model can be regarded as an Ising model with two- and fourspin interactions (Wu, 1971; Kadanoff and Wegner, 1971; Baxter, 1982). To see this, we associate an Ising spin σ_{ij} with each site (i, j) of the dual lattice; the site (i, j) of the dual lattice is connected with the site (i, j) of the original square lattice by shifting in both directions by a half-lattice spacing. An upward or right arrow corresponds to the cases where the adjacent σ -spins are parallel; otherwise, the adjacent σ -spins are antiparallel. The condition (1.1b) ensures that this correspondence is consistent. To any arrow configuration, there correspond two σ -spin configurations, which are related to each other by the transformation defined by $\sigma_{i,j} \rightarrow -\sigma_{ij}$ for all i, j.

The Hamiltonian of the Ising model is given by

$$E = -\sum_{ij} \left(J\sigma_{i,j+1}\sigma_{i+1,j} + J'\sigma_{ij}\sigma_{i+1,j+1} + J''\sigma_{ij}\sigma_{i+1,j}\sigma_{i+1,j+1}\sigma_{i,j+1} \right)$$
(1.2)

where next-nearest neighbor spins are coupled by J and J', depending on the direction of the diagonal; the factor J'' couples four spins. The four boltzmann weights in (1.1*a*) is related to J, J', and J'' as follows:

$$\exp\left[\frac{4J}{k_BT}\right] = \frac{ad}{bc}, \quad \exp\left[\frac{4J'}{k_BT}\right] = \frac{ac}{bd}, \quad \exp\left[\frac{4J''}{k_BT}\right] = \frac{ab}{cd} \tag{1.3}$$

It is noted that when a, b, c, and d satisfy the relation

$$ab = cd \tag{1.4}$$

this Ising model factors into two independent nearest-neighbor Ising models (Fig. 3.2).

Equilibrium crystal shapes (ECS's) and their roughening transition phenomena have been attracted much attention in recent years. The first exact analysis of ECS's was done for the square lattice nearest-neighbor Ising model (Rottman and Wortis, 1981; Avron et al., 1982). Zia and Avron (1982) found that the ECS of this model is represented as a simple algebraic curve. For example, when the interactions are isotropic, the ECS is given by

$$\cosh\left(\Lambda X/k_BT\right) + \cosh\left(\Lambda Y/k_BT\right) = C_I \tag{1.5a}$$

$$C_I = \cosh\left(2J/k_BT\right)/\tanh\left(2J/k_BT\right) \tag{1.5b}$$

where (X, Y) is the position vector of a point on the ECS; Λ is a scale factor; J is the interaction constant. Zia (1986) also showed that ECS's of the triangular and

– 56 –

honeycomb lattice nearest-neighbor Ising models are represented as an algebraic curve like (1.5).

For the Ising models on the planar lattices without bond crossings, Holzer (1990) and Akutsu and Akutsu (1990) pointed out that the interface can be represented as a free-random-walk defined on the dual lattice. This random-walk representation is derived by the use of Feynman-Vdovichenko's method (Vdovichenko, 1964; Feynman, 1972). The form (1.5) characterizes the random-walk. Furthermore, Akutsu and Akutsu re-examined the facet shape of the BCSOS model (or equivalently the ECS of the six-vertex model), and found that the facet shape can be written into the form (1.5a), with C_I replaced by

$$C_{BC} = k^{1/2}(x) + k^{-1/2}(x)$$
(1.6a)

where k(x) is defined as

$$k(x) = 4x \prod_{n=1}^{\infty} \left[\frac{1+x^{4n}}{1+x^{4n-2}} \right]^4$$
(1.6b)

and x are given by (4.3). From this result, they suggested the possibility of representing the step of the BCSOS model as a free-random-walk characterized by (1.5*a*), with C_I replaced by (1.6). At this time, however, the correspondence between the step and the random-walk is not so clear, since the BCSOS model can not be solved by Feynman-Vdovichenko's method.

In connection with these problems, it is significant to consider the eight-vertex model, which contains the square lattice nearest-neighbor Ising model and the six-vertex (or BCSOS) model as special limits. In Chapter 3 we calculate the anisotropic interfacial tension of the eight-vertex model and derive the ECS of this model by the use of Wulff's construction.

This chapter is organized as follows. In the calculation of the interfacial tension, we use Baxter's commuting transfer matrices argument (Baxter, 1972, 1982), which is summarized in Section 2. The interfacial tension of the eight-vertex model for a special direction has been calculated by Baxter(1973). This analysis is extended by the shift operator method given in Section 4.3 of Chapter 2 (Fujimoto, 1990b). In the first place of Section 3 inhomogeneous systems are introduced. Then, we define a one-parameter family of commuting transfer matrices, and derive an equation for eigenvalues of the transfer matrix. In Section 4, using this equation, we determine the explicit forms of the eigenvalues. It is shown that a doublet of the largest eigenvalues are asymptotically degenerate when the width of the system becomes large. The anisotropic interfacial tension is calculated from the finite size correction terms in this limit. In Section 5 the ECS of the eight-vertex model is found by the use of Wulff's construction. We discuss a relation between the algebraic curve (1.5a)and the elliptic solution of the interfacial tension given in Section 4. In Appendix the definitions of elliptic functions are listed.

2. Commuting transfer matrices argument

Baxter (1972, 1982) solved the eight-vertex model as follows. First, a oneparameter family of commuting transfer matrices was found. Then, an equation for the transfer matrix was derived. Using the equation, he determined the explicit forms of their eigenvalues. In this section we review Baxter's commuting transfer matrices argument.

The eight-vertex model on a square lattice of M columns and N rows with toroidal boundary conditions is considered (M: even). Let $\{\alpha_1, \alpha_2, \dots, \alpha_M\}$ and $\{\beta_1, \beta_2, \dots, \beta_M\}$ be the arrow-spins on two successive rows of vertical edges; $\{\mu_1, \mu_2, \dots, \mu_M\}$ be the arrow-spins on the horizontal edges which connect the vertices jointing the two successive rows of the vertical edges. The row-row transfer matrix has elements

$$[\mathbf{V}]_{\{\alpha\}}^{\{\beta\}} = \sum_{\{\mu\}} \prod_{j=1}^{M} W\left(\mu_{j}, \alpha_{j} \middle| \beta_{j}, \mu_{j+1}\right)$$
(2.1)

where W's are given by (1.1) and $\mu_{M+1} = \mu_1$ (Fig. 3.3). We want to find a series of transfer matrices with different values of a, b, c, and d which commute with **V**.

We define transfer matrix \mathbf{V}' by (2.1), with (a, b, c, d) replaced by (a', b', c', d'). The corresponding Boltzmann weight W is denoted by W'. Consider the matrix products \mathbf{VV}' and $\mathbf{V'V}$. The elements of \mathbf{VV}' are

$$\sum_{\{\gamma\}} \left[\mathbf{V} \right]_{\{\alpha\}}^{\{\gamma\}} \left[\mathbf{V}' \right]_{\{\gamma\}}^{\{\beta\}} = \sum_{\{\gamma\}, \{\mu\}, \{\nu\}} \prod_{j=1}^{M} W\left(\mu_j, \alpha_j \big| \gamma_j, \mu_{j+1} \right) W'\left(\nu_j, \gamma_j \big| \beta_j, \nu_{j+1} \right) \\ = \operatorname{Tr} \left\{ \mathbf{R}\left(\alpha_1, \beta_1 \right) \mathbf{R}\left(\alpha_2, \beta_2 \right) \cdots \mathbf{R}\left(\alpha_M, \beta_M \right) \right\}$$
(2.2)

where $\mathbf{R}(\alpha, \beta)$ is a four-by-four matrix with rows labeled by (μ, ν) , columns labeled

-59 –

by (μ', ν') , and elements

$$\left[\mathbf{R}(\alpha,\beta)\right]_{\mu,\nu}^{\mu',\nu'} = \sum_{\gamma} W\left(\mu,\alpha\big|\gamma,\mu'\right) W'\left(\nu,\gamma\big|\beta,\nu'\right)$$
(2.3)

Similarly, $\mathbf{V'V}$ is given by (2.2) and (2.3), with W's and W's interchanged:

$$\sum_{\{\gamma\}} \left[\mathbf{V}' \right]_{\{\alpha\}}^{\{\gamma\}} \left[\mathbf{V} \right]_{\{\gamma\}}^{\{\beta\}} = \sum_{\{\gamma\}, \{\mu\}, \{\nu\}} \prod_{j=1}^{M} W' \left(\mu_j, \alpha_j \big| \gamma_j, \mu_{j+1} \right) W \left(\nu_j, \gamma_j \big| \beta_j, \nu_{j+1} \right) \\ = \operatorname{Tr} \left\{ \mathbf{R}' \left(\alpha_1, \beta_1 \right) \mathbf{R}' \left(\alpha_2, \beta_2 \right) \cdots \mathbf{R}' \left(\alpha_M, \beta_M \right) \right\}$$
(2.4)

where

$$\left[\mathbf{R}'(\alpha,\beta)\right]_{\mu,\nu}^{\mu',\nu'} = \sum_{\gamma} W'\left(\mu,\alpha\big|\gamma,\mu'\right) W\left(\nu,\gamma\big|\beta,\nu'\right)$$
(2.5)

The transfer matrices \mathbf{V} and \mathbf{V}' commute with each other if there exists a four-byfour nonsingular matrix \mathbf{M} such that

$$\mathbf{R}(\alpha,\beta) = \mathbf{M}\mathbf{R}'(\alpha,\beta)\mathbf{M}^{-1}$$
(2.6)

for all $\alpha, \beta = \pm 1$. We post-multiply (2.6) by **M**, and write the element of **M** labeled by (μ, ν) and (μ', ν') as $W''(\nu, \mu | \nu', \mu')$. Then, (2.6) becomes the star-triangle relation

$$\sum_{\gamma,\mu'',\nu''} W(\mu,\alpha|\gamma,\mu'') W'(\nu,\gamma|\beta,\nu'') W''(\nu'',\mu''|\nu',\mu')$$

=
$$\sum_{\gamma,\mu'',\nu''} W''(\nu,\mu|\nu'',\mu'') W'(\mu'',\alpha|\gamma,\mu') W(\nu'',\gamma|\beta,\nu')$$
(2.7)

for all $\alpha, \beta, \mu, \nu, \mu', \nu' = \pm 1$ (Fig 3.4). It is assumed that $W''(\nu, \alpha | \beta, \mu)$ is given by (1.1), with (a, b, c, d,) replaced by (a'', b'', c'', d''). For given values of (a, b, c, d) and (a', b', c', d'), we consider the problem of finding a third set (a'', b'', c'', d'') which satisfies (2.7).

– 60 –

Baxter showed that there exists a nontrivial solution (a'', b'', c'', d'') if $\Delta = \Delta'$ and $\Gamma = \Gamma'$, where

$$\Delta = \left(a^2 + b^2 - c^2 - d^2\right)/2(ab + cd)$$

$$\Gamma = (ab - cd)/(ab + cd)$$
(2.8)

and Δ' , Γ' are defined by (2.8) with (a, b, c, d) replaced by (a', b', c', d'). Eliminating d between the two equations of (2.8), we obtain

$$2\Delta(1+\gamma)ab = a^2 + b^2 - c^2 - a^2b^2\gamma^2/c^2$$
(2.9a)

where

$$\gamma = (1 - \Gamma)/(1 + \Gamma) = cd/ab \tag{2.9b}$$

Given Δ and γ , (2.9*a*) is a symmetric biquadratic relation between a/c and b/c. It is convenient to parametrize this relation in terms of elliptic functions. Explicitly, we use the parametrization by four variables ρ , k, λ , and u:

$$a = -i\rho\Theta(i\lambda)H[i(\lambda - u)/2]\Theta[i(\lambda + u)/2]$$

$$b = -i\rho\Theta(i\lambda)\Theta[i(\lambda - u)/2]H[i(\lambda + u)/2]$$

$$c = -i\rho H(i\lambda)\Theta[i(\lambda - u)/2]\Theta[i(\lambda + u)/2]$$

$$d = -i\rho H(i\lambda)H[i(\lambda - u)/2]H[i(\lambda + u)/2]$$

(2.10)

and

$$\Gamma = \left(1 + k \mathrm{sn}^2 i \lambda\right) / \left(1 - k \mathrm{sn}^2 i \lambda\right)$$

$$\Delta = -\operatorname{cn} i \lambda / \left(1 - k \mathrm{sn}^2 i \lambda\right)$$
(2.11)

where ρ is a normalization factor of the partition function; λ and u appear as arguments of the elliptic functions; k is the modulus of the elliptic functions. The corresponding half-periods are denoted by I and I'. The definitions of the elliptic

functions and relations among them are listed in Appendix. Define (a', b', c', d')and (a'', b'', c'', d'') by (2.10), with u replaced by u' and u' - u, respectively. Then, it is verified that these three sets of Boltzmann weights satisfy (2.7) by the use of addition formulae

$$\frac{\operatorname{sn}(a-u)\operatorname{sn}(a-v) - \operatorname{sn}u\operatorname{sn}v}{1-k^2\operatorname{sn}u\operatorname{sn}v\operatorname{sn}(a-u)\operatorname{sn}(a-v)} = \operatorname{sn}a\operatorname{sn}v$$

$$\frac{\operatorname{sn}v\operatorname{sn}(a-v) - \operatorname{sn}u\operatorname{sn}(a-u)}{\operatorname{sn}(a-u)\operatorname{sn}v - \operatorname{sn}(a-v)\operatorname{sn}u} = \frac{\operatorname{sn}(a-u-v)}{\operatorname{sn}a}$$
(2.12)

Thus, we obtain the one-parameter family of commuting transfer matrices

$$\left[\mathbf{V}(u)\right]_{\{\alpha\}}^{\{\beta\}} = \sum_{\{\mu\}} \prod_{j=1}^{M} W\left(\mu_{j}, \alpha_{j} \middle| \beta_{j}, \mu_{j+1} \middle| u\right)$$
(2.13)

Baxter derived an equation for the transfer matrix by considering 2^{M} -dimensional column vectors $\mathbf{y}(u)$. The vector $\mathbf{y}(u)$ is represented as a direct product of two-dimensional vectors $\mathbf{g}_{1}(u), \mathbf{g}_{1}(u), \cdots, \mathbf{g}_{M}(u)$:

$$\mathbf{y}(u) = \mathbf{g}_1(u) \otimes \mathbf{g}_2(u) \otimes \cdots \otimes \mathbf{g}_M(u)$$
(2.14)

where

$$\mathbf{g}_{j}(u) = \begin{pmatrix} g_{j}(+|u) \\ g_{j}(-|u) \end{pmatrix} = \begin{pmatrix} \Theta \left[is_{j} + i(u+\lambda)\zeta_{j}/2 \right] \\ (-)^{j+1}iH \left[is_{j} + i(u+\lambda)\zeta_{j}/2 \right] \end{pmatrix}$$
(2.15)

Each ζ_j has a value +1 or -1 and ζ_j 's satisfy the condition

$$\zeta_1 + \zeta_2 + \dots + \zeta_M = 0 \tag{2.16}$$

The variables s_j 's are defined for $j = 1, 2, \dots, M + 1$ as

$$s_j = \begin{cases} s, & j = 1\\ s + \lambda(\zeta_1 + \zeta_2 + \dots + \zeta_{j-1}), & j = 2, 3, \dots, M+1 \end{cases}$$
(2.17)

with an arbitrary constant s. There are many 2^{M} -dimensional vectors $\mathbf{y}(u)$, corresponding to different choices of s and ζ_{j} 's. The product $\mathbf{V}(u)\mathbf{y}(u)$ is represented as

$$\sum_{\{\beta\}} \left[\mathbf{V}(u) \right]_{\{\alpha\}}^{\{\beta\}} \left[\mathbf{y}(u) \right]_{\{\beta\}} = \sum_{\{\beta\},\{\gamma\}} \prod_{j=1}^{M} W\left(\mu_{j}, \alpha_{j} \middle| \beta_{j}, \mu_{j+1} \middle| u \right) g_{j}\left(\beta_{j} \middle| u\right)$$
$$= \operatorname{Tr} \left\{ \mathbf{G}\left(\alpha_{1} \middle| u\right) \mathbf{G}\left(\alpha_{2} \middle| u\right) \cdots \mathbf{G}\left(\alpha_{M} \middle| u\right) \right\}$$
(2.18)

where $\mathbf{G}_{j}(\alpha|u)$ is a two-by-two matrix with elements

$$\left[\mathbf{G}_{j}(\alpha|u)\right]_{\mu}^{\mu'} = \sum_{\beta} W\left(\mu, \alpha \big| \beta, \mu' \big| u\right) g_{j}\left(\beta \big| u\right)$$
(2.19)

Baxter found that $\mathbf{G}_j(\alpha|u)$ satisfies the relation

$$\mathbf{G}_{j}(\alpha|u)\mathbf{p}_{j+1} = g'_{j}(\alpha|u)\mathbf{p}_{j}$$
(2.20)

where

$$g'_{j}(+|u) = \rho h \left[(\lambda - u)/2 \right] \Theta \left[i s_{j} + i \zeta (u + 3\lambda)/2 \right]$$

$$(2.21a)$$

$$g'_{j}(-|u) = \rho h [(\lambda - u)/2](-)^{j} i H [is_{j} + i\zeta(u + 3\lambda)/2]$$
(2.21b)

$$h(u) = -i\Theta(0)\Theta(iu)H(iu)$$
(2.22)

and for $j = 1, 2, \dots, M + 1$

$$\mathbf{p}_{j} = \begin{pmatrix} \Theta \left[is_{j} \right] \\ (-)^{j+1} i H \left[is_{j} \right] \end{pmatrix}$$
(2.23)

Two-by-two matrices $\mathbf{P}_1, \mathbf{P}_2, \dots, \mathbf{P}_{M+1}$ are defined as follows: the first column of \mathbf{P}_j is the vector \mathbf{p}_j ; the second column is determined suitably so that det $\mathbf{P}_j = 1$.

Then, \mathbf{P}_{j} and \mathbf{P}_{j+1} transform $\mathbf{G}_{j}(\alpha|u)$ into a two-by-two matrix whose lower-left element is zero:

$$\mathbf{G}_{j}(\alpha|u) = \mathbf{P}_{j}\mathbf{H}_{j}(\alpha|u)\mathbf{P}_{j+1}^{-1}$$
(2.24)

where

$$\mathbf{H}_{j}(\alpha|u) = \begin{pmatrix} g_{j}'(\alpha|u) & g_{j}'''(\alpha|u) \\ 0 & g_{j}''(\alpha|u) \end{pmatrix}$$
(2.25)

$$g_j''(+|u) = \rho h \left[(\lambda + u)/2 \right] \Theta \left[i s_j + i \zeta (u - \lambda)/2 \right]$$
(2.26a)

$$g_j''(-|u) = \rho h [(\lambda + u)/2](-)^j i H [is_j + i\zeta(u - \lambda)/2]$$
(2.26b)

and the explicit form of $g_{j}^{\prime\prime\prime}(\alpha|u)$ is not important here. Note that $\mathbf{P}_{M+1} = \mathbf{P}_{1}$ because of the condition (2.16). Substituting (2.24) into (2.18), we get

$$\sum_{\{\beta\}} \left[\mathbf{V}(u) \right]_{\{\alpha\}}^{\{\beta\}} \left[\mathbf{y}(u) \right]_{\{\beta\}} = \operatorname{Tr} \left\{ \mathbf{H} \left(\alpha_1 | u \right) \mathbf{H} \left(\alpha_2 | u \right) \cdots \mathbf{H} \left(\alpha_M | u \right) \right\}$$
(2.27)

since $\mathbf{P}_1, \mathbf{P}_2, \cdots, \mathbf{P}_{M+1}$ cancels out of the trace. After some calculations, it follows that

$$\mathbf{V}(u)\mathbf{y}(u) = \phi(\lambda - u)\mathbf{y}(u + 2\lambda') + \phi(\lambda + u)\mathbf{y}(u - 2\lambda')$$
(2.28)

where $\lambda' = \lambda + 2iI'$ and

$$\phi(u) = [\rho h(u/2)]^M$$
(2.29)

Using the complete set of vectors $\mathbf{y}(u)$, Baxter constructed a non-singular matrix $\mathbf{Q}(u)$, which has some useful properties. Each columns of $\mathbf{Q}(u)$ is represented as a linear combination of vectors $\mathbf{y}(u)$. Eq. (2.28) yields the equation for the transfer matrix

$$\mathbf{V}(u)\mathbf{Q}(u) = \phi(\lambda - u)\mathbf{Q}(u + 2\lambda') + \phi(\lambda + u)\mathbf{Q}(u - 2\lambda')$$
(2.30)
- 64 -

The matrix $\mathbf{Q}(u)$ commutes with $\mathbf{Q}(u')$ and $\mathbf{V}(u'')$ for all values of u, u', and u''. Therefore, (2.30) gives the eigenvalue equation

$$V(u)q(u) = \phi(\lambda - u)q(u + 2\lambda') + \phi(\lambda + u)q(u - 2\lambda')$$
(2.31)

where V(u) and q(u) are eigenvalues of $\mathbf{V}(u)$ and $\mathbf{Q}(u)$, respectively.

Two matrices **S** and **R** are introduced. The matrix **S** is the diagonal matrix which has entries +1 (-1) for arrow configurations of an even (odd) number of down arrows, and **R** is the matrix which has the effect of reversing all arrows. We shall use **R** to impose the antiperiodic boundary conditions on the lattice in Section 4. The matrices **S**, **R**, **Q**(u), and **V**(u') commute with each other for all values of u and u'. The eigenvalue of **S** (or **R**) corresponding to V(u) and q(u) is denoted by s (or r). Both s and r take values of +1 or -1. The matrix **Q**(u) satisfies the relations

$$\mathbf{Q}(u)\mathbf{S} = \mathbf{Q}(u+4iI) \tag{2.32a}$$

$$\mathbf{Q}(u)\mathbf{SR} = q^{M/4} \exp(-M\pi u/4I)\mathbf{Q}(u+2I')$$
(2.32b)

From these relations, we found the periodicity relations

$$q(u+4iI) = sq(u) \tag{2.33a}$$

$$q(u+2I') = srq^{-M/4} \exp(M\pi u/4I)q(u)$$
(2.33b)

The eigenvalue q(u) is represented as a linear combination of the elements of $\mathbf{Q}(u)$, which are entire functions of u. Detailed investigation shows that q(u) must be of the form

$$q(u) = \exp(\tau u) \prod_{j=1}^{m} h\left(\frac{u - v_j}{2}\right)$$
(2.34)

-65 -

where m = M/2, τ is a constant, and v_j $(j = 1, 2, \dots, m)$ are zeros of q(u) determined by the condition that the rhs of (2.31) vanishes:

$$\left\{\frac{h[(\lambda - v_k)/2]}{h[(\lambda + v_k)/2]}\right\}^M = -\exp(-4\tau\lambda')\prod_{j=1}^m \frac{h[(v_k - v_j - 2\lambda')/2]}{h[(v_k - v_j + 2\lambda')/2]}$$
(2.35)

for $k = 1, 2, \dots, m$. The periodicity relations (2.33) require that v_j 's and τ satisfy the sum-rules

$$v_1 + v_2 + \dots + v_m$$

= $\frac{1}{2}(s - 1 + 2m)I' + i(rs - 1 + 2m)I + 2p'I' + 4piI$ (2.36a)

$$\tau = \pi (s - 1 + 2m + 4p')/8I \tag{2.36b}$$

where p and p' are integers. We can determine the explicit form of V(u) first by solving (2.35), and then by using (2.34) in (2.31) with the solution v_1, v_2, \dots, v_m . There are many eigenvalues, corresponding to the different solutions of (2.35).
3. Shift operator method

In this section we explain how to calculate the anisotropic interfacial tension of the eight-vertex model. At the first place, we introduce inhomogeneous systems (Fujimoto, 1990b). Then, the commuting transfer matrices argument given in Section 2 is applied to the inhomogeneous systems.

A square lattice with $(1+\eta)M$ ($0 < \eta < \infty$) columns and N rows are assumed. We impose on it periodic boundary conditions along the horizontal direction and antiperiodic boundary conditions along the vertical direction. In the preceding section the system is homogeneous: the four parameters ρ , k, λ , and u are common to all the vertices. This condition is relaxed. We assume that ρ and u can vary from column to column. The values of ρ and u on the *j*th column are denoted by ρ_j and u_j , respectively. We consider two inhomogeneous systems: $u_1 = u_2 =$ $\cdots = u_M = u_0, u_{M+1} = u_{M+2} = \cdots = u_{(1+\eta)M} = \mp \lambda, \rho_1 = \rho_2 = \cdots = \rho_M = \rho_0,$ $\rho_{M+1} = \rho_{M+2} = \cdots = \rho_{(1+\eta)M} = i/\Theta(0)\Theta(i\lambda)H(i\lambda)$. The system with the upper (or lower) sign is called (A) (or (B)).

Because of various symmetry properties, we restrict ourselves to the regime

$$0 < k < 1, \qquad 0 < \lambda < I', \qquad |u_0| < \lambda, \qquad \rho_0 > 0$$
 (3.1)

without loss of generality (Baxter, 1982; Fan and Wu, 1970). Then, the eightvertex region where $u_j = u_0$ for 1 < j < M is in an antiferroelectric ordered state dominated by the vertices 5 and 6. When M and N become large under the condition that $(1 + \eta)M$ and N are even with η fixed to be constant, there is an interface across the eight-vertex region. In the region $u_j = -\lambda$ (or λ) for

– 67 –

 $M + 1 < j < (1 + \eta)M$, the arrow configuration around the site (i, j) is identical with that of the site (i + 1, j + 1) (or (i + 1, j - 1)). Therefore, the region $u_j = -\lambda$ (or λ) for $M + 1 < j < (1 + \eta)M$ has the effect of shifting the right end point of the interface downward (or upward) by $M\eta$ lattice spacings (Fig. 3.5). We denote by θ_{\perp} the angle between the horizontal axis and the normal vector of the interface drawn from the lower phase toward the upper phase. The parameter η is related to θ_{\perp} by

(A)
$$\eta = 1/\tan\theta_{\perp}, \qquad 0 < \theta_{\perp} < \pi/2$$
 (3.2a)

(B)
$$\eta = -1/\tan\theta_{\perp}, \qquad \pi/2 < \theta_{\perp} < \pi$$
 (3.2b)

We calculate the interfacial tension as a function of θ_{\perp} .

The commuting transfer matrices argument given in Section 2 is applied to the inhomogeneous systems (Baxter, 1972, 1982). First, the systems (A) and (B) are generalized. We set u_j 's to be $u_1 = u_2 = \cdots = u_M = v$, $u_{M+1} = u_{M+2} = \cdots = u_{(1+\eta)M} = v - u_0 \mp \lambda$, where v is a complex variable. The upper (or lower) sign corresponds to the generalized system (A) (or (B)). (In the following we use this convention.) The row-row transfer matrix is defined as

$$\left[\mathbf{V}_{IH}(v)\right]_{\alpha,\beta} = \sum_{\mu} \prod_{j=1}^{M} W\left(\mu_{j}, \alpha_{j} \left|\beta_{j}, \mu_{j+1}\right| v\right)$$
$$\times \prod_{k=M+1}^{(1+\eta)M} W\left(\mu_{k}, \alpha_{k} \left|\beta_{k}, \mu_{k+1}\right| v - u_{0} \mp \lambda\right)$$
(3.3)

where $\mu_{(1+\eta)M+1} = \mu_1$ and W's are given by (1.1) and (2.10). It is noted that in the star-triangle relation (2.7) the third pair (a'', b'', c'', d'') is parametrized by

- 68 -

difference u' - u. Substitute $\mathbf{V}_{IH}(v)$, $\mathbf{V}_{IH}(v')$ into (2.2) and (2.4) as \mathbf{V} , \mathbf{V}' . It follows, from the star-triangle relation, that $\mathbf{V}_{IH}(v)$ and $\mathbf{V}_{IH}(v')$ commute with each other for all values of v and v'. The one-parameter family of $\mathbf{V}_{IH}(v)$ is simultaneously diagonalized for all v. The eigenvalues of $\mathbf{V}_{IH}(v)$ are denoted by $V_{IH}(v)$.

Secondly, an equation for $V_{IH}(v)$ is derived. We define a complete set of $2^{(1+\eta)M}$ -dimensional vectors $\mathbf{y}_{IH}(v)$. Each vector $\mathbf{y}_{IH}(v)$ is the form

$$\mathbf{y}_{IH}(v) = \mathbf{g}_1(v) \otimes \mathbf{g}_2(v) \otimes \cdots \otimes \mathbf{g}_M(v)$$
$$\otimes \mathbf{g}_{M+1}(v - u_0 \mp \lambda) \otimes \cdots \otimes \mathbf{g}_{(1+\eta)M}(v - u_0 \mp \lambda)$$
(3.4)

where $\mathbf{g}_j(v)$'s are given by (2.15)~(2.17) with M replaced by $(1 + \eta)M$. The argument from (2.18) to (2.27) is repeated for $\mathbf{V}_{IH}(v)$ and $\mathbf{y}_{IH}(v)$. It is found that

$$\mathbf{V}_{IH}(v)\mathbf{y}_{IH}(v) = \phi_1(v)\mathbf{y}_{IH}(v+2\lambda') + \phi_2(v)\mathbf{y}_{IH}(v-2\lambda')$$
(3.5)

where

$$\phi_1(v) = \{\rho_1 h[(\lambda - v)/2]\}^M \{\rho_{M+1} h[(\lambda - v + u_0 \pm \lambda)/2]\}^{M\eta}$$
(3.6a)

$$\phi_2(v) = \{\rho_1 h[(\lambda + v)/2]\}^M \{\rho_{M+1} h[(\lambda + v - u_0 \mp \lambda)/2]\}^{M\eta}$$
(3.6b)

Using the vectors $\mathbf{y}_{IH}(v)$, we construct a non-singular matrix $\mathbf{Q}_{IH}(v)$, which satisfies the matrix equation

$$\mathbf{V}_{IH}(v)\mathbf{Q}_{IH}(v) = \phi_1(v)\mathbf{Q}_{IH}(v+2\lambda') + \phi_2(v)\mathbf{Q}_{IH}(v-2\lambda')$$
(3.6)

Since $\mathbf{Q}_{IH}(v)$ commutes with $\mathbf{Q}_{IH}(v')$ and $\mathbf{V}_{IH}(v'')$ for all values of v, v', and v'', we obtain

$$V_{IH}(v)q_{IH}(v) = \phi_1(v)q_{IH}(v+2\lambda') + \phi_2(v)q_{IH}(v-2\lambda')$$
(3.7)
- 69 -

where $q_{IH}(v)$ is the eigenvalue of $\mathbf{Q}_{IH}(v)$ corresponding to $V_{IH}(v)$. The function $q_{IH}(v)$ is the form given by (2.34), with *m* replaced by $m_{IH} = (1+\eta)M$. The zeros of q_{IH} , v_j $(j = 1, 2, \dots, m_{IH})$, are determined by the equations

$$\left\{\frac{h[(\lambda - v_k)/2]}{h[(\lambda + v_k)/2]}\right\}^M \left\{\frac{h[(\lambda - v_k + u_0 \pm \lambda)/2]}{h[(\lambda + v_k - u_0 \mp \lambda)/2]}\right\}^{M\eta} = -\exp(-4\tau\lambda') \prod_{j=1}^{m_{IH}} \frac{h[(v_k - v_j - 2\lambda)/2]}{h[(v_k - v_j + 2\lambda)/2]}$$
(3.8)

for $k = 1, 2, \dots, m_{IH}$. The zeros v_j 's and the constant τ satisfy the sum-rules

$$v_1 + v_2 + \dots + v_{m_{IH}} - \frac{M}{2}\eta(u_0 \pm \lambda)$$

= $\frac{1}{2}(s - 1 + 2m_{IH})I' + i(rs - 1 + 2m_{IH})I + 2p'I' + 4piI$ (3.9a)

$$\tau = \pi (s - 1 + 2m_{IH} + 4p')/8I \tag{3.9b}$$

where p and p' are integers. The eigenvalues $V_{IH}(v)$ can be calculated by the use of Eqs. (3.7)~(3.9). Then, letting $v = u_0$, we can get necessary informations to analyze the original inhomogeneous systems (A) and (B).

4. Anisotropic interfacial tension

Following the program given in Section 3, we calculate the anisotropic interfacial tension of the eight-vertex model. Since the calculational methods are almost the same for any values of u_0 , it is sufficient to consider the case $u_0 = 0$. In the case $u_0 = 0$, the generalized system (A) contains both original systems (A) and (B) as special limits: the system (A) corresponds to the $v \to 0$ limit; if we re-defined ρ_j 's as $\rho_1 = \rho_2 = \cdots = \rho_M = i/\Theta(0)\Theta(i\lambda)H(i\lambda), \ \rho_{M+1} = \rho_{M+2} = \cdots = \rho_{(1+\eta)M} = \rho_0$, the generalized system (A) reduces to the system (B) as $v \to \lambda$. For the system (B) given by the $v \to \lambda$ limit, (3.2b) should be replaced by

(B)
$$\eta = -\tan \theta_{\perp}, \qquad \pi/2 < \theta_{\perp} < \pi$$
 (3.2b')

We investigate the commuting transfer matrices argument for the generalized system (A). Eqs. (3.7)~(3.9) are used with $u_0 = 0$ and the upper sign. For convenience, (3.7) is rewritten as

$$V_{IH}(v)q_{IH}(v) = \phi_2(v)q_{IH}(v - 2\lambda')[1 + P(v)]$$
(4.1a)

$$=\phi_1(v)q_{IH}(v+2\lambda')[1+1/P(v)]$$
(4.1b)

$$P(v) = \phi_1(v)q_{IH}(v + 2\lambda')/\phi_2(v)q_{IH}(v - 2\lambda')$$
(4.1c)

Analysis is restricted to the regime

$$0 < k < 1, \qquad 0 < \lambda < I', \qquad 0 < \operatorname{Re}(v) < \lambda, \qquad \rho_0 > 0$$
 (4.2)

After $V_{IH}(v)$ is calculated, we take two limits $v \to 0$ and λ . In the regime (4.2) two antiferroelectric ordered state dominated by the vertices 5 and 6 are degenerate. It

– 71 –

is expected that a doublet of the largest eigenvalues of $\mathbf{V}_{IH}(v)$ are asymptotically degenerate as $M \to \infty$. In the low-temperature limit analysis, these eigenvalues are found. Then, we return to non-zero temperature and determine the leading behavior of the doublet of the largest eigenvalues as $M \to \infty$. Next, their finite size correction terms in this limit are calculated by the use of an integral equation. The anisotropic interfacial tension is obtained from the finite size correction terms (Baxter, 1973, 1982).

In the parametrization (2.10) the low-temperature limit corresponds to the $k \to 0, I', \lambda, v \to \infty$ limit, with the ratios λ/I' and v/I' being order of unity. It is supposed that $0 < \operatorname{Re}(v_j) < \lambda$ for all j. Then, the low-temperature limit analysis of (3.8) and (3.9) shows that

$$\tau = 0, \qquad s = (-1)^{m_{IH}} \qquad \prod_{j=1}^{m_{IH}} z_j = r x^{M\eta/2}$$
(4.3)

where

$$z_j = \exp(-\pi v_j/2I), \qquad x = \exp(-\pi\lambda/2I) \tag{4.4}$$

Because of the sum-rules (3.9), τ and $\prod_{j=1}^{m_{IH}} z_j$ take discrete values. The eigenvalue s takes a value of +1 or -1. We expect that τ , s, and $\prod_{j=1}^{m_{IH}}$ keep their low-temperature limit values (4.3) throughout the regime (4.2) without discontinuous changes. In the low-temperature limit it is also found, from (3.8) and (3.9), that

$$v_j \sim \frac{2I}{m_{IH}} i[2j - m_{IH} - (r+1)/2] + \frac{\eta}{1+\eta}\lambda$$
 (4.5)

and that

$$P(v) \sim r(-1)^{m_{IH}} z^{m_{IH}} x^{-M\eta/2},$$

-72 –

$$-\min\left\{0, 2 - \frac{2+3\eta}{1+\eta}\frac{\lambda}{I'}\right\} < \operatorname{Re}\left(\frac{v}{I'}\right) < \min\left\{\frac{\lambda}{I'}, 2 - \frac{2+\eta}{1+\eta}\frac{\lambda}{I'}\right\} (4.6a)$$

$$\sim q^{m_{IH}} x^{-2m_{IH}}, \qquad 2 - \frac{2+\eta}{1+\eta} \frac{\lambda}{I'} < \operatorname{Re}\left(\frac{v}{I'}\right) < \frac{\lambda}{I'}$$

$$(4.6b)$$

$$\sim q^{-m_{IH}} x^{2m_{IH}}, \qquad 0 < \operatorname{Re}\left(\frac{v}{I'}\right) < \frac{2+3\eta}{1+\eta} \frac{\lambda}{I'} - 2$$

$$(4.6c)$$

where

$$z = \exp(-\pi v/2I) \tag{4.7}$$

The region of applicability of the three equations (4.6) are shown in Fig. 3.6. We get two eigenvalues, corresponding to $r = \pm 1$. Using (4.5) and (4.6) in (4.1*a*), we find that the two eigenvalues behave in the low-temperature limit as

$$V_{IH;r}(v) \sim r\rho_1^M \rho_{M+1}^{M\eta} q^{m_{IH}/2} x^{-2m_{IH}} \sim r \prod_{j=1}^{(1+\eta)M} c_j$$
(4.8)

Note that in the low-temperature limit

$$c_j \gg a_j, b_j, d_j$$
 for all j (4.9)

where a_j , b_j , c_j , and d_j are given by (2.10), with ρ and u replaced by ρ_j and u_j . From (4.8) and (4.9), the two eigenvalues $V_{IH;r}(v)$ are identified with the doublet of the largest eigenvalues.

Here, we leave the low-temperature limit. In the regime (4.2) the asymptotic behavior of the doublet of the largest eigenvalues $V_{IH;r}(v)$ as $M \to \infty$ is calculated. We start with assuming that

(i) for large M a contour C defined by |P(v)| = 1 is found in the region $0 < \operatorname{Re}(v) < \lambda; v_j$'s lie on the contour C

- (ii) there exists a real positive number δ such that P(v) is exponentially larger than 1 as M → ∞ if v is between the contour C and the line Re(v)= -δ;
 P(v) is exponentially smaller than 1 if v is between the contour C and the line Re(v)= λ + δ,
- (iii) $V_{IH;r}(v)$ is analytic and non-zero (ANZ) for $0 \leq \operatorname{Re}(v) \leq \lambda$.

From (4.6) and (4.8), the assumptions (i) \sim (iii) seem to be correct for sufficient low-temperature. It will be shown that these assumptions are satisfied throughout the regime (4.2).

Two functions $X_+(v)$ and $X_-(v)$ are defined by

$$\ln X_{+}(v) = \frac{1}{4iI} \int_{\lambda+\beta-2iI}^{\lambda+\beta+2iI} \frac{\ln[1+P(v')]}{\exp[\pi(v-v')/2I] - 1} dv', \quad \operatorname{Re}(v) > \lambda+\beta \ (4.10a)$$
$$\ln X_{-}(v) = \frac{-1}{4iI} \int_{\lambda+\beta'-2iI}^{\lambda+\beta'+2iI} \frac{\ln[1+P(v')]}{\exp[\pi(v-v')/2I] - 1} dv', \quad \operatorname{Re}(v) < \lambda+\beta'(4.10b)$$

with $0 < \beta < \beta' < \delta$. Then, 1 + P(v) is factorized as

$$X_{+}(v)X_{-}(v) = 1 + P(v)$$
(4.11)

Using (4.11), we define $X_+(v)$ for $\operatorname{Re}(v) \leq \lambda + \beta$ and $X_-(v)$ for $\operatorname{Re}(v) \geq \lambda + \beta'$. From the assumption (ii), $X_+(v)$ is ANZ if v is in the rhs of the contour C, and $X_-(v)$ is ANZ for $\operatorname{Re}(v) < \lambda + \delta$. Substituting (4.11) into (4.1a), we find that

$$V_{IH;r}(v) = \phi_2(v)q_{IH}(v - 2\lambda')X_+(v)X_-(v)/q_{IH}(v)$$
(4.12)

The functions $\phi_2(v)$ and $q_{IH}(v)$ is rewritten as

$$\phi_2(v) = \rho_1^M \rho_{M+1}^{M\eta} \gamma^{2m_{IH}} z^{-m_{IH}} x^{-m_{IH}} \exp\left[-\frac{m_{IH}\pi}{2I} \frac{\eta}{1+\eta}\lambda\right] - 74 -$$

$$\times A(\lambda + v)A^{\eta}(v)A(2I' - \lambda - v)A^{\eta}(2I' - \lambda)$$
(4.13)

$$q_{IH}(v) = \gamma^{m_{IH}} \exp[\pi (m_{IH}v - v_1 - v_2 - \dots - v_{m_{IH}})/4I]$$

$$\times F(v)G(v - 2I') \qquad (4.14a)$$

$$= (-\gamma)^{m_{IH}} \exp[\pi (v_1 + v_2 + \dots + v_{m_{IH}} - m_{IH}v)/4I]$$

$$\times F(v + 2I')G(v) \qquad (4.14b)$$

where

$$\gamma = q^{1/4} \Theta(0) \prod_{n=1}^{\infty} (1 - q^{2n})^2$$
(4.15)

$$A(v) = \prod_{n=0}^{\infty} [1 - q^n \exp(-\pi v/2I)]^M$$
(4.16)

$$F(v) = \prod_{j=1}^{m_{IH}} \prod_{n=0}^{\infty} \{1 - q^n \exp[-\pi(v - v_j)/2I]\}$$
(4.17)

$$G(v) = \prod_{j=1}^{m_{IH}} \prod_{n=0}^{\infty} \{1 - q^n \exp[\pi(v - v_j)/2I]\}$$
(4.18)

Substitute (4.13) and (4.14) into (4.12). We use (4.14a) for $q_{IH}(v)$ and (4.14b) for $q_{IH}(v-2\lambda')$. It follows that

$$V_{IH;r}(v) = r\rho_1^M \rho_{M+1}^{M\eta} \gamma^{2m_{IH}} x^{-2m_{IH}} L_+(v) L_-(v)$$
(4.19)

where

$$L_{+}(v) = A(\lambda + v)A^{\eta}(v)F(v + 2I' - 2\lambda)X_{+}(v)/F(v)$$
(4.20)

$$L_{-}(v) = A(2I' - \lambda - v)A^{\eta}(2I' - v)G(v - 2\lambda)X_{-}(v)/G(v - 2I') \quad (4.20b)$$

From the assumption (i) and (iii), it is found that $L_+(v)$ is ANZ for $\operatorname{Re}(v) > 0$, and that $L_-(v)$ is ANZ for $\operatorname{Re}(v) < \delta'$; $\delta' = \min\{(2I' - \lambda), 2\lambda, \lambda + \delta\}$.

We also define $Y_+(v)$ and $Y_-(v)$ by

$$\ln Y_{+}(v) = \frac{1}{4iI} \int_{-\beta-2iI}^{-\beta+2iI} \frac{\ln[1+1/P(v')]}{\exp[\pi(v-v')/2I] - 1} dv', \quad \text{Re} > -\beta \qquad (4.21a)$$

$$\ln Y_{-}(v) = \frac{-1}{4iI} \int_{-\beta'-2iI}^{-\beta'+2iI} \frac{\ln[1+1/P(v')]}{\exp[\pi(v-v')/2I] - 1} dv', \quad \text{Re} < -\beta' \quad (4.21b)$$

Then, 1 + 1/P(v) is factorized as

$$Y_{+}(v)Y_{-}(v) = 1 + 1/P(v)$$
(4.22)

Eq. (4.1b) is rewritten as

$$V_{IH;r}(v) = \phi_1(v)q_{IH}(v+2\lambda')Y_+(v)Y_-(v)/q_{IH}(v)$$
(4.23)

Using the expressions (4.14) and

$$\phi_{1}(v) = \rho_{1}^{M} \rho_{M+1}^{M\eta} \gamma^{2m_{IH}} z^{m_{IH}} x^{-m_{IH}} \exp\left[\frac{m_{IH}\pi}{2I} \frac{\eta}{1+\eta}\lambda\right] \\ \times A(\lambda - v) A^{\eta}(2\lambda - v) A(2I' - \lambda + v) A^{\eta}(2I' - 2\lambda + v)$$
(4.24)

we obtain

$$V_{IH;r}(v) = r\rho_1^M \rho_{M+1}^{M\eta} \gamma^{2m_{IH}} x^{-2m_{IH}} M_+(v) M_-(v)$$
(4.25)

where

$$M_{+}(v) = A(2I' - \lambda + v)A^{\eta}(2I' - 2\lambda + v)F(v + 2\lambda)Y_{+}(v)/F(v + 2I')(4.26a)$$
$$M_{-}(v) = A(\lambda - v)A^{\eta}(2\lambda - v)G(v + 2\lambda - 2I')Y_{-}(v)/G(v)$$
(4.26b)

The function $M_+(v)$ is ANZ for $\operatorname{Re}(v) > \lambda - \delta'$; $M_-(v)$ is ANZ for $\operatorname{Re}(v) < \lambda$.

Compare (4.19) with (4.25). It is found that

$$M_{+}(v)/L_{+}(v) = L_{-}(v)/M_{-}(v)$$
(4.27)

The lhs of (4.27) is ANZ for $\operatorname{Re}(v) > 0$, and the rhs of (4.27) is ANZ for $\operatorname{Re}(v) < \lambda$. Thus, both sides of (4.27) are entire. Moreover, they are bounded in the $\operatorname{Re}(v) \rightarrow \pm \infty$ limit. From Liouville's theorem, it follows that they are constant. The fact that the rhs of (4.27) \rightarrow 1 as $\operatorname{Re}(v) \rightarrow \infty$ shows that this constant is 1. Finally, we obtain

$$M_{+}(v) = L_{+}(v), \qquad M_{-}(v) = L_{-}(v)$$
 (4.28)

The first equation gives the recursion relation of $S_+(v)$:

$$S_{+}(v) = S_{+}(v + 2I' - 2\lambda)X_{+}(v)/Y_{+}(v)$$
(4.29)

where

$$S_{+}(v) = F(v+2\lambda)F(v)/A(v+\lambda)A^{\eta}(v)$$
(4.30)

Eq. (4.29) is solved as

$$S_{+}(v) = \prod_{n=0}^{\infty} X_{+}[v + 2n(I' - \lambda)]/Y_{+}[v + 2n(I' - \lambda)]$$
(4.31)

Regarding (4.30) as a recursion relation for F(v), we get

$$F(v) = \prod_{n=0}^{\infty} \frac{A[v + (4n+1)\lambda]A^{\eta}(v + 4n\lambda)S_{+}(v + 4n\lambda)}{A[v + (4n+3)\lambda]A^{\eta}[v + (4n+2)\lambda]S_{+}[v + (4n+2)\lambda]}$$
(4.32)

Similarly, it follows, from the second equation in (4.28), that

$$S_{-}(v) = G(v)G(v - 2\lambda)/A(\lambda - v)A^{\eta}(2\lambda - v)$$

= $\prod_{n=0}^{\infty} Y_{-}[v - 2n(I' - \lambda)]/X_{-}[v - 2n(I' - \lambda)]$ (4.33)

$$G(v) = \prod_{n=0}^{\infty} \frac{A[(4n+1)\lambda - v]A^{\eta}[(4n+2)\lambda - v]S_{-}(v - 4n\lambda)}{A[(4n+3)\lambda - v]A^{\eta}[(4n+4)\lambda - v]S_{-}[v - (4n+2)\lambda]}$$
(4.34)

Substitute (4.13), (4.14), and (4.24) into (4.1c). Eq. (4.14a) is used for $q_{IH}(v + 2\lambda')$, and (4.14b) for $q_{IH}(v - 2\lambda')$. Then, by the use of (4.32) and (4.34), P(v) can be expressed in terms of A(v) and $S_{\pm}(v)$. After some calculations, we obtain

$$P(v) = rp^{M}(v)p^{M\eta}(v-\lambda)$$

$$\times \prod_{n=0}^{\infty} \frac{S_{+}[v+(4n+2)\lambda]S_{+}(v+2I'+4n\lambda)}{S_{+}[v+(4n+4)\lambda]S_{+}[v+2I'+(4n-2)\lambda]}$$

$$\times \prod_{n=0}^{\infty} \frac{S_{-}[v-2I'-(4n-2)\lambda]S_{-}[v-(4n+4)\lambda]}{S_{-}(v-2I'-4n\lambda)S_{-}[v-(4n+2)\lambda]}$$
(4.35)

where

$$p(v) = (-z)^{1/2} f(xz^{-1}, x^4) / f(xz, x^4)$$
(4.36)

and z is related to v by (4.7); f(w, x) is given by (2.30) of Chapter 2. Eq. (4.31) shows that, when M becomes large and v is in the rhs of the contour C, $S_+(v)$ behaves as

$$S_{+}(v) \sim 1 + e^{-\varepsilon M} \tag{4.37}$$

with $\varepsilon > 0$. From (4.33) it is found that, if v is in the lbs of C, $S_{-}(v)$ behaves for large M as

$$S_{-}(v) \sim 1 + \mathrm{e}^{-\varepsilon M} \tag{4.38}$$

with $\varepsilon > 0$. We define three regions a, b, and c as follows: for a given point v, choose a point v_C on C such that $\operatorname{Im}(v)=\operatorname{Im}(v_C)$; v is in the region a if $|\operatorname{Re}(v)-\operatorname{Re}(v_C)| <$ $\min\{2\lambda, 2I'-2\lambda\}$; in the region b if $2I'-2\lambda < \operatorname{Re}(v)-\operatorname{Re}(v_C) < 2\lambda$; in the region c if $2\lambda < \operatorname{Re}(v)-\operatorname{Re}(v_C) < 2I'-2\lambda$ (Fig. 3.7). For $v \in$ the region a and M large, $S_+(v)$'s and $S_-(v)$'s in the rhs of (4.35) can be replaced by unity. It follows that

– 78 –

as $M \to \infty$

$$P(v) \sim r p^M(v) p^{M\eta}(v-\lambda), \qquad v \in \text{the region } a$$
 (4.39a)

For $v \in$ the regions b and c, using the periodicity relation

$$q_{IH}(v+2I') = srq^{-(1+\eta)M/4} \exp\left\{\left[(1+\eta)Mv - M\eta\lambda\right]\pi/4I\right\}q_{IH}(v)$$
(4.40)

we can determine the leading behavior of P(v) in the $M \to \infty$ limit as

$$P(v) \sim 1, \qquad v \in \text{the region } b \qquad (4.39b)$$
$$\sim p^{M}(v)p^{M}(v-2I')p^{M\eta}(v-\lambda)p^{M\eta}(v-\lambda-2I'), \qquad v \in \text{the region } c \qquad (4.39c)$$

Replace $L_{-}(v)$ by $M_{-}(v)$ in (4.19). Then, substituting (4.20*a*), (4.26*b*) into (4.19), using (4.32) and (4.34), and neglecting exponentially small corrections as $M \to \infty$, we find that for $0 \leq \text{Re}(v) \leq \lambda$

$$V_{IH;r}(v) \sim rV_0(v) \tag{4.41}$$

where

$$V_{0}(v) = (\gamma \rho_{1}/x)^{M} \prod_{n=0}^{\infty} \frac{A[v + (4n+3)\lambda]A[v + 2I' + (4n-1)\lambda]}{A[v + (4n+5)\lambda]A[v + 2I' + (4n+1)\lambda]}$$

$$\times \prod_{n=0}^{\infty} \frac{A[(4n+3)\lambda - v]A[(4n-1)\lambda - v + 2I']}{A[(4n+5)\lambda - v]A[(4n+1)\lambda - v + 2I']}$$

$$\times (\gamma \rho_{M+1}/x)^{M\eta} \prod_{n=0}^{\infty} \frac{A^{\eta}[v + (4n+2)\lambda]A^{\eta}[v + 2I' + (4n-2)\lambda]}{A^{\eta}[v + (4n+4)\lambda]A^{\eta}[v + 2I' + 4n\lambda]}$$

$$\times \prod_{n=0}^{\infty} \frac{A^{\eta}[(4n+4)\lambda - v]A^{\eta}[4n\lambda - v + 2I']}{A^{\eta}[(4n+6)\lambda - v]A^{\eta}[(4n+2)\lambda - v + 2I']}$$
(4.42)

The leading behavior as $M \to \infty$ (4.39) and (4.41) show that the three assumptions (i)~(iii) are always satisfied without the restriction to the sufficient lowtemperature. Therefore, the argument from (4.10) to (4.42) makes sense throughout the regime (4.2). It is verified that (4.39) and (4.41) reproduce (4.6) and (4.8) in the low-temperature limit.

In (4.41) the leading terms of $V_{IH;r}(v)$ as $M \to \infty$ are equal in magnitude and opposite in sign. The calculation of the finite size correction terms shows that they are asymptotically degenerate as $M \to \infty$. Returning to the derivation of (4.41), and keeping all the contributions from $S_{\pm}(v)$, $X_{\pm}(v)$, and $Y_{\pm}(v)$, we get the integral equation

$$\ln[rV_{IH;r}(v)/V_0(v)] = \frac{1}{8iI} \int_{\lambda-2iI}^{\lambda+2iI} dv' \ln[1+P(v')]D(v-v') - \frac{1}{8iI} \int_{-2iI}^{+2iI} dv' \ln[1+1/P(v')]D(v-v') = \frac{1}{4iI} \int_{\lambda-2iI}^{\lambda+2iI} dv' \ln[1+P(v')]D(v-v'), 0 < \operatorname{Re}(v) < \lambda$$
(4.43)

where

$$D(v) = 1 + 2\sum_{n=0}^{\infty} (-1)^n \left\{ \frac{x^{2n} z^{-1}}{1 - x^{2n} z^{-1}} + \frac{x^{2n+2} z}{1 - x^{2n+2} z} \right\}$$
(4.44)

In the deformation into the third line of (4.43), we assumed the relation

$$P(v+2\lambda) = 1/P(v) \tag{4.45}$$

which holds in the leading order (4.39). The integral equation (4.43) can be used to calculate the finite size correction terms as $M \to \infty$.

-80 -

For $0 < \lambda/I' < 1/2$, the asymptotic degeneracy is easily found. From (4.39*a*), it follows that as $M \to \infty$

$$\ln[1 + P(v')] \sim r p^{M}(v') p^{M\eta}(v' - \lambda)$$
(4.46)

For large M, we can put (4.46) into (4.43) and integrate by steepest descent. Consequently, we obtain

$$rV_{IH;r}(v)/V_0(v) \sim 1 + \alpha(v)rp^M(v_s)p^{M\eta}(v_s - \lambda) + \cdots$$
 (4.47)

where v_s is the saddle point of $|p(v)p^{\eta}(v-\lambda)|$, determined by

$$\eta = -\frac{f(z_s, x^4)f(x^2z_s, x^4)f(-xz_s, x^4)f(-x^3z_s, x^4)}{f(-z_s, x^4)f(-x^2z_s, x^4)f(xz_s, x^4)f(x^3z_s, x^4)}, \quad z_s = \exp\left(-\frac{\pi v_s}{2I}\right) \quad (4.48a)$$

with the condition

$$v_s = \lambda + 2iI, \qquad \eta = 0 \tag{4.48b}$$

The function $\alpha(v)$ is to be determined by D(v) and the derivative of p(v). Eq. (4.47) shows that the doublet of the largest eigenvalues $V_{IH;r}(v)$ are asymptotically degenerate as $M \to \infty$.

For $1/2 < \lambda/I' < 1$, it happens that the saddle point v_s determined by (4.48) is in the region c, where the expansion (4.46) does not hold. If we replace (4.39a) by (4.39c) in (4.46), it is found that $V_{IH;+}(v)/V_{IH;-}(v) = 1$ within the leading order as $M \to \infty$. To investigate the asymptotic degeneracy, the higher order contributions neglected in the derivation of (4.39c) must be considered.

The function P(v) for r = +1 (or -1) is denoted by $P_+(v)$ (or $P_-(v)$). Instead of (4.43), it is useful to consider the equation

$$\ln[-V_{IH;+}(v)/V_{IH;-}(v)] \sim \frac{1}{4iI} \int_{\lambda-2iI}^{\lambda+2iI} dv' [P_{+}(v') - P(v')]D(v-v') \qquad (4.49)$$
$$-81 -$$

The asymptotic form (4.39a) shows that

$$P_{+}(v) - P_{-}(v) \sim 2p^{M}(v)p^{M\eta}(v-\lambda)$$
(4.50)

for $v \in$ the region *a*. Assuming that the saddle point v_s determined by (4.48) is in the region *c*, we show that Eq. (4.50) hold in the region *c*.

Eq. (4.39c) is re-derived with all the contributions from $S_{\pm}(v)$ as

$$\ln[P(v)/p^{M}(v)p^{M}(v-2I')p^{M\eta}(v-\lambda)p^{M\eta}(v-\lambda-2I')]$$

= $\ln[1+P(v-2I'+2\lambda)] + \ln[1+P(v)]$
+ $\frac{1}{4iI} \int_{\lambda-2iI}^{\lambda+2iI} dv' \ln[1+P(v')][D(v-v'-2I')+D(v'-v)]$ (4.51)

for $v \in$ the region c, $\operatorname{Re}(v) < \lambda$. Keeping only the dominant terms as $M \to \infty$, we obtain

$$\ln[P_{+}(v)/P_{-}(v)] \sim [P_{+}(v+2\lambda-2I') - P_{-}(v+2\lambda-2I')] + \frac{1}{4iI} \int_{\lambda-2iI}^{\lambda+2iI} dv' [P_{+}(v') - P_{-}(v')] [D(v-v'-2I') + D(v'-v)] \quad (4.52)$$

A line segment connecting the points v_s and v_s^* is denoted by l; v_s^* is a point on the contour C such that $\operatorname{Im}(v_s)=\operatorname{Im}(v_s^*)$. In the rhs of (4.52), suppose that the contribution from the integral is always negligibly smaller than that from the square bracket in a region containing l. It follows, from (4.39*a*) and (4.39*c*), that Eq. (4.50) is correct in this region. Moreover, substituting (4.50) into the integrand of (4.52), and evaluating the integral by steepest descent around v_s , we find that this integral is dominated by the square bracket for v on l. We expect that the asymptotic form of $P_+(v) - P_-(v)$ as $M \to \infty$ is given by (4.50) in a region containing l though it can not be proved rigorously. Therefore, the result (4.47) is unchanged even if the saddle point v_s is in the region c.

Now, setting v = 0 and λ , and choosing the values of ρ_j 's suitably, we consider the systems (A) and (B). When M and N becomes large under the condition that $(1+\eta)M$ and N are even with η fixed to be constant, the partition functions of the systems (A) and (B) are estimated as

$$Z = \text{Tr} \left[\mathbf{V}_{IH}^{N}(v) \mathbf{R}^{n} \right]$$

 $\sim \left\{ \left[1 + (-1)^{n} \right] + \left[1 - (-1)^{n} \right] N \alpha(v) p^{M}(v_{s}) p^{M\eta}(v_{s} - \lambda) \right\} V_{0}^{N}(v),$
 $v = 0, \lambda$ (4.53)

where **R** is inserted to impose two different boundary conditions along the vertical direction: the case $n \equiv 0 \pmod{2}$ corresponds to periodic boundary conditions, and $n \equiv 1 \pmod{2}$ antiperiodic boundary conditions. The second term in the brace of (4.53) gives an excess free energy above the bulk free energy when the antiperiodic boundary conditions are imposed. From the excess free energy, the anisotropic interfacial tension is calculated. After some calculations, we get

$$-\sigma/k_B T = \cos\theta_{\perp} \ln p(v_s - \lambda) + \sin\theta_{\perp} \ln p(v_s), \quad -\pi < \theta_{\perp} < \pi$$
(4.54)

where σ is the interfacial tension and v_s is determined as a function of θ_{\perp} by (4.48), with η replaced by $1/\tan \theta_{\perp}$. The saddle point v_s satisfies the relations

$$v_s(\theta_{\perp} + \pi/2) = v_s(\theta_{\perp}) - \lambda, \qquad v_s(-\theta_{\perp}) = -v_s(\theta_{\perp}) - 2\lambda \tag{4.55}$$

These relations assure the symmetry relations of σ

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

$$-83 -$$

$$(4.56)$$

5.Equilibrium crystal shape

We derive the ECS of the eight-vertex model from the anisotropic interfacial tension (4.54). Using Wulff's construction (4.56a) of Chapter 2, we find that

$$\frac{\Lambda X}{k_B T} = -\ln \left| (-x^{-1} z_s)^{1/2} \frac{f(x^2 z_s, x^4)}{f(z_s, x^4)} \right|$$
(5.1*a*)

$$\frac{\Lambda Y}{k_B T} = -\ln \left| (-z_s)^{1/2} \frac{f(x z_s^{-1}, x^4)}{f(x z_s, x^4)} \right|$$
(5.1*b*)

where (X, Y) is the position vector of a point on the ECS and Λ is a scale factor. As temperature is lowered, the ECS deformed into a square from a sphere near the critical temperature (Fig. 3.8). It is helpful to calculate the radius of curvature. We can calculate the radii of curvature at $\theta_{\perp} = 0$ and $\pi/4$. A facet (or corner) appears at $\theta_{\perp} = 0$ (or $\pi/4$) in the low-temperature limit. At $\theta_{\perp} = 0$, we obtain

$$\frac{\rho}{R} = \frac{f^4(x, x^4)}{f^4(-x, x^4)} \bigg/ \ln \left[x^{-1/2} \frac{f(-x^2, x^4)}{f(-1, x^4)} \right]$$
(5.2)

where ρ is the radius of curvature and $R = (X^2 + Y^2)^{1/2}$. In the low-temperature limit, where $x \to 0$, it is found that

$$\rho/R \sim -2/\ln x \tag{5.3}$$

Near the critical temperature, where I becomes large and λ is order of unity, ρ/R behaves as

$$\rho/R \sim 1 - (16/3) \exp(-2\pi I/\lambda)$$
 (5.4)

Similarly, the radius of curvature at $\theta = \pi/4$ is calculated as

$$\frac{\rho}{R} = x^{-1/2} \frac{f^2(x, x^4) f^2(-x, x^4)}{f^2(-1, x^4) f^2(-x^2, x^4)} \frac{f(x^{1/2}, x^4) f(x^{3/2}, x^4)}{f(-x^{1/2}, x^4) f(-x^{3/2}, x^4)} \\ \left/ \ln \left[x^{-1/4} \frac{f(-x^{3/2}, x^4)}{f(-x^{1/2}, x^4)} \right] \right.$$
(5.5)

-84-

It follows that in the low-temperature limit

$$\rho/R \sim 1/x^{1/2} \ln x \tag{5.6}$$

and that near the critical temperature

$$\rho/R \sim 1 + (16/3) \exp(-2\pi I/\lambda)$$
(5.7)

The ECS (5.1) can be written into the simple closed form

$$\cosh\left[\Lambda(X+Y)/k_BT\right] + \cosh\left[\Lambda(X-Y)/k_BT\right] = k^{1/2}(x) + k^{-1/2}(x)$$
(5.8)

where k(x) is defined by (1.6b). As we mentioned in Section 1, the eight-vertex model contains the six-vertex model and the square lattice nearest-neighbor Ising model as special limits. It follows, from (2.10), that the six-vertex model corresponds to the $q \to 0$ limit of the eight-vertex model. The expressions of the anisotropic interfacial tension (4.54) and the ECS (5.1), however, are independent of q. Rotating the coordinate axes through $\pi/4$, we find that (5.8) and (1.5*a*), with C_I replaced by C_{BC} , are the same within the scale factor Λ . Similarly, (1.4) and (2.10) show that, when $q = x^4$, the eight-vertex model factors into the two independent nearest-neighbor Ising models. At this time, (1.3) gives the relation

$$\sinh(2J/k_B T) = \sinh(2J'/k_B T) = k^{-1/2}(x)$$
 (5.9)

Using this relation, we can reproduce the ECS (1.5) from (5.8).

Until now from the beginning of the Section 4, we consider the special case $u_0 = 0$. The calculation in Section 4 can be easily extended for the general case

-85 -

 $|u_0| < \lambda$. There, the ECS (5.1) is generalized as

$$\frac{\Lambda X}{k_B T} = -\ln \left| (-a^{-1} x^{-1} z')^{1/2} \frac{f(x^2 a^{-1} z', x^4)}{f(a^{-1} z', x^4)} \right|$$
(5.10a)

$$\frac{\Lambda Y}{k_B T} = -\ln\left|(-z')^{1/2} \frac{f(xz'^{-1}, x^4)}{f(xz', x^4)}\right|$$
(5.10b)

where

$$a = \exp(-\pi u_0/2I)$$
 (5.11)

As the variable z' moves in the interval $-x^3 < z' < -x^{-1}$, (X, Y) in (5.10) draw a closed curve. The ECS (5.10) is also rewritten into the compact form

$$\cosh\left[\Lambda(X+Y)/k_BT\right] + B\cosh\left[\Lambda(X-Y)/k_BT\right] = 2D \tag{5.12}$$

Instead of showing the explicit forms of C and D, we point out that (5.10) can be regarded as a natural parametrization of (5.12). To see this, we rewrite (5.12) as

$$\alpha^2 \beta^2 + 1 + B\alpha\beta(\alpha + \beta) = 2D\alpha\beta \tag{5.13}$$

where

$$\alpha = \exp(-\Lambda X/k_B T), \qquad \beta = \exp(-\Lambda Y/k_B T)$$
 (5.14)

Eq. (5.13) is a symmetric biquadratic relation between α and β . It is known that this relation is naturally parametrized in terms of Jacobian elliptic functions as

$$\alpha = k^{1/2} \operatorname{sn}(\zeta + \eta), \qquad \beta = k^{1/2} \operatorname{sn}\zeta$$

$$B = -1/k \operatorname{sn}^2 \eta, \qquad D = -\operatorname{cn}\eta \operatorname{dn}\eta/k \operatorname{sn}^2\eta$$
(5.15)

where the elliptic functions are given by (A.4) (Baxter, 1982). Replace the norm of the elliptic function by x^2 , and set

$$z' = x \exp(-i\pi\zeta/I), \qquad \eta = i(u_0 + \lambda)/2$$
 (5.16)
- 86 -

Then, the expression (5.10) is reproduced. It is shown that the elliptic functions in (5.10) reflects the ECS (5.12).

Appendix

The theta functions with the norm q and the argument u are given by

$$H(u) = 2q^{1/4} \sin \frac{\pi u}{2I} \prod_{n=1}^{\infty} \left(1 - 2q^{2n} \cos \frac{\pi u}{I} + q^{4n} \right) (1 - q^{2n})$$
(A.1a)

$$H_1(u) = 2q^{1/4} \cos \frac{\pi u}{2I} \prod_{n=1}^{\infty} \left(1 + 2q^{2n} \cos \frac{\pi u}{I} + q^{4n} \right) (1 - q^{2n}) \tag{A.1b}$$

$$\Theta(u) = \prod_{n=1}^{\infty} \left(1 - 2q^{2n-1} \cos \frac{\pi u}{I} + q^{4n-2} \right) (1 - q^{2n}) \tag{A.1c}$$

$$\Theta_1(u) = \prod_{n=1}^{\infty} \left(1 + 2q^{2n-1} \cos \frac{\pi u}{I} + q^{4n-2} \right) (1 - q^{2n}) \tag{A.1d}$$

The half-periods are

$$I = \frac{\pi}{2} \prod_{n=1}^{\infty} \left(\frac{1+q^{2n-1}}{1-q^{2n-1}} \frac{1-q^{2n}}{1+q^{2n}} \right)^2$$
(A.2a)

$$I' = -\pi^{-1} I \ln q \tag{A.2b}$$

The modulus k and the conjugate modulus k' are

$$k = 4q^{1/2} \prod_{n=1}^{\infty} \left(\frac{1+q^{2n}}{1+q^{2n-1}}\right)^4 \tag{A.3a}$$

$$k' = \prod_{n=1}^{\infty} \left(\frac{1 - q^{2n-1}}{1 + q^{2n-1}} \right)^4 \tag{A.3b}$$

The Jacobian elliptic functions are

$$\operatorname{sn} u = k^{-1/2} H(u) / \Theta(u) \tag{A.4a}$$

$$\operatorname{cn} u = (k'/k)^{1/2} H_1(u) / \Theta(u)$$
 (A.4b)

$$\mathrm{dn}u = k^{\prime 1/2} \Theta_1(u) / \Theta(u) \tag{A.4c}$$

- 88 -

Chapter 4. Summary and Discussion

In Chapter 2, to calculate the anisotropic correlation length of the hardhexagon model, we proposed a new method. In this method, the shift operator and the transfer matrix were used simultaneously. The anisotropic correlation length was calculated from the ratios between the largest and next-largest eigenvalues of the transfer matrix and those of the shift operator. For $z > z_c$, a similar method was applied to the calculation of the anisotropic interfacial tension of the hard-hexagon model. There, systems with a mismatched vertical seam were considered, and the shift operator was used to tilt the seam. In the ordered state of the hard-hexagon model three phases degenerate. Noting this point, we calculated the interfacial tension between the A-phase and the B-phase from the extra factors appearing in the eigenvalues of the transfer matrix and the shift operator.

The anisotropic interfacial tension was also found by another method, where an inhomogeneous system was considered. The inhomogeneous system was defined on a square lattice of (1+v)M columns and N rows with toroidal boundary conditions. The lhs of the (M + 1)th column was the hard-hexagon model and the rhs of the (M + 1)th column had the effect of shifting the particle configuration of a column downward: if the particle configuration of the (M + 1)th column was shifted by Mv lattice spacings downward, it was identical with that of the first column. It was shown that a triplet of the largest eigenvalues of the row-row transfer matrix

4. SUMMARY AND DISCUSSION

are asymptotically degenerate as $M \to \infty$ under the condition that $(1 - v)M \equiv 0$ (mod 3), with v being fixed to be constant. The anisotropic interfacial tension was calculated from the finite size correction terms in this limit.

From the anisotropic interfacial tension, the equilibrium shape of a droplet of A-phase embedded inside the B-phase was derived by the use of Wulff's construction. It was found that the equilibrium crystal shape is a simple algebraic curve. Considering the radius of curvature at some special points on the equilibrium shape, we showed the roughening transition in the $z \to \infty$ limit.

In Chapter 3 the shift operator method of calculating the anisotropic interfacial tension was applied to the eight-vertex model. We considered an inhomogeneous eight-vertex model. It was found that a doublet of the largest eigenvalues of the transfer matrix are asymptotically degenerate as the width of the system becomes large. The finite size correction terms in this limit gave the anisotropic interfacial tension. The equilibrium crystal shape of the eight-vertex model was obtained from the calculated anisotropic interfacial tension via Wulff's construction. The eight-vertex model contains the six-vertex model and the square lattice Ising model as the $q \rightarrow 0$ and x^4 limits, respectively. The equilibrium crystal shapes of these two models had been derived, and shown that they are essentially the same. In the framework of the eight-vertex model, this fact was extended to the q-independence of the equilibrium crystal shape. We regarded the equilibrium crystal shape of the eight-vertex model as a symmetric biquadratic relation between $\alpha = \exp(-\Lambda X/k_BT)$ and $\beta = \exp(-\Lambda Y/k_BT)$. It was shown that the elliptic solution of the anisotropic interfacial tension is a natural parametrization of this relation.

4. SUMMARY AND DISCUSSION

Here, we make an addition about the equilibrium crystal shape of the hardhexagon model (4.59) of Chapter 2. It is known that the symmetric biquadratic relations between α and β

$$A_1 \alpha^2 \beta^2 + A_2 \alpha \beta (\alpha + \beta) + A_3 (\alpha^2 + \beta^2) + A_4 \alpha \beta + A_5 (\alpha + \beta) + A_6 = 0$$
(1)

are naturally parametrized in terms of elliptic theta functions, the general form being

$$\alpha = \phi(u+\eta), \qquad \beta = \phi(u) \tag{2a}$$

where

$$\phi(u) = \xi H(u+a)H(u-a)/H(u+b)H(u-b)$$
(2b)

and H(u) is the elliptic theta function defined by (A.1a) in Appendix of Chapter 3; ξ , a, and b are constants (p. 471 of Baxter, 1982). Eq. (4.59) of Chapter 2 can be rewritten as

$$\alpha^2 \beta^2 - C\alpha\beta + (\alpha + \beta) = 0 \tag{3a}$$

where

$$\alpha = \exp\left[-\sqrt{3}\Lambda\left(X + \sqrt{3}Y\right)/2\right], \qquad \beta = \exp\left[-\sqrt{3}\Lambda\left(X - \sqrt{3}Y\right)/2\right] \qquad (3b)$$

Eq. (3a) is a special case of (1) with $A_1 = A_5 = 1$, $A_4 = -C$, $A_2 = A_3 = A_6 = 0$. Set $\xi = x^{1/3}$, $a = -\eta = -2iI'/3$, and b = 0 in (2). The norm q and the argument u of the theta functions are related to x and a_s by

$$q^2 = x^3, \qquad \exp(-i\pi u/I) = a_s x^{-1}$$
 (4)
- 91 -

4. SUMMARY AND DISCUSSION

Then, the expression (4.58) of Chapter 2 is reproduced. The elliptic solutions of the anisotropic interfacial tension of the hard-hexagon model is also regarded as a natural parametrization of the symmetric biquadratic relation (3a).

Besides the hard-hexagon model and the eight-vertex model, there are some models whose interfacial tension had been calculated for special direction (Pearce and Baxter, 1984; Suzuki, 1989). It is known that the interfacial tension of these models are represented in terms of elliptic functions. These elliptic solutions are also expected to be related to simple equilibrium crystal shapes. We hope that these facts will be clarified in further investigation.

Acknowledgments

My study of the exactly solvable models started with a seminar by Prof. J. Kanamori. Application of the shift operator method to the equilibrium crystal shape problem was suggested by Prof. Y. Akutsu. I would like to express my appreciation for their useful advice and continuous encouragement.

Prof. S. Sasaki gave me a hint about the analysis presented in Section 4.3 of Chapter 2. Profs. P. A. Pearce and R. J. Baxter sent me detailed explanation of their paper, which was helpful in this analysis. I wish to thank them.

At last, I would like to thank Profs. A. Kotani, J. Igarashi, K. Suzuki, and T. Jo for their instruction at Kanamori Lab..

References

- Abraham, D. B. and Reed, P. (1974). Phys. Rev. Lett. 33, 377-379.
- Abraham, D. B. and Reed, P. (1976). Commun. Math. Phys. 49, 35-46.
- Akutsu, Y. and Akutsu, N. (1986). J. Phys. A: Math. Gen. 19, 2813-2820.
- Akutsu, Y. and Akutsu, N. (1990). Phys. Rev. Lett. 64, 1189-1192.
- Andrews, G. E., Baxter, R. J. and Forrester, P. J. (1984). J. Stat. Phys. 35, 193-266.
- Avron, J. E., van Beijeren, H., Schulman, L. S. and Zia, R. K. P. (1982). J.
 Phys. A: Math. Gen. 15, L81-L86.
- Baxter, R. J. (1971). Phys. Rev Lett. 26, 832-833.
- Baxter, R. J. (1972). Ann. Phys (N.Y.). 70, 193-228.
- Baxter, R. J. (1976). J. Stat. Phys. 15, 485-503.
- Baxter, R. J. (1973). J. Stat. Phys. 8, 25-55.
- Baxter, R. J. (1980). J. Phys. A: Math. Gen. 13, L61-L70.
- Baxter, R. J. (1982). "Exactly Solved Models in Statistical Mechanics". Academic Press, London.
- o Baxter, R. J. and Pearce, P. A. (1982). J. Phys. A: Math. Gen. 15, 897-910.
- Bethe, H. A. (1931). Z. Physik. 71, 205-226.
- Burton, W. K., Carbera, N. and Frank, F. C. (1951). Trans. R. Soc. A243, 229-358.

REFERENCES

- Cahn, J. W. and Hoffman, D. W. (1974). Acta. Met. 22, 1205-1214.
- Cheng, H. and Wu, T. T. (1967). Phys. Rev. 164, 719-735.
- Dobrushin, R. L. (1972). Theory Prob. Appl. 17, 582-600.
- Fan, C. and Wu. F. Y. (1970). Phys. Rev. B2, 723-733.
- Feynman, R. P. (1972). "Statistical Mechanics". Benjamin, Reading, Mass.
- Fradkin, E., Huberman, B. A. and Shenker, S. H. (1978). *Phys. Rev.* B18, 4789-4813.
- Fujimoto, M. (1990a). J. Stat. Phys. 59, 1355-1381.
- Fujimoto, M. (1990b). J. Stat. Phys. 61, 1297-1306.
- Gallavotti, G. (1972). Commun. Math. Phys. 27, 103-136.
- o Gaunt, D. S. (1967). J. Chem. Phys. 46, 3237-3259.
- Hoffman, D. W. and Cahn, J. W. (1972). Surf. Sci. 31, 368-388.
- Holzer, M. (1990). Phys. Rev. Lett. 64, 653-656.
- Jayaprakash, C., Saam, W. F. and Teitel, S. (1983). Phys. Rev. Lett. 50, 2017-2020.
- Kadanoff, L. P. and Wegner, F. J. (1971). Phys. Rev. B4, 3989-3993.
- Kasteleyn, P. W. (1961). *Physica* 27, 1209-1225.
- Kasteleyn, P. W. (1963). J. Math. Phys. 4, 287-293.
- Kuniba, A., Akutsu, Y. and Wadati, M. (1986). J. Phys. Soc. Jpn. 55, 3338-3353, and references therein.
- Lieb, E. H. (1967a). Phys. Rev. 162, 162-172.
- Lieb, E. H. (1967b). *Phys. Rev. Lett.* 18, 1046-1048.
- Lieb, E. H. (1967c). *Phys. Rev. Lett.* **19**, 108-110.

-95 -

- McCoy, B. M. and Wu, T. T. (1973). "The Two-Dimensional Ising Model".
 Harvard University Press, Cambridge, Mass.
- Onsager, L. (1944). Pys. Rev. 65, 117-149.
- Pearce, P. A. and Baxter, R. J. (1984). J. Phys. A: Math. Gen. 17, 2095-2108.
- Rottman, C. and Wortice, M. (1981). Pys. Rev. B24, 6274-6277.
- Runnels, L. K. and Combs, L. L. (1966). J. Chem. Phys. 45, 2482-2492.
- Stephenson, J. (1964). J. Math. Phys. 8, 1009-1024.
- Stroganov, Y, G. (1979). Phys. Lett. 74A, 116-118.
- Sutherland, B. (1970). J. Math. Phys. 11, 3183-3186.
- Sutherland, B., Yang, C. N. and Yang, C. P. (1967). *Phys. Rev. Lett.* 19, 586-591.
- Suzuki, J. (1989). J. Phys. Soc. Jpn. 58, 3111-3122.
- van Beijeren, H. (1977). Phys. Rev. Lett. 38, 993-996.
- Vdovichenko, N. V. (1964). Zh. Eksp. Teor. Fiz. 47, 715-719. [(1965). Sov.
 Phys. JETP 20, 477-479.]
- von Laue, M. (1944). Z. Krist. 105, 124-133.
- Weeks, J. D., Gilmer, G. H. and Leamy, H. J. (1973). Phys. Rev. Lett. 31, 549-551.
- Wu, F. Y. (1971). *Phys. Rev.* **B4**, 2312-2314.
- Wulff, G. (1901). Z. Krist. Mineral. 34, 449-530.
- Yang, C. P. (1967). Phys. Rev. Lett. 19, 586-588.
- Zia, R. K. P. (1978). *Phys. Lett.* A64, 345-347.

REFERENCES

- Zia, R. K. P. (1986). J. Stat. Phys. 45, 801-813.
- Zia, R. K. P. and Avron, J. E. (1982). Phys. Rev. B25, 2042-2045.

Figure Captions

- Fig. 2.1. A typical configuration of the hard-hexagon model. Occupied sites are denoted by solid circles and unoccupied sites are denoted by open circles.
- Fig. 2.2. (a) A typical configuration of the hard-square model. (b) Boltzmann weight around a face.
- Fig. 2.3. Graphical representation of the star-triangle relation of the hard-square model.
- Fig. 2.4. Mismatched vertical seams in the z → ∞ limit. (a) M ≡ 1 (mod 3), and (b) M ≡ 2 (mod 3). The starting points of the seams are denoted by S, and the end points are denoted by E. Three shift operators are inserted above the tenth row of each lattice. They tilt the seams by moving the points S and E along the horizontal direction.
- Fig. 2.5. Typical configurations of the inhomogeneous systems in the z → ∞ limit. (a)
 N ≡ 2 (mod 3). (b) N ≡ 1 (mod 3). The lhs of the tenth column is the hard-hexagon model, and the rhs of the tenth column works as the downward shift operator.
- Fig. 2.6. The polar plot of σ/ζ denoted by Σ in the $z \to \infty$ limit. All the figures $\bar{S}_1, \bar{S}_2, \bar{S}_3, \cdots$ satisfy the condition (4.52). The equilibrium shape is determined as the similar figure of the innermost figure \bar{S}_1 .
- Fig. 2.7. (a) The polar plot of the interfacial tension, and (b) the equilibrium crystal shape of the hard-hexagon model. We choose the chemical potential ζ as the

-98 –

FIGURE CAPTIONS

scale factor Λ . 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.

- Fig. 3.1. The eight possible arrow configurations around a vertex, and the corresponding Boltzmann weights.
- Fig. 3.2. The Ising model with two- and four-spin interactions. The solid lines are the square lattice where the eight-vertex model is defined. When J'' = 0, the dual lattice is divided into two sublattices; the sites of one sublattice is represented by open circles and the sites of the other sublattice by closed circle. The nearest-neighbor pairs on each sublattice are connected by interactions J and J', which are shown by dash dotted lines and broken lines, respectively.
- Fig. 3.3. The transfer matrix of the eight-vertex model.
- Fig. 3.4. Graphical representation of the star-triangle relation of the eight-vertex model.
- Fig. 3.5. Typical configuration of the inhomogeneous system (A) in the low-temperature limit. The eight-vertex region is represented by solid lines, and the region $u_j = -\lambda$ broken line. In the eight-vertex region two antiferroelectric ordered phases dominated by the vertices 5 and 6 coexist. Across the eight-vertex region, there is an interface. The interface consists of the vertices 1 and 3, which are shown by open circles. Because of the region $u_j = -\lambda$, the interface is tilted.
- Fig. 3.6. The regions of the applicability of the three formulae (3.5).
- Fig. 3.7. The three region a, b, and c in (4.40). (a) For a given point v, choose a point v_C on the contour C so that $\text{Im}(v)=\text{Im}(v_C)$. (b) Then, using $\text{Re}(v/I')-\text{Re}(v_C/I')$, we define three regions a, b, and c.

-99 -

Fig. 3.8. The equilibrium crystal shape of the eight-vertex model. We choose $k_B T \ln C$ as the scale factor Λ ; C is defined by (1.6*a*). From the outermost figure, $x = 1.0 \times 10^{-6}$, 1.0×10^{-4} , 0.001, 0.004, 0.01, 0.02, 0.04, 0.07, and 0.12, successively.



Fig. 2.1







(Ъ)




Fig. 2.3





(a)

T-1

Fig. 2.4



(a)



Fig. 2.5

(**b**)



Fig. 2.6







Fig. 3.1



Fig. 3.2



Fig. 3.3



Fig. 3.4



Fig. 3.5



Fig. 3.6



Fig. 3.7