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Equilibrium crystal shape of hard squares with diagonal attractions

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Abstract. We exactly calculate the anisotropic interfacial tension of a square lattice gas model with nearest-neighbour exclusion and next-nearest-neighbour attractions. This is achieved by a method which introduces the shift operator into the standard transfer matrix argument. From the calculated anisotropic interfacial tension the equilibrium crystal shape (ECS) is derived by the use of the Wulff construction. The ECS is a closed curve in the X–Y plane, represented as $\cosh[\Lambda(X+Y)/k_{\rm B}T] + A_3\cosh[\Lambda(X-Y)/k_{\rm B}T] + A_4/2 = 0$ with a scale factor Λ and constants A_3, A_4. We argue that this shape is a universal one which appears as the ECSs of a wide class of models.

1. Introduction

In connection with the roughening transition phenomena the equilibrium crystal shape (ECS) has attracted much attention [1]. A traditional method for finding the ECS is the Wulff construction [2], where the interfacial tension with its full anisotropy (anisotropic interfacial tension) is needed. A statistical mechanical model is solvable if it yields a parametrized family of solutions to the Yang–Baxter equation [3,4]. We have many such solutions to the Yang–Baxter equation and hence many solvable models [4]. Within the framework of the standard transfer matrix argument [3], we can obtain the interfacial tension of solvable models along a special direction. Analysis of the anisotropy, however, is a very complicated problem there. Recently, we developed a new method for finding the anisotropic interfacial tension [5,6]. The new method introduces the shift operator into the standard transfer matrix argument.

In a previous paper [7] we calculated the anisotropic interfacial tension of the eight-vertex model using the shift operator method. From the anisotropic interfacial tension we derived the ECS via the Wulff construction. The ECS of this model is represented as

$$\alpha^2\beta^2 + 1 + A_3^{(8v)}(\alpha^2+\beta^2) + A_4^{(8v)}\alpha\beta = 0 \qquad (1.1a)$$

with

$$\alpha = (-\Lambda X/k_{\rm B}T) \qquad \beta = (-\Lambda Y/k_{\rm B}T) \qquad (1.1b)$$

where (X, Y) is the position vector of a point on the ECS and Λ is a scale factor. The eight-vertex model contains the square lattice Ising model and the six-vertex model as special

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limits with respect to a parameter q [3]. Showing that the coefficients $A_3^{(8v)}$ and $A_4^{(8v)}$ are independent of q, we extend the fact that the ECSs of the square lattice Ising model and the six-vertex model are essentially the same [8]. Equation (1.1a) is a symmetric biquadratic relation between α and β. The symmetric biquadratic relation is naturally parametrized in terms of the Jacobian elliptic functions. We pointed out that an elliptic function $p(v)$ in the expression of the interfacial tension is directly related to the sn function in this parametrization. (For definition of $p(v)$, see (3.11) of [7].) In other words, the symmetric biquadratic relation (1.1a) is a source of the elliptic function $p(v)$.

In solving the hard-hexagon model, Baxter [3, 9–11] considered a square lattice gas model with nearest-neighbour exclusion (thus 'hard-squares') and next-nearest-neighbour interactions: an occupation number $\sigma_i (= 0, 1)$ is assigned to each site i of a square lattice; $\sigma_i = 0$ if the site i is empty; $\sigma_i = 1$ if the site i is occupied by a particle. When occupation numbers around a face are a, b, c and d counterclockwise starting from the bottom-left corner, the Boltzmann weight of the face is

$$W(a,b,c,d) = \begin{cases} mz^{(a+b+c+d)/4} \mathrm{e}^{Kac+Lbd} t^{-a+b-c+d} & \text{if } ab = bc = cd = da = 0 \\ 0 & \text{otherwise} \end{cases} \quad (1.2a)$$

There are five independent Boltzmann weights around a face:

$$\begin{aligned} \omega_1 &= W(0,0,0,0) = m \\ \omega_2 &= W(1,0,0,0) = W(0,0,1,0) = mz^{1/4}/t \\ \omega_3 &= W(0,1,0,0) = W(0,0,0,1) = mz^{1/4}t \\ \omega_4 &= W(1,0,1,0) = mz^{1/2}\mathrm{e}^K/t^2 \\ \omega_5 &= W(0,1,0,1) = mz^{1/2}\mathrm{e}^L t^2 \end{aligned} \quad (1.2b)$$

In (1.2) m is a trivial normalization factor and t is a parameter which cancels out of the partition function. For given values of one-particle activity z and diagonal interactions K, L, we can determine the thermal equilibrium state of the hard-square model. In the three-dimensional (z, K, L) space this model is solvable on a two-dimensional manifold defined by

$$z = (1 - \mathrm{e}^{-K})(1 - \mathrm{e}^{-L})/(\mathrm{e}^{K+L} - \mathrm{e}^K - \mathrm{e}^L) \quad (1.3)$$

Baxter divided the manifold (1.3) into six regimes I–VI.

The connection between $p(v)$ and (1.1a) in the eight-vertex model makes the ECSs of regimes III and IV very interesting. The manifold (1.3) corresponds to regimes III and IV in the case of attractive diagonal interactions: $K, L > 0$. Regime III is a first-order transition surface separating a disordered fluid phase and $c(2 \times 2)$ ordered solid phases, where one of the two sublattices is preferentially occupied by particles [11, 12]. Regime IV is an analytic continuation of regime III beyond a line of tricritical points but lies entirely in the $c(2 \times 2)$ ordered solid phase. For regimes III and IV Baxter and Pearce (BP) [11] calculated the interfacial tension along a special direction by standard transfer matrix argument. In both regimes the interfacial tension is expressed in terms of essentially the same elliptic function as $p(v)$. In the present paper we investigate the ECSs of regimes III and IV. The anisotropic interfacial tension of regimes III and IV is found by the shift operator method. Then, the ECSs are derived via the Wulff construction. The shift operator method is also used to show a simple thermodynamic relation between the anisotropic interfacial tension and the anisotropic correlation length.

The layout of this paper is as follows. In section 2 we are concerned with regime IV, and in section 3 regime III. Finally, section 4 is devoted to a summary and discussion, where we argue that (1.1) is a universal shape which appears as the ECSs of a wide class of models.

2. Regime IV

2.1. Anisotropic interfacial tension

In this section we consider a system where two $c(2 \times 2)$ ordered solid phases coexist with a phase separation line (or an interface). We denote the interfacial tension between the two solid phases by $\gamma(S-S)$. We start with reviewing the analysis of $\gamma(S-S)$ by BP [11], where its anisotropy does not enter. Suppose a square lattice of M columns and N rows with periodic boundary conditions in both directions. When $M \equiv 1 \pmod 2$ and $N \equiv 0 \pmod 2$, reflecting the existence of a mismatched vertical interface (figure 1(*a*)), extra factors appear in the largest eigenvalues of the transfer matrix. BP obtained $\gamma(S-S)$ along the vertical direction from the extra factors.

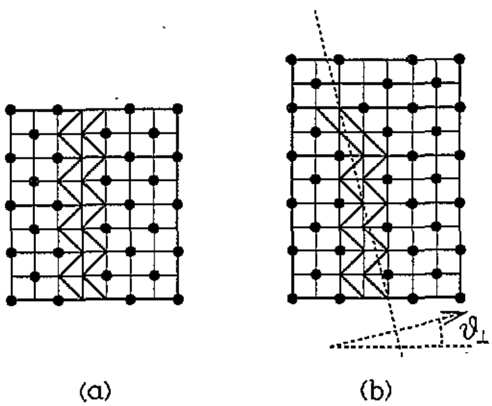

Figure 1. Mismatched vertical seam (or interface) in the $x \to 0$ limit. (*a*) When $M \equiv 1 \pmod 2$ and $N \equiv 0 \pmod 2$, there exists a mismatched vertical interface in the system. (*b*) The shift operator is inserted into a system with a mismatched vertical interface. The shift operator tilts the interface by moving the endpoint on the first row from that on the $(N+1)$th row along the horizontal direction.

To find the anisotropy of $\gamma(S-S)$, we repeat the argument in sections 3.1 and 3.2 of [5]. We tilt the vertical interface by inserting the shift operator into the lattice (figure 1(*b*)). The shift operator has the effect of moving the particle configuration on a row to the right along the horizontal direction by a lattice spacing. It is convenient to define the transfer matrices $\mathbf{T}(w)$ [10] as

$$[\mathbf{T}(w)]_{\sigma,\sigma'} = \left[-\frac{\omega_1(w)}{\omega_4(w)\omega_5(w)}\right]^M \prod_{i=1}^{M} W(\sigma_i, \sigma_{i+1}, \sigma'_{i+1}, \sigma'_i|w) \qquad (2.1)$$

where $\sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_M\}$ and $\sigma' = \{\sigma'_1, \sigma'_2, \ldots, \sigma'_M\}$ are the particle configurations of two successive periodic rows of M sites; the five Boltzmann weights ωs in (1.2b) are parametrized by (3.11) of [10] with $1 < w < x^{-2}$ and $-1 < x < 0$. In the $w \to 1$ limit $\mathbf{T}(w)$ reduces to the shift operator. By the use of $\mathbf{T}(w)$, the anisotropic interfacial tension is represented as

$$-\gamma(S-S)/k_\mathrm{B}T = \lim_{M,N\to\infty} \frac{1}{N\sqrt{1+\eta^2}} \ln \frac{1}{M\kappa^{MN}(w)} \mathrm{Tr}[\mathbf{T}(w)\mathbf{T}(1)^\eta]^N$$

$$= \lim_{M,N\to\infty} \frac{1}{N\sqrt{1+\eta^2}} \ln \frac{1}{M\kappa^{MN}(w)} \sum_p [T_p(w)T_p(1)^\eta]^N \tag{2.2a}$$

where the limit is taken under the conditions that $M \equiv 1 \pmod 2$ and $N(1+\eta) \equiv 0 \pmod 2$, with η fixed to be constant; $T_p(w)$ $(p = 1, 2, \ldots)$ is the pth eigenvalue of $\mathbf{T}(w)$ in decreasing order of magnitude; $\kappa(w)$ is the partition function per face, given by

$$\kappa(w) = \lim_{M\to\infty} T_1^{1/M}(w). \tag{2.2b}$$

The explicit forms of $T_p(w)$ were determined in section 3.1 of BP. Substituting them into (2.2), we get

$$-\gamma(S-S)/k_\mathrm{B}T = \lim_{N\to\infty} \frac{1}{N\sqrt{1+\eta^2}} \ln \frac{1}{4\pi\mathrm{i}} \oint_{|b|=1} \frac{\mathrm{d}b}{b} \rho(b)\phi^N(w/b)\phi^{N\eta}(1/b) \tag{2.3}$$

where

$$\phi(w) = w^{-1/2} f(xw, x^4)/f(xw^{-1}, x^4) \tag{2.4a}$$

$$f(p,q) = (1-p)\prod_{n=1}^{\infty}(1-pq^n)(1-p^{-1}q^n)(1-q^n). \tag{2.4b}$$

In the $M \to \infty$ limit $T_p(w)/\kappa^M(w)$ and $T_p(1)$ in (2.2a) become $\phi(w/b)$ and $\phi(1/b)$, respectively. We denote the continuous distribution of the eigenvalues on two sheets of Riemann surface by $\rho(b)$. The explicit form of $\rho(b)$ is unknown. Here, it is sufficient to assume its analyticity.

The integral in the right-hand side of (2.3) is estimated by the method of steepest descent. It follows that

$$\gamma(S-S|\theta_\perp)/k_\mathrm{B}T = \cos\theta_\perp \ln\phi(b_\mathrm{s}/w) + \sin\theta_\perp \ln\phi(b_\mathrm{s}) \quad -\pi/2 < \theta_\perp < \pi/2 \tag{2.5}$$

where $\theta_\perp$ is the angle between the horizontal direction and the normal direction of the line connecting the two endpoints of the interface (figure 1(b)); η is related to $\theta_\perp$ as

$$\eta = \tan\theta_\perp \tag{2.6}$$

and b_s is a saddle point of $|\phi(w/b)\phi^\eta(1/b)|$, given by

$$\tan\theta_\perp = -\left.\frac{f(xb,x^4)f(x^3b,x^4)f(-xb/w,x^4)f(-x^3b/w,x^4)}{f(-xb,x^4)f(-x^3b,x^4)f(xb/w,x^4)f(x^3b/w,x^4)}\right|_{b=b_\mathrm{s}} \tag{2.7a}$$

with the condition

$$b_\mathrm{s} = -xw \qquad \theta_\perp = 0. \tag{2.7b}$$

From the relation $\gamma(S-S|\theta_\perp+\pi) = \gamma(S-S|\theta_\perp)$, it is found that the expression (2.5) is analytically continued into $-\pi < \theta_\perp < \pi$, with b_s regarded as a function of $\theta_\perp$.

2.2. Equilibrium crystal shape

We now draw the ECS in the X–Y plane. Suppose that a droplet of one solid phase whose area is fixed to be constant is embedded inside a sea of the other solid phase. The ECS is the droplet shape of the minimum energy obtained from the anisotropic interfacial tension $\gamma(S-S)$ via the Wulff construction [1,2]:

$$\begin{aligned}\Lambda X &= \cos\theta_\perp \gamma(S-S|\theta_\perp) - \sin\theta_\perp \, \mathrm{d}\gamma(S-S|\theta_\perp)/\mathrm{d}\theta_\perp \\ \Lambda Y &= \sin\theta_\perp \gamma(S-S|\theta_\perp) + \cos\theta_\perp \, \mathrm{d}\gamma(S-S|\theta_\perp)/\mathrm{d}\theta_\perp\end{aligned} \tag{2.8}$$

where Λ is a scale factor adjusted to yield the area of the ECS; the position vector of a point on the ECS, denoted by (X, Y), is represented as a function of $\theta_\perp$; (X, Y) sweeps out the ECS as $\theta_\perp$ varies from $-\pi$ to π. Substituting (2.5) into (2.8), we get

$$\Lambda X/k_\mathrm{B}T = \ln\phi(b_\mathrm{s}/w) \qquad \Lambda Y/k_\mathrm{B}T = \ln\phi(b_\mathrm{s}). \tag{2.9}$$

Note that $\phi(w)$ is essentially the same elliptic function as $p(v)$ given by (3.11) of [7]. We can write (2.9) into the symmetric biquadratic relation (1.1a), where the two coefficients $A_3^{(8\mathrm{v})}$ and $A_4^{(8\mathrm{v})}$ are replaced by

$$\begin{aligned}A_3^{(\mathrm{IV})} &= -wf^2(x^2w, x^4)/xf^2(w, x^4) \\ A_4^{(\mathrm{IV})} &= w^{1/2}f^3(x^2, x^4)f(w^2, x^4)/xf^3(w, x^4)f(wx^2, x^4)\end{aligned} \tag{2.10}$$

and $\phi(w)$ corresponds to the sn function which naturally parametrizes the symmetric biquadratic relation (1.1a). Comparing (2.10) with (4.22) of [7], we find that the ECS (2.9) is identical to that of the eight-vertex model with

$$a^{(8\mathrm{v})} = -1/xw \qquad x^{(8\mathrm{v})} = -x \tag{2.11}$$

where $a^{(8\mathrm{v})}$ and $x^{(8\mathrm{v})}$ are the variables of the eight-vertex model defined by (4.18b) and (3.5) of [7], respectively.

2.3. Anisotropic correlation length

We suppose a sufficiently large lattice of M columns and N rows with periodic boundary conditions in both directions [$M \equiv N \equiv 0 \pmod 2$]. The pair correlation function between the site $(0, 0)$ and the site (l, m) is expected to decay exponentially to zero as $r = \sqrt{l^2 + m^2}$ becomes large. The correlation length ξ is defined by

$$\langle\sigma_{00}\sigma_{lm}\rangle - \langle\sigma_{00}\rangle\langle\sigma_{lm}\rangle \sim r^{-\tau}\mathrm{e}^{-r/\xi} \qquad \text{as } r \to \infty \tag{2.12}$$

where τ is a constant and the limit is taken with the ratio m/l ($= \eta = \tan\theta_\perp$) fixed. BP [11] calculated ξ for $\theta_\perp = 0$ to find that

$$1/\xi = 2\gamma(S-S)/k_\mathrm{B}T \qquad \text{for } \theta_\perp = 0 \tag{2.13}$$

The correlation length ξ is dependent on the direction $\theta_\perp$. In this section we extend the analysis of BP into general directions. It is shown that the thermodynamic relation (2.13) is satisfied for all $\theta_\perp$.

Using the standard transfer matrix argument BP represented the expectation value of the product $\sigma_{00}\sigma_{lm}$ as

$$\langle\sigma_{00}\sigma_{lm}\rangle = \sum_p \tilde{S}_0(1,p)\tilde{S}_m(p,1)[T_p(w)/T_1(w)]^l \tag{2.14}$$

where $T_p(w)$ $(p = 1, 2, \ldots)$ is the pth eigenvalue of the transfer matrix $\mathbf{T}(w)$ given by (2.1) in decreasing order of magnitude. For $\theta_\perp = 0$, considering the $l \to \infty$ limit with $m = 0$ in (2.14), we can obtain ξ from the ratios between the largest and next-largest eigenvalues of $\mathbf{T}(w)$. To find ξ for general $\theta_\perp$, the coefficients $\tilde{S}_0(1,p)\tilde{S}_m(p,1)$ are also important as well as the ratios of the eigenvalues. Calculating $\tilde{S}_0(1,p)\tilde{S}_m(p,1)$ is a very complicated problem, however. As was shown in section 2.1 of [5], we can overcome this difficulty by introducing the shift operator. Noting that $\mathbf{T}(w)$ reduces to the shift operator in the $w \to 1$ limit, we rewrite (2.14) as

$$\langle\sigma_{00}\sigma_{lm}\rangle = \sum_p \tilde{S}_0(1,p)\tilde{S}_0(p,1)\left[\frac{T_p(w)}{T_1(w)}\left(\frac{T_p(1)}{T_1(1)}\right)^\eta\right]^l. \tag{2.14'}$$

Using expression (2.14′), we can calculate the anisotropic correlation length from the ratios between the largest and next-largest eigenvalues of the transfer matrix $\mathbf{T}(w)$ and those of the shift operator $\mathbf{T}(1)$.

Substituting the explicit forms of $T_p(w)$ obtained in section 3.1 of BP into (2.14′), and after some calculations, we find that

$$-\frac{1}{\xi} = \lim_{l\to\infty}\frac{\cos\theta_\perp}{l}\ln\left\{\left(\frac{1}{4\pi\mathrm{i}}\right)^2\oint_{|b_1|=1}\frac{\mathrm{d}b_1}{b_1}\oint_{|b_2|=1}\frac{\mathrm{d}b_2}{b_2}\rho(b_1,b_2)\right.$$
$$\left.\times\,[\phi(w/b_1)\phi^\eta(1/b_1)]^l[\phi(w/b_2)\phi^\eta(1/b_2)]^l\right\} \tag{2.15}$$

where $\phi(w/b_1)\phi(w/b_2)$ and $\phi(1/b_1)\phi(1/b_2)$ correspond to $T_p(w)/T_1(w)$ and $T_p(1)/T_1(1)$ in (2.14′), respectively; the function $\phi(w)$ is defined by (2.4). The summation in (2.14′) becomes integrals along unit circles on two sheets of Riemann surface because of the continuous distribution of the eigenvalues in the $M \to \infty$ limit. The function $\rho(b_1, b_2)$ is determined from the distribution of the eigenvalues and the coefficients $\tilde{S}_0(1,p)\tilde{S}_0(p,1)$ in (2.14′). Its explicit form is not important here.

We can estimate the integral in the right-hand side of (2.15) by the method of steepest descent, which is the same calculation given in section 2.1. As a result, we get

$$1/\xi = 2\gamma(S - S)/k_\mathrm{B}T \qquad \text{for all } \theta_\perp. \tag{2.16}$$

3. Regime III

3.1. Anisotropic interfacial tension

In this and the following sections, the shift operator method in [6] is applied to the calculation of the anisotropic interfacial tension of regime III. As mentioned in section 1, regime III is a first-order transition surface where a disordered fluid phase and two $c(2 \times 2)$ ordered solid phases can coexist. Therefore, two types of interfacial tension are possible: one is the interfacial tension $\gamma(S-S)$ between the two solid phases; and the other is the interfacial tension $\gamma(F-S)$ between the fluid phase and a solid phase. Investigating $\gamma(S-S)$ is too complicated a problem to be treated here. Analysis is restricted to $\gamma(F-S)$. In this section we explain the shift operator method to calculate the anisotropic interfacial tension $\gamma(F-S)$. We introduce two inhomogeneous systems; each inhomogeneous system consists of two regions; one of the two regions works as the 'column–column' shift operator. For each inhomogeneous system we examine a one-parameter family of commuting transfer matrices [3, 10, 11]. The eigenvalues of the transfer matrix satisfy a functional equation. In the next section, by solving the functional equation, we obtain the anisotropic interfacial tension $\gamma(F-S)$. We shall use the parametrization of the five Boltzmann weights ωs in (1.2*b*) given by (3.14) of [10] with w and x $(0<x<1)$.

We consider two inhomogeneous systems to define the anisotropic interfacial tension. Suppose a square lattice of $(1+\eta)M$ columns and N rows wound on a cylinder ($M \equiv M\eta \equiv 0 \pmod 2$). We also assume that w can vary from column to column. The value of w between the jth column and the $(j+1)$th column is denoted by w_j. The two inhomogeneous systems are given by

$$w_1 = w_2 = \cdots = w_M = w_0 \qquad w_{M+1} = w_{M+2} = \cdots = w_{(1+\eta)M} = x^r$$

where $x < w_0 < 1$ and $r = 0$ or 1. The inhomogeneous system with $r = 0$ is called (A), and the system with $r = 1$ (B). Hereafter, the new parameter w_0 is abbreviated to w.

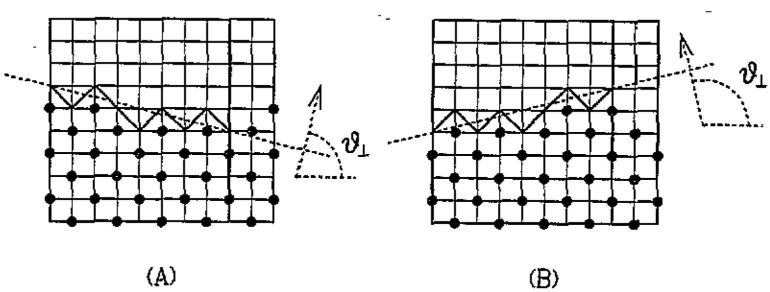

Figure 2. Typical configurations of the inhomogeneous systems (A) and (B) in the $x \to 0$ limit. There exists an interface across the region $w_j = w$ for $1 \leqslant j \leqslant M$. In the system (A) (or (B)) the region $w_j = 1$ (or x) for $M+1 \leqslant j \leqslant (1+\eta)M$ shifts the endpoint of the interface on the $(M+1)$th column from that on the first column downward (or upward) by ηM lattice spacings.

We fix the boundary particle configurations of the inhomogeneous systems as follows:

$$\sigma_t = \{0, 0, \ldots, 0\} \qquad \sigma_b = \{0, 1, 0, 1, \ldots, 0, 1\}$$

where σ_t and σ_b are the particle configurations on the top row and the bottom row, respectively. Then, there exists an interface F–S across the region $w_j = w$ for $1 \leqslant j \leqslant M$ (figure 2). In (A) (or (B)) the region $w_j = 1$ (or x) for $M+1 \leqslant j \leqslant (1+\eta)M$ tilts the interface by shifting the endpoint on the $(M+1)$th column from that on the first column downward (or upward) by ηM lattice spacings. We represent the average tilt of the interface by $\theta_\perp$, which is the angle between the horizontal direction and the normal direction of the line connecting the two endpoints of the interface. The parameter η is related to $\theta_\perp$ by

$$\text{(A)} \qquad \eta = 1/\tan\theta_\perp \qquad 0 < \theta_\perp < \pi/2 \tag{3.1a}$$

$$\text{(B)} \qquad \eta = -1/\tan\theta_\perp \qquad \pi/2 < \theta_\perp < \pi \tag{3.1b}$$

Let $Z_{MN}(\theta_\perp)$ $(0 < \theta_\perp < \pi)$ be the partition function of (A) and (B) with the boundary conditions. The anisotropic interfacial tension is defined by

$$\gamma(F-S|\theta_\perp) = -k_{\rm B}T\sin\theta_\perp \lim_{M,N\to\infty} M^{-1}\ln[Z_{MN}(\theta_\perp)/N\kappa^{M(N-1)}] \qquad (3.2)$$

where the limit is taken with $\theta_\perp$ (or η) fixed to be constant; κ is the partition function per face in the region $w_j = w$.

To calculate $Z_{MN}(\theta_\perp)$ in (3.2), we construct a one-parameter family of commuting transfer matrices for each inhomogeneous system [3, 10, 11]. The inhomogeneous systems (A) and (B) are generalized: we set the w_j to be

$$w_1 = w_2 = \cdots = w_M = wv/x^r \qquad w_{M+1} = w_{M+2} = \cdots = w_{(1+\eta)M} = v$$

where $r = 0$ (or 1) for the generalized system (A) (or (B)); using the convention of r, we deal with the inhomogeneous systems (A) and (B) in parallel. If $\sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_{(1+\eta)M}\}$ and $\sigma' = \{\sigma'_1, \sigma'_2, \ldots, \sigma'_{(1+\eta)M}\}$ are the particle configurations of two successive periodic rows, the transfer matrix is defined by elements as

$$[\mathbf{T}_{\rm IH}(v)]_{\sigma,\sigma'} = \left[-\frac{\omega_1(wv/x^r)}{\omega_4(wv/x^r)\omega_5(wv/x^r)}\right]^M \prod_{i=1}^{M} W(\sigma_i, \sigma_{i+1}, \sigma'_{i+1}, \sigma'_i|wv/x^r)$$
$$\times \left[-\frac{\omega_1(v)}{\omega_4(v)\omega_5(v)}\right]^{M\eta} \prod_{j=M+1}^{(1+\eta)M} W(\sigma_j, \sigma_{j+1}, \sigma'_{j+1}, \sigma'_j|v). \qquad (3.3)$$

Unless otherwise mentioned, we regard v as a complex variable and x, w as constants $(0 < x < w < 1)$. For all complex variables v and v', $\mathbf{T}_{\rm IH}(v)$ and $\mathbf{T}_{\rm IH}(v')$ commute with each other, being simultaneously diagonalized. We denote the eigenvalues of $\mathbf{T}_{\rm IH}(v)$ by $T_{\rm IH}(v)$. From the same derivation of (3.5) in [10], it follows that the eigenvalues $T_{\rm IH}(v)$ must satisfy the functional equation

$$T_{\rm IH}(v)T_{\rm IH}(xv) = 1 + T_{\rm IH}(x^3v). \qquad (3.4)$$

We also find the periodicity relation

$$T_{\rm IH}(x^5v) = T_{\rm IH}(v). \qquad (3.5)$$

Assuming some analytic properties of the eigenvalues $T_{\rm IH}(v)$ and, using (3.4) and (3.5), we can determine the explicit forms of $T_{\rm IH}(v)$. After the eigenvalues $T_{\rm IH}(v)$ are determined, we can get the necessary information for obtaining the anisotropic interfacial tension by setting $v = x^r$.

3.2. Anisotropic interfacial tension 2

Let us now calculate the eigenvalues $T_{\rm IH}(v)$. First, we consider the forms of $T_{\rm IH}(v)$ in the $x \to 0$ limit, which give some useful insights into their large-M behaviour. Then, using the functional equation (3.4) and the periodicity relation (3.5), we determine the asymptotic behaviour of $T_{\rm IH}(v)$ as M becomes large. From the asymptotic behaviour of $T_{\rm IH}(v)$, we can estimate the partition function in (3.2). The anisotropic interfacial tension is given by the finite-size correction terms of the largest eigenvalues as $M \to \infty$. Since methods are almost the same, we explain only the analysis for (A) with $r = 0$, and omit that for (B). Calculation in this section is an extension of section 2 of BP [11].

To obtain the anisotropic interfacial tension, we wish to investigate the largest eigenvalues in the annulus $x/w \leqslant |v| \leqslant 1$. There, a disordered fluid phase and two $c(2\times 2)$ ordered solid phases are degenerate. From this fact it is expected that a triplet of the largest eigenvalues are asymptotically degenerate as M becomes large. Such eigenvalues are found in the $x \to 0$ limit: In this limit there exist a triplet of eigenvalues $T_{\mathrm{IH};\pm}(v)$ and $T_{\mathrm{IH};X}(v)$ which behave as

$$T_{\mathrm{IH};\pm}(v) \sim \begin{cases} 1 & x^{3/2}/w < |v| < x^{-1/2} \quad (3.6a) \\ \pm\sqrt{2}(-wv)^{M/2}(-v)^{\eta M/2}x^{-5(1+\eta)M/4} & \\ \quad \times(1-x^3/wv)^M(1-x^3/v)^{\eta M} & x^4/w < |v| < x^2 \quad (3.6b) \end{cases}$$

$$T_{\mathrm{IH};X}(v) \sim \begin{cases} -1 & x^{3/2}/w < |v| < x^{-1/2} \quad (3.7a) \\ -(-wv)^{M/2}(-v)^{\eta M/2}x^{-(1+\eta)M} & \\ \quad \times(1-x^3/wv)^M(1-x^3/v)^{\eta M} & x^4/w < |v| < x^2 \quad (3.7b) \end{cases}$$

The factors 1 in (3.6a) and -1 in (3.7a) come from superpositions of a vacuum state consisting of the face ω_1 and complete $c(2\times 2)$ ordered ones dominated by the faces ω_4 and ω_5. The right-eigenvectors corresponding to $T_{\mathrm{IH};\pm}(v)$ are

$$|\pm\rangle = \frac{1}{\sqrt{2}}|00\rangle \pm \frac{1}{2}|10\rangle \pm \frac{1}{2}|01\rangle \qquad (3.8)$$

and the right-eigenvector corresponding to $T_{\mathrm{IH};X}(v)$ is

$$|X\rangle = \frac{1}{\sqrt{2}}|10\rangle - \frac{1}{\sqrt{2}}|01\rangle \qquad (3.9)$$

where $|00\rangle$ (respectively $|10\rangle$, $|01\rangle$) is a column vector which has entries 1 for the particle configuration $\{0,0,\ldots,0\}$ (respectively $\{1,0,1,0,\ldots,1,0\}$, $\{0,1,0,1,\ldots,0,1\}$) and 0 for the other particle configurations; transposing the right-eigenvectors gives the left-eigenvectors. We identify $T_{\mathrm{IH};\pm}(v)$ and $T_{\mathrm{IH};X}(v)$ as the triplet of the largest eigenvalues in the annulus $x/w \leqslant |v| \leqslant 1$ since they are indeed so in the $x \to 0$ limit.

The eigenvalues $T_{\mathrm{IH};\pm}(v)$ are important for calculating the anisotropic interfacial tension $\gamma(F-S)$. When M becomes large, we determine the asymptotic behaviour of $T_{\mathrm{IH};\pm}(v)$ as follows. In the beginning we find the leading terms of $T_{\mathrm{IH};\pm}(v)$. The result (3.6) in the $x \to 0$ limit suggests that, for large M, $T_{\mathrm{IH};\pm}(v)$ must be of the form

$$T_{\mathrm{IH};\pm}(v) \sim \begin{cases} 1 & x^{3/2}/w < |v| < x^{-1/2} \quad (3.10a) \\ v^m K(v)(1-x^3/wv)^M(1-x^3/v)^{\eta M} & x^4/w < |v| < x^2 \quad (3.10b) \end{cases}$$

where m is an integer and the function $K(v)$ is analytic and non-zero in the annulus $x^4/w < |v| < x^2$. Consider the annulus $x^3/w < |v| < x^2$. Then, substituting (3.10) into (3.4) gives

$$v^m(xv)^m K(v)K(xv)(1-x^3/wv)^M(1-x^2/wv)^M(1-x^3/v)^{\eta M}(1-x^2/v)^{\eta M} = 2$$
$$x^3/w < |v| < x^2 \qquad (3.11)$$

where we keep only the dominant terms as $M \to \infty$. Taking logarithms of both sides of (3.11), Laurent expanding and equating coefficients, we can determine the integer m and the explicit form of $K(v)$. It follows that

$$T_{\mathrm{IH};\pm} \sim \pm\sqrt{2}\bar{\psi}^M(wv)\bar{\psi}^{\eta M}(v), \qquad x^4/w < |v| < x^2 \tag{3.12}$$

where

$$\bar{\psi}(v) = (-v/x^{1/2})^{1/2} f(xv, x^2)/f(v, x^2) \tag{3.13}$$

and $f(p,q)$ is defined by (2.4b). From (3.10a) and (3.12), using (3.4) with (3.5), we can consistently determine the leading behaviour of $T_{\mathrm{IH};\pm}(v)$ for all v. Furthermore, (3.12) reproduces (3.6b) in the $x \to 0$ limit. These facts show that (3.10a) and (3.12) give the correct leading behaviour of $T_{\mathrm{IH};\pm}(v)$ as $M \to \infty$.

Next, we investigate the finite-size correction terms of $T_{\mathrm{IH};\pm}(v)$ as M becomes large. Consider the annulus $x^{1/2}/w < |v| < x^{-1/2}$, where the second term is exponentially smaller than the unity in the right-hand side of (3.4). Taking logarithms of both sides of (3.4), Laurent expanding, and equating coefficients, we find that

$$\ln T_{\mathrm{IH};\pm}(v) = \frac{1}{2\pi \mathrm{i}} \oint_C \frac{\mathrm{d}v'}{v'} J(v/x^{1/2}v') \ln[1 + T_{\mathrm{IH};\pm}(x^3 v')] \qquad x^{3/2}/w < |v| < x^{-1/2} \tag{3.14}$$

where C is a circle in $x^{1/2}/w < |v| < x^{-1/2}$ and $J(v)$ is defined by

$$J(v) = \frac{1}{2} + \sum_{n=1}^{\infty} \left(\frac{x^{n/2}v^n}{1+x^n} + \frac{x^{n/2}v^{-n}}{1+x^n} \right). \tag{3.15}$$

For large M, using (3.12), we estimate the logarithm in the integrand in the right-hand side of (3.14) as

$$\ln[1 + T_{\mathrm{IH};\pm}(x^3 v')] \sim \pm\sqrt{2}\bar{\psi}^M(xwv')\bar{\psi}^{\eta M}(xv') \tag{3.16}$$

and integrate (3.14) by the method of steepest descent. It follows that

$$T_{\mathrm{IH};\pm}(v) \sim 1 \pm \alpha(v)\sqrt{2}\bar{\psi}^M(xwv_{\mathrm{s}})\bar{\psi}^{\eta M}(xv_{\mathrm{s}}) + \cdots \qquad x^{3/2}/w < |v| < x^{-1/2} \tag{3.17}$$

where v_{s} is a saddle point of $|\bar{\psi}(xwv')\bar{\psi}^{\eta}(xv')|$, given by

$$\tan^{-1}\theta_\perp = -\left.\frac{f(v',x^2)f(xv',x^2)f(-wv',x^2)f(-xwv',x^2)}{f(-v',x^2)f(-xv',x^2)f(wv',x^2)f(xwv',x^2)}\right|_{v'=v_{\mathrm{s}}} \tag{3.18a}$$

with the condition

$$v_{\mathrm{s}} = -1/w \qquad \theta_\perp = \pi/2. \tag{3.18b}$$

The explicit form of $\alpha(v)$, which is determined from $J(v)$ and the derivatives of $\bar{\psi}(v)$, is not important here. Since $|\bar{\psi}(xwv_{\mathrm{s}})\bar{\psi}^{\eta}(xv_{\mathrm{s}})| < 1$, (3.17) shows that $T_{\mathrm{IH};\pm}(v)$ are asymptotically degenerate as $M \to \infty$.

Now, setting $v = 1$, we calculate the anisotropic interfacial tension. When M and N become large ($1 \ll M \ll N \ll \bar{\psi}^{-M}(xwv_s)\bar{\psi}^{-\eta M}(xv_s)$), using the triplet of the largest eigenvalues $T_{\mathrm{IH};\pm}(1)$ and $T_{\mathrm{IH};X}(1)$, we can estimate the partition function $Z_{MN}(\theta_\perp)$ in (3.2) as

$$\begin{aligned} Z_{MN}(\theta_\perp) &= \langle 00|\mathbf{T}_{\mathrm{IH}}^{N-1}(1)|01\rangle \sim \sum_{p=\pm,X} \langle 00|p\rangle T_{\mathrm{IH};p}^{N-1}(1)\langle p|01\rangle \\ &\sim \{\langle 00|+\rangle\langle +|01\rangle + \langle 00|-\rangle\langle -|01\rangle\} + \{\langle 00|+\rangle\langle +|01\rangle - \langle 00|-\rangle\langle -|01\rangle\} \\ &\quad \times (N-1)\alpha(1)\sqrt{2}\bar{\psi}^{M}(xwv_s)\bar{\psi}^{\eta M}(xv_s) + \langle 00|X\rangle\langle X|01\rangle T_{\mathrm{IH};X}^{N-1}(1) + \cdots . \end{aligned} \tag{3.19}$$

Note that $T_{\mathrm{IH};X}(1)$ is a negative eigenvalue: from (3.7) it follows that, as $M \to \infty$, $T_{\mathrm{IH};X}(v)$ is of the form

$$T_{\mathrm{IH};X}(v) = -1 + O(x^{-\varepsilon M}) \qquad x^2/w < |v| < x^{-1} \tag{3.20}$$

with $\varepsilon > 0$. The asymptotic behaviour of $Z_{MN}(\theta_\perp)$ is expected to occur regardless of whether N is even or odd, which suggests that the contribution from the third term is very small in the right-hand side of (3.19). In the $\eta \to 0$ and ∞ limits $\langle 00|X\rangle$ is exactly zero. For general η, numerical diagonalization of $\mathbf{T}_{\mathrm{IH}}(1)$ for finite-size systems shows that

(i) $\langle 00|X\rangle$ decays to zero more rapidly than the finite-size correction terms of $T_{\mathrm{IH};\pm}(1)$ as M becomes large (numerical diagonalization also shows that the first term is negligible in the right-hand side of (3.19));

(ii) for large M, $\langle 00|+\rangle\langle +|01\rangle$ (> 0) and $\langle 00|-\rangle\langle -|01\rangle$ are equal in magnitude and opposite in sign.

The facts (i) and (ii) are consistent with (3.9) and (3.8) in the $x \to 0$ limit, respectively. Although we cannot rigorously prove them we are certain of the properties (i) and (ii). Using these properties in the right-hand side of (3.19), we obtain for sufficient large M and N

$$Z_{MN}(\theta_\perp) \sim 2\sqrt{2}N\langle 00|+\rangle\langle +|01\rangle\alpha(1)\bar{\psi}^{M}(xwv_s)\bar{\psi}^{\eta M}(xv_s). \tag{3.19$'$}$$

On the other hand, the partition function per face is calculated as

$$\kappa = \lim_{M\to\infty} T_{\mathrm{IH};+}^{1/M}(1) = 1. \tag{3.21}$$

Substituting (3.19′) and (3.21) into (3.2), we get

$$\gamma(F-S|\theta_\perp)/k_{\mathrm{B}}T = \cos\theta_\perp \ln\bar{\psi}(v_s) + \sin\theta_\perp \ln\bar{\psi}(wv_s) \qquad 0 < \theta_\perp < \pi/2. \tag{3.22}$$

Combining the result of the inhomogeneous system (B), and using the relation $\gamma(F-S|\theta_\perp + \pi) = \gamma(F-S|\theta_\perp)$, we find that (3.22) is analytically continued into $-\pi < \theta_\perp < \pi$, with v_s regarded as a function of $\theta_\perp$.

3.3. Equilibrium crystal shape

We are in a position to derive the ECS in this regime. Here, we assume that a droplet of a solid phase is embedded inside a sea of the fluid phase (or *vice versa*). Replacing $\gamma(S-S)$ by $\gamma(F-S)$ in (2.8), and substituting (3.22), we obtain

$$\Lambda X/k_{\rm B}T = \ln\bar{\psi}(v_{\rm s}) \qquad \Lambda Y/k_{\rm B}T = \ln\bar{\psi}(wv_{\rm s}). \tag{3.23}$$

Similarly to (2.9), it is found that (3.23) can be rewritten in the symmetric biquadratic relation (1.1*a*), with the two coefficients $A_3^{(8v)}$ and $A_4^{(8v)}$ replaced by

$$\begin{aligned} A_3^{(\rm III)} &= wf^2(xw,x^2)/x^{1/2}f^2(w,x^2) \\ A_4^{(\rm III)} &= -w^{1/2}f^3(x,x^2)f(w^2,x^2)/x^{1/2}f^3(w,x^2)f(xw,x^2). \end{aligned} \tag{3.24}$$

The elliptic function $\bar{\psi}(v)$ is essentially the sn function which naturally parametrizes the symmetric biquadratic relation (1.1*a*). Compare (3.24) with (4.22) of [7]. It follows that (3.23) corresponds to the ECS of the eight-vertex model with

$$a^{(8v)} = w/x^{1/2} \qquad x^{(8v)} = x^{1/2} \tag{3.25}$$

where the variables of the eight-vertex model $a^{(8v)}$ and $x^{(8v)}$ are defined by (4.18*b*) and (3.5) of [7], respectively.

3.4. Anisotropic correlation length

To find the anisotropic correlation length, we repeat the analysis in section 2.3. Suppose a sufficiently large lattice of M columns and N rows with periodic boundary conditions in both directions ($M \equiv N \equiv 0 \pmod 2$). Using the expression (2.14′), we estimate the asymptotic behaviour of the pair correlation function between the site (0,0) and the site (l,m) from the ratios between the largest and next-largest eigenvalues of the transfer matrix $\mathbf{T}(w)$ and those of the shift operator $\mathbf{T}(1)$; the transfer matrix $\mathbf{T}(w)$ is defined by (2.1), with the five Boltzmann weights ωs parametrized by (3.14) of [10] with $0<w<x<1$; and $\mathbf{T}(w)$ reduces to the shift operator in the $w\to 1$ limit. The explicit forms of the eigenvalues of $\mathbf{T}(w)$ were determined in section 3.1 of BP [11]. Substitute them into (2.14′). It follows that

$$\begin{aligned} -\frac{1}{\xi} = \lim_{l\to\infty}\frac{\cos\theta_\perp}{l}\ln\Bigg\{\left(\frac{1}{4\pi{\rm i}}\right)^2\oint_{|d_1|=1}\frac{{\rm d}d_1}{d_1}\oint_{|d_2|=1}\frac{{\rm d}d_2}{d_2}\rho(d_1,d_2) \\ \times[\psi(w/d_1)\psi^\eta(1/d_1)]^l[\psi(w/d_2)\psi^\eta(1/d_2)]^l\Bigg\} \end{aligned} \tag{3.26}$$

where $\psi(d) = -{\rm i}\bar{\psi}(x^{1/2}d)$ and $\eta = m/l = \tan\theta_\perp$. Calculating the integral in the right-hand side of (3.26) by the method of steepest descent, we find that

$$1/\xi = 2\gamma(F-S)/k_{\rm B}T \qquad \text{for all } \theta_\perp. \tag{3.27}$$

The thermodynamic relation (3.27) is an extension of (2.46) in BP.

4. Summary and discussion

We calculated the anisotropic interfacial tension of regimes III and IV of the hard-square model defined by Baxter. In regime IV we have investigated the interfacial tension $\gamma(S-S)$ between the two $c(2\times2)$ ordered solid phases, and in regime III the interfacial tension $\gamma(F-S)$ between the disordered fluid phase and a $c(2\times2)$ ordered solid phase. From the calculated anisotropic interfacial tension we obtained the ECSs via the Wulff construction. In both regimes it was found that the ECS is represented by the symmetric biquadratic relation (1.1*a*), which is the same ECS that the eight-vertex model has. Thus, the ECS (1.1*a*) is quite general. As shown in the analyses of the eight-vertex model and the hard-square models, the ECS (1.1*a*) provides a characteristic expression for the interfacial tension: the sn function which naturally parametrizes the symmetric biquadratic relation (1.1*a*) appears in the expression of the interfacial tension. Besides the eight-vertex and the hard-square models, the interfacial tension of the magnetic hard-square model [13] and the Sogo–Akutsu–Abe (SAA) model [14] was calculated along a special direction by a standard transfer matrix argument. There, elliptic functions in the expressions of the interfacial tension are also (essentially) the sn function. It is strongly suggested that the ECSs of the magnetic hard-square model and the SAA model are the symmetric biquadratic relation (1.1*a*).

For regimes III and IV we showed a thermodynamic relation between the anisotropic interfacial tension and the anisotropic correlation length, the form being

$$1/\xi = 2\gamma/k_{\mathrm{B}}T \qquad \text{for all directions} \tag{4.1}$$

where the anisotropic interfacial tension is denoted by γ, and the anisotropic correlation length by ξ. It is known that a simple thermodynamic relation like (4.1) usually holds between the interfacial tension and the correlation length [3, 5, 13–16]. Therefore, the expression for the correlation length can give useful information about the ECS. We make an addition to the above argument; in [17], the correlation length of some solvable models was calculated along a special direction. The correlation length of the solvable models is represented by the use of (essentially) the sn function. From this fact, assuming the thermodynamic relation (4.1), we also expect that the ECSs of the solvable models will be the symmetric biquadratic relation (1.1*a*). To conclude, we expect that (1.1*a*) is a universal shape which appears as the ECSs of a wide class of models. Further study of (1.1*a*) is desirable.

Finally, we considered the critical limit of the ECS (1.1*a*) for the eight-vertex model and regimes III and IV of the hard-square model. The behaviour of the coefficients A_3, A_4 of the eight-vertex model (respectively regimes III, IV) in the critical limit is given by (4.22) of [7] (respectively (3.24), (2.10)) with $I\to\infty$ (respectively $x\to1,-1$). It is convenient to use the conjugate modulus transformation (A.6*b*) of [7]. (See also section 3 of [10] and ch 15 of [3].) Noting that $\Lambda\to0$ in the critical limit, we find that

$$(X+Y)^2/\cos^2(\pi u/2\lambda)+(X-Y)^2/\sin^2(\pi u/2\lambda)\propto 64k_{\mathrm{B}}^2T_{\mathrm{C}}^2 \tag{4.2}$$

where u is the spectral parameter and λ is the crossing parameter; in [7] u and λ parametrizes the Boltzmann weights of the eight-vertex model by (2.1), and later, for calculational convenience, u is rewritten as u_0; for the hard-square model u is related to w by (3.10) of [10], and $\lambda=\pi/5$.

When the interactions are isotropic, two-dimensional lattice models are conformally invariant at the critical point [18]. If we consider such a conformally invariant model on a lattice of M columns and N rows ($1 \ll M \ll N$) wound on a torus, it can be shown that the partition function Z must be of the form

$$\ln Z \sim MNf + (\pi c/6)(N/M) \qquad (4.3)$$

where f is the free energy per site (or face), and c is the conformal anomaly. For most anisotropic systems, where the conformal invariance is restored by a suitable anisotropic rescaling of length, (4.3) is modified as [19]

$$\ln Z \sim MNf + (\pi c/6)(N/M)\Gamma^{-2} \qquad (4.4a)$$

$$\Gamma^2 = \gamma^2 \cos^2\theta + \gamma^{-2}\sin^2\theta \qquad (4.4b)$$

where γ^2 represents the required rescaling, and θ is the angle between the vertical axis and the direction along which the system is rescaled. For the eight-vertex and hard-square models, (4.2) shows that

$$\gamma^2 = \sin(\pi u/2\lambda)/\cos(\pi u/2\lambda) \qquad \theta = \pi/4. \qquad (4.5a)$$

Substituting (4.5a) into (4.4b), we get

$$\Gamma^2 = \sin^{-1}(\pi u/\lambda). \qquad (4.5b)$$

Kim and Pearce (KP) [20] discussed Γ^2 from several solvable models, using the corner transfer matrices. They showed that (4.5b) is a general expression satisfied by the eight-vertex, hard-square, magnetic hard-square, and the q-state Potts models. For the eight-vertex and hard-square models, the expression (4.5b) is closely related to the symmetric biquadratic relation (1.1a) through parametrization by the Jacobian elliptic functions. This fact renders the ECSs of the q-state Potts models, which are not solvable except at the critical point, extremely interesting. I hope that this problem will be clarified in a future publication.

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