Staggered ice-rule vertex model (on a square lattice)

1976 J. Phys. A: Math. Gen. 9 1685

(http://iopscience.iop.org/0305-4470/9/10/020)

J. Phys. A: Math. Gen., Vol. 9, No. 10, 1976. Printed in Great Britain. © 1976

Staggered ice-rule vertex model†

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Received 21 April 1976

Abstract. We have studied the staggered ice-rule vertex model on a square lattice which allows different vertex weights for the four sublattices of the square lattice. The most general Pfaffian solution is given. It is shown that our model may exhibit up to three phase transitions. The specific heat diverges with an exponent $\frac{1}{2}$ either above or below each transition temperature. The exact isotherm of an antiferroelectric model in the presence of both direct and staggered fields at a particular temperature is obtained. As the fields are varied, the system undergoes transitions among states of zero, partial and complete direct polarization.

1. Introduction

Recently Wu and Lin (1975) considered the staggered ice-rule vertex model on a square lattice which allows different vertex weights for the two sublattices. They studied the most general Pfaffian solution and found that the system may exhibit up to two phase transitions. The specific heat diverges with an exponent $\frac{1}{2}$ either above or below each transition temperature. They also obtained the exact isotherm of an antiferroelectric model at a particular temperature in the presence of both direct and staggered fields. As the fields are varied, the system undergoes transitions among states of zero, partial and complete direct polarization. Lin (1975) obtained similar results for the staggered vertex model on a Kagomé lattice.

The purpose of this paper is to generalize the results of Wu and Lin to the staggered ice-rule vertex model which allows four different vertex weights for the four sublattices of the square lattice. Our model is described in § 2. Symmetry relations are discussed in § 3. When the vertex weights satisfy the free-fermion condition, the model can be solved by the Pfaffian method (Montroll 1964). The Pfaffian solution is given in § 4. There are eighteen cases where the free-fermion condition is satisfied at all temperatures. These cases are examined in § 5. The exact isotherm of an antiferroelectric model is discussed in § 6. Our conclusion is given in § 7.

2. Definition of the model

Place arrows on the bonds of a square lattice L of N sites subject to the ice rule that there are always two arrows pointing away and two arrows pointing into each site. In figure 1,

† Supported in part by the National Science Council, Republic of China.

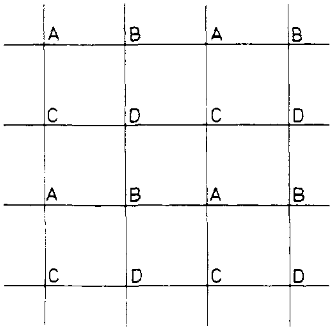

Figure 1. The square lattice with four sublattices A, B, C and D.

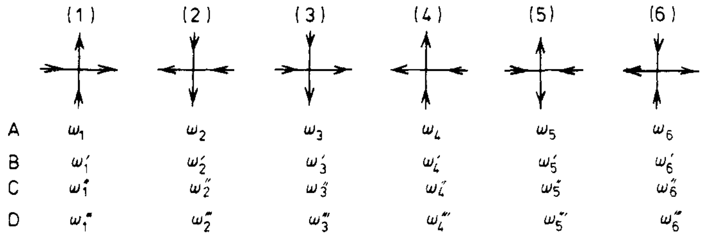

Figure 2. The six ice-rule configurations and the associated vertex weights.

the four sublattices of L are denoted by A, B, C and D. The six configurations allowed at each vertex are shown in figure 2, where each vertex is assigned a weight. Let the vertex weights be

$$
\begin{aligned}
\{\omega\} &= \{\omega_1, \omega_2, \ldots, \omega_6\} && \text{on A} \\
\{\omega'\} &= \{\omega'_1, \omega'_2, \ldots, \omega'_6\} && \text{on B} \\
\{\omega''\} &= \{\omega''_1, \omega''_2, \ldots, \omega''_6\} && \text{on C} \\
\{\omega'''\} &= \{\omega'''_1, \omega'''_2, \ldots, \omega'''_6\} && \text{on D.}
\end{aligned}
\tag{1}
$$

The partition function is

$$
Z = \sum \left(\prod \omega_{\omega_i}^{n_i}\right)\left(\prod \omega_i'^{n_i'}\right)\left(\prod \omega_i''^{n_i''}\right)\left(\prod \omega_i'''^{n_i'''}\right) \tag{2}
$$

where the summation is extended to all allowed arrow configurations on L, and $n_i(n'_i, n''_i, n'''_i)$ is the number of the ith-type sites on A(B, C, D). The aim is to calculate the 'free energy'

$$
\psi = \lim_{N\to\infty} \frac{1}{N} \ln Z. \tag{3}
$$

In a physical model, the vertex weights are interpreted as the Boltzmann factors

$$
\begin{aligned}
\omega'_1 &= \exp(-\beta e_i) & \omega'_i &= \exp(-\beta e'_i) \\
\omega''_i &= \exp(-\beta e''_i) & \omega'''_i &= \exp(-\beta e'''_i)
\end{aligned}
\tag{4}
$$

where $\beta = 1/kT$, k is the Boltzmann constant, T is the temperature, and e_i, e'_i, e''_i, e'''_i are the vertex energies.

3. Symmetry relations

The partition function Z possesses some symmetry relations which follow from general considerations. Translational invariance of the square lattice implies that Z is invariant under each of the following transformations:

$$\begin{array}{lll} (1) & \{\omega\}\leftrightarrow\{\omega'\} & \{\omega''\}\leftrightarrow\{\omega'''\} \\ (2) & \{\omega\}\leftrightarrow\{\omega''\} & \{\omega'\}\leftrightarrow\{\omega'''\} \\ (3) & \{\omega\}\leftrightarrow\{\omega'''\} & \{\omega'\}\leftrightarrow\{\omega''\}. \end{array} \tag{5}$$

We write

$$Z = Z(123456, 1'2'3'4'5'6', 1''2''3''4''5''6'', 1'''2'''3'''4'''5'''6''') \tag{6}$$

where i, i', i'', i''' denote respectively ω_i, ω'_i, ω''_i, ω'''_i. Reflectional symmetry in the horizontal or vertical direction implies

$$\begin{aligned} Z &= Z(432156, 4'3'2'1'5'6', 4''3''2''1''5''6'', 4'''3'''2'''1'''5'''6''') \\ &= Z(341256, 3'4'1'2'5'6', 3''4''1''2''5''6'', 3'''4'''1'''2'''5'''6'''). \end{aligned} \tag{7}$$

Reversing all arrows implies

$$Z = Z(214365, 2'1'4'3'6'5', 2''1''4''3''6''5'', 2'''1'''4'''3'''6'''5'''). \tag{8}$$

Reflectional symmetry in the diagonal directions implies

$$\begin{aligned} Z &= Z(213465, 2''1''3''4''6''5'', 2'1'3'4'6'5', 2'''1'''3'''4'''6'''5''') \\ &= Z(1'''2'''4'''3'''6'''5''', 1'2'4'3'6'5', 1''2''4''3''6''5'', 124365). \end{aligned} \tag{9}$$

Finally there is the weak-graph symmetry (Nagle and Temperley 1968) which is a local property of a lattice and is valid even if the weights are site dependent.

4. Pfaffian solution

A vertex model can be solved by the Pfaffian method if the free-fermion condition is satisfied at each vertex (Fan and Wu 1970). In our model, the condition reads

$$\begin{aligned} &\omega_1\omega_2 + \omega_3\omega_4 = \omega_5\omega_6 \\ &\omega'_1\omega'_2 + \omega'_3\omega'_4 = \omega'_5\omega'_6 \\ &\omega''_1\omega''_2 + \omega''_3\omega''_4 = \omega''_5\omega''_6 \\ &\omega'''_1\omega'''_2 + \omega'''_3\omega'''_4 = \omega'''_5\omega'''_6. \end{aligned} \tag{10}$$

Under this condition the partition function is equal to a Pfaffian which is evaluated in appendix 1. The result is

$$\psi = \frac{1}{8\pi^2} \int_{-\pi}^{\pi} \mathrm{d}\theta \int_{-\pi}^{\pi} \mathrm{d}\phi \, \ln|F(\theta, \phi)| \tag{11}$$

where

$$F = a + b\,\mathrm{e}^{\mathrm{i}\theta} + b'\,\mathrm{e}^{-\mathrm{i}\theta} + c\,\mathrm{e}^{\mathrm{i}\phi} + c'\mathrm{e}^{-\mathrm{i}\phi} - f\,\mathrm{e}^{\mathrm{i}(\theta+\phi)} - f'\,\mathrm{e}^{-\mathrm{i}(\theta+\phi)} - g\,\mathrm{e}^{\mathrm{i}(\theta-\phi)} - g'\,\mathrm{e}^{\mathrm{i}(\phi-\theta)} \tag{12}$$

with

$$\begin{aligned}
&a = \omega_1\omega_3'\omega_4''\omega_2''' + \omega_2\omega_4'\omega_3''\omega_1''' + \omega_3\omega_1'\omega_2''\omega_4''' + \omega_4\omega_2'\omega_1''\omega_3''' + \omega_5\omega_6'\omega_6''\omega_5''' + \omega_6\omega_5'\omega_5''\omega_6''' \\
&b = b_1 + b_2 \qquad b_1 = \omega_2\omega_4'\omega_2''\omega_4''' \qquad b_2 = \omega_4\omega_2'\omega_4''\omega_2''' \\
&b' = b_1' + b_2' \qquad b_1' = \omega_1\omega_3'\omega_1''\omega_3''' \qquad b_2' = \omega_3\omega_1'\omega_3''\omega_1''' \\
&c = c_1 + c_2 \qquad c_1 = \omega_2\omega_2'\omega_3''\omega_3''' \qquad c_2 = \omega_3\omega_3'\omega_2''\omega_2''' \\
&c' = c_1' + c_2' \qquad c_1' = \omega_1\omega_1'\omega_4''\omega_4''' \qquad c_2' = \omega_4\omega_4'\omega_1''\omega_1''' \\
&f = \omega_2\omega_2'\omega_2''\omega_2''' \qquad f' = \omega_1\omega_1'\omega_1''\omega_1''' \qquad g = \omega_4\omega_4'\omega_4''\omega_4''' \qquad g' = \omega_3\omega_3'\omega_3''\omega_3'''.
\end{aligned} \tag{13}$$

The special case of $\omega_i = \omega_i' = \omega_i'' = \omega_i'''$ has been considered by Fan and Wu (1970). The special case of $\omega_i = \omega_i'''$ and $\omega_i' = \omega_i''$ was considered by Wu and Lin (1975), in this case it is readily verified that $F(\theta, \phi)$ can be factorized into two factors:

$$F(\theta,\phi) = (A + B\,\mathrm{e}^{\mathrm{i}\alpha} + C\,\mathrm{e}^{-\mathrm{i}\alpha} - D\,\mathrm{e}^{\mathrm{i}\beta} - E\,\mathrm{e}^{-\mathrm{i}\beta})(A - B\,\mathrm{e}^{\mathrm{i}\alpha} - C\,\mathrm{e}^{-\mathrm{i}\alpha} + D\,\mathrm{e}^{\mathrm{i}\beta} + E\,\mathrm{e}^{-\mathrm{i}\beta}) \tag{14}$$

with

$$\begin{aligned}
&\theta = -\alpha - \beta \qquad \phi = \beta - \alpha \qquad A = \omega_5\omega_6' + \omega_6'\omega_5 \\
&B = \omega_1\omega_1' \qquad C = \omega_2\omega_2' \qquad D = \omega_3\omega_3' \qquad E = \omega_4\omega_4'
\end{aligned}$$

and our solution (12) indeed reduces to the previously known expressions (Wu and Lin 1975).

Notice that although there are 20 independent vertex weights to start with, the final expression (12) contains only nine independent parameters. The free-fermion condition (10) implies the following inequalities (see appendix 2):

$$\tfrac{1}{2}a \geq (bb')^{1/2} + (c_1c_1')^{1/2} + (c_2c_2')^{1/2} + (ff')^{1/2} + (gg')^{1/2} \tag{15}$$

$$\tfrac{1}{2}a \geq (b_1b_1')^{1/2} + (b_2b_2')^{1/2} + (cc')^{1/2} + (ff')^{1/2} + (gg')^{1/2} \tag{16}$$

$$\tfrac{1}{2}a \geq b + c + f + g \qquad \text{if } b = b',\ c = c',\ f = f',\ g = g'. \tag{17}$$

It follows from definitions that

$$b_1b_2 = fg \qquad b_1'b_2' = f'g' \qquad c_1c_2 = fg' \qquad c_1'c_2' = f'g. \tag{18}$$

The analytic properties of ψ are given by the following theorems†.

Theorem 1

If a, $b + b'$, $c + c'$ and $f + f' + g + g'$ cannot form a polygon, then $F(\theta, \phi) \neq 0$ for all θ and

† These theorems are proved by K Y Lin in appendix 2.

ϕ which implies ψ has no singularity and

$$\begin{aligned}\psi &= \tfrac{1}{2}\ln\max\{b_1, b_2, b_1', b_2'\} && \text{if } b+b' > a+c+c'+f+f'+g+g' \\ &= \tfrac{1}{2}\ln\max\{c_1, c_2, c_1', c_2'\} && \text{if } c+c' > a+b+b'+f+f'+g+g' \\ &= \tfrac{1}{2}\ln\max\{f, f', g, g'\} && \text{if } f+f'+g+g' > a+b+b'+c+c' \\ &= \frac{1}{8\pi^2}\int_0^{2\pi} d\theta \int_0^{2\pi} d\phi \ln[a - 2(bb')^{1/2}\cos\theta - 2(cc')^{1/2}\cos\phi \\ &\quad -2(ff')^{1/2}\cos(\theta+\phi) - 2(gg')^{1/2}\cos(\theta-\phi)] \\ &\quad \text{if } a > b+b'+c+c'+f+f'+g+g',\ bcf' = b'c'f \text{ and } bc'g' = b'cg.\end{aligned} \tag{19}$$

Theorem 2
If a, $b+b'$, $c+c'$, and $f+f'+g+g'$ form a polygon, then $F(\theta, \phi)=0$ has either one or three solutions (θ_i, ϕ_i) such that $-\pi \leqslant \theta_i(\phi_i) \leqslant \pi (i=1, 2, 3)$ where (θ_i, ϕ_i) and $(-\theta_i, -\phi_i)$ are considered as the same solution. In the special case of $bcf' = b'c'f$, $bc'g' = b'cg$, $bb' \geqslant cc' = 4ff' = 4gg'$, there is exactly one solution.

If $F(\theta, \phi) = 0$ has only one solution (θ_1, ϕ_1), we can write

$$\begin{aligned}\psi &= \frac{1}{2\pi}\int_0^{|\phi_1|} \ln|z_1(\phi)|\, d\phi + \tfrac{1}{2}\ln\max\{b_1, b_2, f, g\} && \text{if } b+f+g > b'+f'+g' \\ &= \frac{1}{2\pi}\int_0^{|\phi_1|} \ln|z_2(\phi)^{-1}|\, d\phi + \tfrac{1}{2}\ln\max\{b_1', b_2', f', g'\} && \text{if } b'+f'+g' > b+f+g\end{aligned} \tag{20}$$

where z_1, $z_2(|z_1| \geqslant |z_2|)$ are the roots of

$$(b - f\,e^{i\phi} - g\,e^{-i\phi})z^2 + (a + c\,e^{i\phi} + c'\,e^{-i\phi})z + b' - f'\,e^{-i\phi} - g'e^{i\phi} = 0;$$

when the polygon degenerates into a straight line, namely

$$\Delta \equiv a+b+b'+c+c'+f+f'+g+g' - 2\max\{a, b+b', c+c', f+f'+g+g'\} = 0. \tag{21}$$

$F(\theta, \phi) = 0$ has only one solution where

$$\begin{aligned}\theta &= \phi = \pi && \text{if } a = b+b'+c+c'+f+f'+g+g' \\ \theta &= \pi, \phi = 0 && \text{if } b+b' = a+c+c'+f+f'+g+g' \\ \theta &= 0, \phi = \pi && \text{if } c+c' = a+b+b'+f+f'+g+g' \\ \theta &= \phi = 0 && \text{if } f+f'+g+g' = a+b+b'+c+c'.\end{aligned} \tag{22}$$

ψ is non-analytic if and only if the parameters satisfy the critical condition (21). Besides, we have

$$\psi_{\text{singular}} \sim \Delta^2 \ln(-\Delta) \qquad \Delta \to 0^- \qquad \text{if } b=b', c=c', f=f', g=g' \tag{23}$$

$$\sim \Delta^{3/2} \qquad \Delta \to 0^+ \qquad \text{otherwise.} \tag{24}$$

The physical interpretations of these theorems are given in the following two sections.

5. Exactly soluble models

In physical models, the vertex weights (1) are interpreted as the Boltzmann factors (4). In this section we consider the cases where the free-fermion condition (10) is valid for all temperatures so that the models are exactly solved.

There are four distinct classes of exactly soluble models (others are related to them by symmetry relations given in § 3):

$$\begin{array}{llll}
\text{A:} & \omega_1\omega_2=\omega_1'\omega_2'=\omega_1''\omega_2''=\omega_1'''\omega_2'''=0 & & \omega_3\omega_4=\omega_5\omega_6 \\
 & \omega_3'\omega_4'=\omega_5'\omega_6' & \omega_3''\omega_4''=\omega_5''\omega_6'' & \omega_3'''\omega_4'''=\omega_5'''\omega_6''' \\
\text{B:} & \omega_1\omega_2=\omega_1'\omega_2'=\omega_3''\omega_4''=\omega_1'''\omega_2'''=0 & & \omega_3\omega_4=\omega_5\omega_6 \\
 & \omega_3'\omega_4'=\omega_5'\omega_6' & \omega_1''\omega_2''=\omega_5''\omega_6'' & \omega_3'''\omega_4'''=\omega_5'''\omega_6''' \\
\text{C:} & \omega_1\omega_2=\omega_1'\omega_2'=\omega_3''\omega_4''=\omega_3'''\omega_4'''=0 & & \omega_3\omega_4=\omega_5\omega_6 \\
 & \omega_3'\omega_4'=\omega_5'\omega_6' & \omega_1''\omega_2''=\omega_5''\omega_6'' & \omega_1'''\omega_2'''=\omega_5'''\omega_6''' \\
\text{D:} & \omega_1\omega_2=\omega_3'\omega_4'=\omega_3''\omega_4''=\omega_1'''\omega_2'''=0 & & \omega_3\omega_4=\omega_5\omega_6 \\
 & \omega_1'\omega_2'=\omega_5'\omega_6' & \omega_1''\omega_2''=\omega_5''\omega_6'' & \omega_3'''\omega_4'''=\omega_5'''\omega_6'''.
\end{array} \tag{25}$$

Each class has four or five different cases, overall we have 18 different models to consider:

$$\begin{array}{lll}
(1) & \omega_1=\omega_4'=\omega_3''=\omega_2'''=0(\text{class D}) & F=a \\
(2) & \omega_1=\omega_2'=\omega_3''=\omega_4'''=0(\text{class C}) & F=a+c_2\,e^{i\phi}+c_2'\,e^{-i\phi} \\
(3) & \omega_1=\omega_2'=\omega_2''=\omega_1'''=0(\text{class A}) & F=a-g\,e^{i(\theta-\phi)}-g'\,e^{i(\phi-\theta)} \\
(4) & \omega_1=\omega_1'=\omega_3''=\omega_2'''=0(\text{class B}) & F=a+b_1\,e^{i\theta}+c_2'\,e^{-i\phi}-g\,e^{i(\theta-\phi)} \\
(5) & \omega_1=\omega_2'=\omega_3''=\omega_1'''=0(\text{class B}) & F=a+b_1\,e^{i\theta}+c_2\,e^{i\phi}-g\,e^{i(\theta-\phi)} \\
(6) & \omega_1=\omega_3'=\omega_4''=\omega_1'''=0(\text{class D}) & F=a+b_1\,e^{i\theta}+c_1\,e^{i\phi}-f\,e^{i(\theta+\phi)} \\
(7) & \omega_1=\omega_3'=\omega_3''=\omega_2'''=0(\text{class D}) & F=a+b_1\,e^{i\theta}+c_2'\,e^{-i\phi}-g\,e^{i(\theta-\phi)} \\
(8) & \omega_1=\omega_3'=\omega_3''=\omega_1'''=0(\text{class D}) & F=a+b\,e^{i\theta}-f\,e^{i(\theta+\phi)}-g\,e^{i(\theta-\phi)} \\
(9) & \omega_1=\omega_1'=\omega_2''=\omega_2'''=0(\text{class A}) & F=a+c_1\,e^{i\phi}+c_2'\,e^{-i\phi} \\
 & & \quad -g\,e^{i(\theta-\phi)}-g'\,e^{i(\phi-\theta)} \\
(10) & \omega_1=\omega_2'=\omega_4''=\omega_3'''=0(\text{class C}) & F=a+b_1\,e^{i\theta}+b_2'\,e^{-i\theta} \\
 & & \quad +c_2\,e^{i\phi}+c_2'\,e^{-i\phi} \\
(11) & \omega_1=\omega_3'=\omega_4''=\omega_2'''=0(\text{class D}) & F=a+b_1\,e^{i\theta}+b_2'\,e^{-i\theta} \\
 & & \quad +c_1\,e^{i\phi}+c_2'\,e^{-i\phi} \\
(12) & \omega_1=\omega_1'=\omega_2''=\omega_1'''=0(\text{class A}) & F=a+b_2\,e^{i\theta}+c_1\,e^{i\phi} \\
 & & \quad -g\,e^{i(\theta-\phi)}-g'\,e^{i(\phi-\theta)} \\
(13) & \omega_1=\omega_1'=\omega_4''=\omega_3'''=0(\text{class C}) & F=a+b_1\,e^{i\theta}+c_2\,e^{i\phi} \\
 & & \quad +c_2'\,e^{-i\phi}-f\,e^{i(\theta+\phi)}
\end{array}$$

(14)	$\omega_1=\omega_1'=\omega_3''=\omega_1'''=0$(class B)	$F=a+b\,e^{i\theta}+c_2\,e^{i\phi}-f\,e^{i(\theta+\phi)}-g\,e^{i(\theta-\phi)}$
(15)	$\omega_1=\omega_1'=\omega_4''=\omega_2'''=0$(class B)	$F=a+b_1\,e^{i\theta}+c_1\,e^{i\phi}+c_2'\,e^{-i\phi}-g'\,e^{i(\phi-\theta)}$
(16)	$\omega_1=\omega_1'=\omega_3''=\omega_3'''=0$(class C)	$F=a+b\,e^{i\theta}+c_2\,e^{i\phi}+c_2'\,e^{-i\phi}-f\,e^{i(\theta+\phi)}-g\,e^{i(\theta-\phi)}$
(17)	$\omega_1=\omega_1'=\omega_4''=\omega_4'''=0$ (class C)	$F=a+c\,e^{i\phi}+c_2'\,e^{-i\phi}-f\,e^{i(\theta+\phi)}-g'\,e^{i(\phi-\theta)}$
(18)	$\omega_1=\omega_1'=\omega_1''=\omega_1'''=0$(class A)	$F=a+b\,e^{i\theta}+c\,e^{i\phi}-f\,e^{i(\theta+\phi)}-g\,e^{i(\theta-\phi)}-g'\,e^{i(\phi-\theta)}$.

The free energies of these models are discussed in the following subsections, where similar models are discussed together.

5.1. Model 1

In this model we have $\psi=\frac{1}{2}\ln a$ and there is no phase transition.

5.2. Models 2 and 3

These models are identical to the model b of Wu and Lin (1975). The system is in a frozen state at all temperatures.

5.3. Models 4–7

The free energies of these models can all be expressed in the form

$$\psi=\frac{1}{8\pi^2}\int_{-\pi}^{\pi}d\alpha\int_{-\pi}^{\pi}d\beta\,\ln|A-B\,e^{i(\alpha+\beta)}+C\,e^{i\alpha}+D\,e^{i\beta}|. \tag{26}$$

This integral has been evaluated by Hsue *et al* (1975). Models 4 and 5 are identical to model 11 of Lin (1975). Models 6 and 7 are similar to model 11 of Lin except that A is now the sum of four Boltzmann factors instead of three The system may exhibit up to two phase transitions.

5.4. Model 8

The free energy is

$$\psi=\frac{1}{8\pi^2}\int_{-\pi}^{\pi}d\theta\int_{-\pi}^{\pi}d\phi\,\ln|b+a\,e^{-i\theta}-f\,e^{i\phi}-g\,e^{-i\phi}|. \tag{27}$$

This model is similar to the modified KDP model of Wu (1971) except that here a is the sum of four Boltzmann factors instead of one. The critical temperature T_c is determined by the critical condition

$$\Delta(T_c)\equiv b+a+f+g-2\max\{a,b,f+g\}=0. \tag{28}$$

In Wu's model there is only one transition. In our model the system may exhibit up to two transitions. To see this, we denote

$$\begin{aligned} a &= \sum_{i=1}^{4} \exp(-\beta\epsilon_i) \qquad & b &= \exp(-\beta\epsilon_5) + \exp(-\beta\epsilon_6) \\ f &= \exp(-\beta\epsilon_7) \qquad & g &= \exp(-\beta\epsilon_8) \end{aligned} \tag{29}$$

where $\epsilon_1+\epsilon_2=\epsilon_3+\epsilon_4$ and $\epsilon_5+\epsilon_6=\epsilon_7+\epsilon_8$. Equation (28) has two solutions if $\epsilon_1+\epsilon_2<\epsilon_5+\epsilon_6$ and

$$\min\{\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4\} > \min\{\epsilon_5, \epsilon_6, \epsilon_7, \epsilon_8\}. \tag{30}$$

5.5. Models 9–11

The free energies can be written in the form

$$\psi = \frac{1}{8\pi^2}\int_{-\pi}^{\pi} d\alpha \int_{-\pi}^{\pi} d\beta \ln|A + B\,e^{i\alpha} + C\,e^{-i\alpha} + D\,e^{i\beta} + E\,e^{-i\beta}|. \tag{31}$$

This integral has been evaluated by Wu and Lin (1975). The system may exhibit up to two transitions.

5.6. Models 12–14

The free energies can be written in the form

$$\psi = \frac{1}{8\pi^2}\int_{-\pi}^{\pi} d\alpha \int_{-\pi}^{\pi} d\beta \ln|A + B\,e^{i\alpha} + C\,e^{-i\beta} - D\,e^{i(\alpha+\beta)} - E\,e^{-i(\alpha+\beta)}|. \tag{32}$$

These models are similar to the model 15 of Lin (1975) except that here A is the sum of three (models 12 and 13) Boltzmann factors instead of two and C is the sum of three (model 14) factors instead of one. The system has either one or three transitions.

5.7. Model 15

The free energy can be rewritten in the form

$$\psi = \frac{1}{8\pi^2}\int_{-\pi}^{\pi} d\alpha \int_{-\pi}^{\pi} d\beta \ln|a + b_1\,e^{-i\alpha} + c_1\,e^{i\beta} + c_2'\,e^{-i\beta} - g'\,e^{i(\alpha+\beta)}| \tag{33}$$

which is a special case of the general model discussed by Lin (1975). The system may exhibit up to two phase transitions.

5.8. Model 16

We denote

$$\begin{aligned} &A(\phi) = a_1 + a_2 + c_2\,e^{i\phi} + c_2'\,e^{-i\phi} \\ &B(\phi) = b_1 + b_2 - f\,e^{i\phi} - g\,e^{-i\phi} \\ &a_1 = \omega_5\omega_6'\omega_6''\omega_5''' \qquad a_2 = \omega_6\omega_5'\omega_5''\omega_6''' \end{aligned} \tag{34}$$

where $a_1a_2=c_2c_2'$ and $b_1b_2=fg$. The free energy is

$$\psi=\frac{1}{8\pi^2}\int_{-\pi}^{\pi}\mathrm{d}\phi\int_{-\pi}^{\pi}\mathrm{d}\theta\,\ln|A+\mathrm{e}^{\mathrm{i}\theta}B|=\frac{1}{4\pi}\int_{-\pi}^{\pi}\mathrm{d}\phi\,\ln\max\{|A|,|B|\}$$

$$=\tfrac{1}{2}\ln\max\{a_1,a_2,b_1,b_2,c_2,c_2',f,g\}\qquad\text{if } a_1+a_2,\, b_1+b_2,\, c_2+c_2',\, f+g \text{ do not form a polygon}\tag{35}$$

$$=\frac{1}{2\pi}\int_0^{\phi_0}\mathrm{d}\phi\,\ln|A(\phi)|+\frac{1}{2\pi}\int_{\phi_0}^{\pi}\mathrm{d}\phi\,\ln|B(\phi)|\qquad\text{otherwise}$$

where $|A(\phi_0)|=|B(\phi_0)|$ has exactly one solution such that $0\leq\phi_0\leq\pi$. The system has exactly one transition temperature T_c determined by the critical condition (21). The specific heat diverges with an exponent† $\alpha=\frac{1}{2}$ above T_c while below T_c the system is in a frozen state.

5.9. *Model 17*

It follows from theorems 1 and 2 that

$$\begin{aligned}\psi&=\tfrac{1}{2}\ln\max\{c_1,c_2,c_2'\} &&\text{if } c+c_2'>a+f+g'\\ &=\tfrac{1}{2}\ln\max\{f,g'\} &&\text{if } f+g'>a+c+c_2'\\ &=\tfrac{1}{2}\ln\{\tfrac{1}{2}[a+(a^2-4cc_2')^{1/2}]\} &&\text{if } a>c+c_2'+f+g'.\end{aligned}\tag{36}$$

The critical condition

$$\Delta(T_c)=a+c+c_2'+f+g'-2\max\{a,c+c_2',f+g'\}=0\tag{37}$$

has either one or three solutions. To see this, we denote

$$\begin{aligned}&c+c_2'=\sum_{i=1}^{3}\exp(-\beta\epsilon_i)\\ &f+g'=\exp(-\beta\epsilon_4)+\exp(-\beta\epsilon_5)\qquad a=\sum_{i=6}^{9}\exp(-\beta\epsilon_i)\end{aligned}\tag{38}$$

where $\epsilon_1+\epsilon_2=\epsilon_4+\epsilon_5$, $\epsilon_1+\epsilon_3=\epsilon_6+\epsilon_7$, $\epsilon_2+\epsilon_3=\epsilon_8+\epsilon_9$. There are two possiblities:

(i)
$$\begin{aligned}&\min\{\epsilon_6,\epsilon_7,\epsilon_8,\epsilon_9\}=\text{lowest energy} &&\text{(1 transition)}\\ &\psi=\tfrac{1}{2}\ln[a+(a^2-4cc_2')^{1/2}]-\tfrac{1}{2}\ln 2 &&T\leq T_c\end{aligned}\tag{39}$$

(ii)
$$\begin{aligned}&\min\{\epsilon_1,\epsilon_2,\epsilon_3,\epsilon_4,\epsilon_5\}=\epsilon_0=\text{lowest energy} &&\text{(1 or 3 transitions)}\\ &\psi=-\tfrac{1}{2}\beta\epsilon_0\text{(frozen state)} &&T\leq T_c^1\\ &\quad=\tfrac{1}{2}\ln[a+(a^2-4cc_2')^{1/2}]-\tfrac{1}{2}\ln 2 &&T_c^3\geq T\geq T_c^2>T_c^1\end{aligned}\tag{40}$$

where T_c^2 may become infinity.

† We use the standard definitions of critical-point exponents (Stanley 1971).

5.10. Model 18

It follows from theorems 1 and 2 that

$$\begin{aligned} \psi &= \tfrac{1}{2}\ln\max\{b_1, b_2\} && \text{if } b > a+c+f+g+g' \\ &= \tfrac{1}{2}\ln\max\{c_1, c_2\} && \text{if } c > a+b+f+g+g' \\ &= \tfrac{1}{2}\ln\max\{f, g, g'\} && \text{if } f+g+g' > a+b+c \\ &= \tfrac{1}{2}\ln\max\{a_1, a_2\} && \text{if } a > b+c+f+g+g' \end{aligned} \tag{41}$$

where $a = a_1 + a_2$, $a_1 = \omega_5\omega_6'\omega_6''\omega_5'''$ and $a_2 = \omega_6\omega_5'\omega_5''\omega_6'''$. The critical condition $\Delta(T_c) = 0$ has exactly one solution. We have

$$\psi = \tfrac{1}{2}\ln\max\{a_1, a_2, b_1, b_2, c_1, c_2, f, g, g'\} \qquad T \leqslant T_c. \tag{42}$$

6. Exact isotherm of an antiferroelectric model

Following Baxter (1970), we use the free-fermion condition (10) to define a temperature at which the Pfaffian solution is valid. Since the validity of condition (10) is independent of the direct and staggered fields, we have an exact isotherm for a general staggered model.

We denote the staggered field by s, the direct fields in the horizontal and vertical directions by h and v such that†

$$\begin{aligned} & e_5 = e_6' = e_6'' = e_5''' = 2s \qquad e_6 = e_5' = e_5'' = e_6''' = -2s \\ & e_1(e_1', e_1'', e_1''') = \epsilon_1(\epsilon_1', \epsilon_1'', \epsilon_1''') - h - v \\ & e_2(e_2', e_2'', e_2''') = \epsilon_1(\epsilon_1', \epsilon_1'', \epsilon_1''') + h + v \\ & e_3(e_3', e_3'', e_3''') = \epsilon_2(\epsilon_2', \epsilon_2'', \epsilon_2''') - h + v \\ & e_4(e_4', e_4'', e_4''') = \epsilon_2(\epsilon_2', \epsilon_2'', \epsilon_2''') + h - v \\ & \max\{\epsilon_1, \epsilon_2\} = \max\{\epsilon_1', \epsilon_2'\} = \max\{\epsilon_1'', \epsilon_2''\} = \max\{\epsilon_1''', \epsilon_2'''\} = \epsilon_{\max} \\ & \min\{\epsilon_1, \epsilon_2\} = \min\{\epsilon_1', \epsilon_2'\} = \min\{\epsilon_1'', \epsilon_2''\} = \min\{\epsilon_1''', \epsilon_2'''\} = \epsilon_{\min}. \end{aligned} \tag{43}$$

The temperature is determined by equation (10):

$$\exp(-2\beta\epsilon_{\max}) + \exp(-2\beta\epsilon_{\min}) = 1. \tag{44}$$

Note that we have the equalities $bcf' = b'c'f$ and $bc'g' = b'cg$. There are four different cases (the others are related to them by symmetry):

(1) $\quad \epsilon_1 = \epsilon_1' = \epsilon_1'' = \epsilon_1''' \qquad \epsilon_2 = \epsilon_2' = \epsilon_2'' = \epsilon_2'''$

(2) $\quad \epsilon_1 = \epsilon_2' = \epsilon_2'' = \epsilon_1''' \qquad \epsilon_2 = \epsilon_1' = \epsilon_1'' = \epsilon_2'''$

(3) $\quad \epsilon_1 = \epsilon_2' = \epsilon_1'' = \epsilon_2''' \qquad \epsilon_2 = \epsilon_1' = \epsilon_2'' = \epsilon_1'''$

(4) $\quad \epsilon_1 = \epsilon_1' = \epsilon_1'' = \epsilon_2''' \qquad \epsilon_2 = \epsilon_2' = \epsilon_2'' = \epsilon_1'''.$

These models are discussed in the following subsections.

† See equation (2) of Baxter (1970).

6.1. *Models 1 and 2*

These models have been discussed in detail by Baxter (1970) and Wu and Lin (1975).

6.2. *Model 3*

The free energy is

$$\psi=\frac{1}{8\pi^2}\int_0^{2\pi}\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\phi\ln|2\cosh S+2C+2B\cos(\theta+\mathrm{i}H)$$
$$+2C\cos(\phi+\mathrm{i}V)-2C\cos(\theta+\mathrm{i}H)\cos(\phi+\mathrm{i}V)| \tag{45}$$

where

$$S=8\beta s \qquad H=4\beta h \qquad V=4\beta v$$
$$B=\exp(-4\beta\epsilon_1)+\exp(-4\beta\epsilon_2) \qquad C=2\exp[-2\beta(\epsilon_1+\epsilon_2)].$$

The staggered and direct polarization $P(S)$, $P(H)$, $P(V)$ can be defined as the derivatives of ψ with respect to S, H, and V (Baxter 1970). We define

$$\Omega_1=\cosh S+C \qquad \Omega_2=B\cosh H$$
$$\Omega_3=C\cosh V \qquad \Omega_4=C\cosh V\cosh H. \tag{46}$$

It follows from theorems 1 and 2 that

$$\psi=\frac{1}{8\pi^2}\int_0^{2\pi}\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\phi\ \ln(2\cosh S+2C+2B\cos\theta+2C\cos\phi-2C\cos\theta\cos\phi)$$
$$\text{if } \Omega_1>\Omega_2+\Omega_3+\Omega_4 \tag{47}$$

where ψ is independent of H and V,

$$\psi=\tfrac{1}{2}|H|-2\beta\min(\epsilon_1,\epsilon_2) \qquad \text{if } \Omega_2>\Omega_1+\Omega_3+\Omega_4 \tag{48}$$

where

$$|P(H)|=\tfrac{1}{2} \qquad P(V)=P(S)=0,$$
$$\psi=\tfrac{1}{2}|H|+\tfrac{1}{2}|V|-\beta(\epsilon_1+\epsilon_2) \qquad \text{if } \Omega_4>\Omega_1+\Omega_2+\Omega_3 \tag{49}$$

where

$$|P(H)|=|P(V)|=\tfrac{1}{2} \qquad P(S)=0,$$
$$\psi=(20) \qquad \text{if } \Omega_1,\Omega_2,\Omega_3,\Omega_4 \text{ form a polygon} \tag{50}$$

where

$$|P(H)|=\tfrac{1}{2}[1-(|\phi_0|/\pi)] \qquad |P(V)|=\tfrac{1}{2}[1-(|\theta_0|/\pi)]$$

and $F(\theta_0,\phi_0)=0$ $(-\pi\leq\theta_0(\phi_0)\leq\pi)$.

6.3. *Model 4*

The free energy is

$$\psi=\frac{1}{8\pi^2}\int_0^{2\pi}\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\phi\ \ln|2\cosh S+2B[1+\cos(\theta+\mathrm{i}H)+\cos(\phi+\mathrm{i}V)]$$
$$-2F\cos(\theta+\phi+\mathrm{i}H+\mathrm{i}V)-2G\cos(\theta-\phi+\mathrm{i}H-\mathrm{i}V)| \tag{51}$$

where

$$B=F+G \qquad F=\exp[-\beta(3\epsilon_1+\epsilon_2)] \qquad G=\exp[-\beta(\epsilon_1+3\epsilon_2)].$$

We define

$$\begin{aligned}&\Omega_1=\cosh S+B \qquad \Omega_2=B\cosh H \qquad \Omega_3=B\cosh V\\&\Omega_4=F\cosh(H+V)+G\cosh(H-V).\end{aligned} \tag{52}$$

It follows from theorems 1 and 2 that

$$\begin{aligned}\psi=\frac{1}{8\pi^2}\int_0^{2\pi}\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\phi\,\ln[2\cosh S+2B(1+\cos\theta+\cos\phi)\\-2F\cos(\theta+\phi)-2G\cos(\theta-\phi) \qquad \text{if } \Omega_1>\Omega_2+\Omega_3+\Omega_4\end{aligned} \tag{53}$$

where $P(H)=P(V)=0$,

$$\psi=\tfrac{1}{2}|H|-\tfrac{1}{2}\beta\min\{3\epsilon_1+\epsilon_2, 3\epsilon_2+\epsilon_1\} \qquad \text{if } \Omega_2>\Omega_1+\Omega_3+\Omega_4 \tag{54}$$

where $|P(H)|=\frac{1}{2}$, $P(V)=P(S)=0$,

$$\psi=\tfrac{1}{2}|V|-\tfrac{1}{2}\beta\min\{3\epsilon_1+\epsilon_2, 3\epsilon_2+\epsilon_1\} \qquad \text{if } \Omega_3>\Omega_1+\Omega_2+\Omega_4 \tag{55}$$

where $|P(V)|=\frac{1}{2}$, $P(H)=P(S)=0$,

$$\psi=\tfrac{1}{2}\max\{|H+V|-\beta(3\epsilon_1+\epsilon_2), |H-V|-\beta(3\epsilon_2+\epsilon_1)\} \qquad \text{if } \Omega_4>\Omega_1+\Omega_2+\Omega_3 \tag{56}$$

where $|P(H)|=|P(V)|=\frac{1}{2}$, $P(S)=0$,

$$\psi=(20) \qquad \text{otherwise} \tag{57}$$

where

$$|P(H)|=\tfrac{1}{2}[1-(|\phi_0|/\pi)] \qquad |P(V)|=\tfrac{1}{2}[1-(|\theta_0|/\pi)]$$

and $F(\theta_0, \phi_0)=0$ $(-\pi\leqslant\theta_0(\phi_0)\leqslant\pi)$.

7. Conclusion

We have generalized the results of Wu and Lin (1975) to the staggered ice-rule vertex model on a square lattice which allows four different vertex weights for the four sublattices. There are eighteen different cases where the vertex weights satisfy the free-fermion condition at all temperatures. We have considered these soluble models and found that the system may exhibit up to three phase transitions. If there is only one transition, then the system is in an ordered or frozen state below T_c, and the specific heat diverges with $\alpha=\frac{1}{2}$ above T_c. If there are two transitions ($T_c^2>T_c^1$), then the system is in an ordered state above T_c^2, and in an ordered state (the free energy is described by the same function for $T>T_c^2$ and $T<T_c^1$) or frozen state below T_c^1 ($\alpha=\frac{1}{2}$ at T_c^1 and $\alpha'=\frac{1}{2}$ at T_c^2). If there are three transitions ($T_c^3>T_c^2>T_c^1$), then the system is frozen below T_c^1, and in an ordered state for $T_c^3\geqslant T\geqslant T_c^2$, while the free energy is described by the same function for both $T>T_c^3$ and $T_c^2>T>T_c^1$ ($\alpha=\frac{1}{2}$ at T_c^3, T_c^1 and $\alpha'=\frac{1}{2}$ at T_c^2).

We also obtained the exact isotherm of a general antiferroelectric model at a particular temperature in the presence of both direct and staggered fields. As the fields are varied, the system undergoes transitions among states of zero, partial and complete direct polarization.

Finally we compare our results with those of Vaks *et al* (1965)†. In the study of the two-dimensional Ising model on the Union Jack lattice, they discovered that their model may exhibit up to three phase transitions. Their model has been generalized by Sacco and Wu (1975) and is equivalent to a special case of the staggered eight-vertex model on a square lattice (Hsue *et al* 1975). In the model of Vaks *et al*, the specific heat diverges logarithmically both above and below each transition temperature and has the exponents $\alpha = \alpha' = 0$. In our model the specific heat has inverse square-root singularities either above ($\alpha = \frac{1}{2}$) or below ($\alpha' = \frac{1}{2}$) each transition temperature.

Appendix 1. Pfaffian solution

Expand each site of the square lattice L into a 'city' of four terminals to form a dimer lattice L^{Δ} whose unit cell is shown in figure 3. Following exactly the same procedure as Wu and Lin (1975), we obtain

$$\psi = \frac{1}{4(2\pi)^2} \int_{-\pi}^{\pi} d\theta \int_{-\pi}^{\pi} d\phi \, \ln[(\omega_2 \omega_2' \omega_2'' \omega_2''')^2 D(\theta, \phi)] \tag{A.1}$$

where

$$D(\theta, \phi) = \begin{vmatrix} 0 & \mathbf{A} \\ -\mathbf{A}^* & 0 \end{vmatrix}$$

$$\mathbf{A} = \begin{vmatrix} u_3 & -u_6 & 1 & 0 & 0 & 0 & 0 & 0 \\ -u_5 & u_4 & 0 & 0 & 0 & e^{i\phi} & 0 & 0 \\ e^{i\theta} & 0 & u_3' & -u_6' & 0 & 0 & 0 & 0 \\ 0 & 0 & -u_5' & u_4' & 0 & 0 & 0 & e^{i\phi} \\ 0 & 0 & 0 & 0 & u_3'' & -u_6'' & 1 & 0 \\ 0 & 1 & 0 & 0 & -u_5'' & u_4'' & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{i\theta} & 0 & u_3''' & -u_6''' \\ 0 & 0 & 0 & 1 & 0 & 0 & -u_5''' & u_4''' \end{vmatrix} \tag{A.2}$$

$$u_i = \omega_i/\omega_2 \qquad u_i' = \omega_i'/\omega_2' \qquad u_i'' = \omega_i''/\omega_2'' \qquad u_i''' = \omega_i'''/\omega_2'''$$

and $\mathbf{A}^*$ is the hermitian conjugate matrix of $\mathbf{A}$. Equation (A.1) reduces to equation (11) in the text after some algebra.

Appendix 2. General properties of ψ

In this appendix we discuss the analytic properties of the free energy

$$\psi = \frac{1}{8\pi^2} \int_{-\pi}^{\pi} d\theta \int_{-\pi}^{\pi} d\phi \, \ln|F(\theta, \phi)| = \frac{1}{8\pi^2} \mathrm{Re} \int_{-\pi}^{\pi} d\theta \int_{-\pi}^{\pi} d\phi \, \ln F(\theta, \phi) \tag{A.3}$$

† A mistake in this reference was corrected by Sacco and Wu (1975).

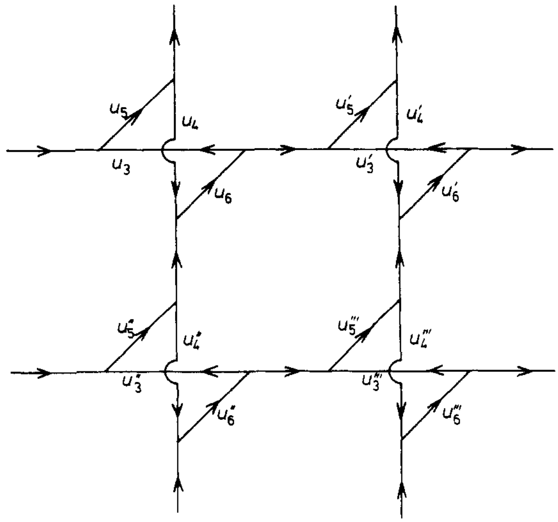

Figure 3. A unit cell of the dimer lattice L^{Δ}.

where

$$F = a + b\,e^{i\theta} + b'\,e^{-i\theta} + c\,e^{i\phi} + c'\,e^{-i\phi} - f\,e^{i(\theta+\phi)} - f'\,e^{-i(\theta+\phi)} - g\,e^{i(\theta-\phi)} - g'\,e^{i(\phi-\theta)}$$

$$b = b_1 + b_2 \qquad b' = b_1' + b_2' \qquad c = c_1 + c_2 \qquad c' = c_1' + c_2'$$

$$b_1 b_2 = fg \qquad b_1' b_2' = f'g' \qquad c_1 c_2 = fg' \qquad c_1' c_2' = f'g$$

and the parameters are defined by equation (13).

Lemma 1.

$$\tfrac{1}{2}a \geqslant (bb')^{1/2} + (c_1 c_1')^{1/2} + (c_2 c_2')^{1/2} + (ff')^{1/2} + (gg')^{1/2} \tag{A.4}$$

$$\tfrac{1}{2}a \geqslant (cc')^{1/2} + (b_1 b_1')^{1/2} + (b_2 b_2')^{1/2} + (ff')^{1/2} + (gg')^{1/2} \tag{A.5}$$

$$\tfrac{1}{2}a \geqslant b + c + f + g \qquad \text{if } b = b',\ c = c',\ f = f',\ g = g'. \tag{A.6}$$

Proof. Let us consider (A.4) first. The free-fermion condition (10) implies

$$\omega_1\omega_2 = \sin^2\alpha\,\omega_5\omega_6 \qquad \omega_3\omega_4 = \cos^2\alpha\,\omega_5\omega_6$$

$$\omega_1'\omega_2' = \cos^2\beta\,\omega_5'\omega_6' \qquad \omega_3'\omega_4' = \sin^2\beta\,\omega_5'\omega_6'$$

$$\omega_1''\omega_2'' = \cos^2\gamma\,\omega_5''\omega_6'' \qquad \omega_3''\omega_4'' = \sin^2\gamma\,\omega_5''\omega_6''$$

$$\omega_1'''\omega_2''' = \sin^2\delta\,\omega_5'''\omega_6''' \qquad \omega_3'''\omega_4''' = \cos^2\delta\,\omega_5'''\omega_6'''.$$

We define x and y by

$$\omega_1\omega_3'\omega_4''\omega_2''' = x^2 AS \qquad \omega_3\omega_1'\omega_2''\omega_4''' = y^2 AC$$

where

$$S = \sin\alpha\,\sin\beta\,\sin\gamma\,\sin\delta \qquad C = \cos\alpha\,\cos\beta\,\cos\gamma\,\cos\delta$$

$$A^2 = \omega_5\omega_6\omega_5'\omega_6'\omega_5''\omega_6''\omega_5'''\omega_6'''.$$

We now rewrite both sides of (A.4) in the form

$$\begin{aligned}\tfrac{1}{2}a &= \tfrac{1}{2}A[S(x^2+x^{-2})+C(y^2+y^{-2})]+\tfrac{1}{2}(\omega_5\omega_6'\omega_6''\omega_5'''+\omega_6\omega_5'\omega_5''\omega_6''') \\ &\geqslant A[(Sx^2+Cy^2)(Sx^{-2}+Cy^{-2})]^{1/2}+A \\ &= A[(S+C)^2+SC(xy^{-1}-yx^{-1})^2]^{1/2}+A\end{aligned}$$

The right-hand side is given by

$$A[(S'+C')^2+SC(xy^{-1}-yx^{-1})^2]^{1/2}+A\ \sin(\alpha+\beta)\sin(\gamma+\delta)$$

where

$$S'=\sin\alpha\ \sin\beta\ \cos\gamma\ \cos\delta \qquad C'=\cos\alpha\ \cos\beta\ \sin\gamma\sin\delta.$$

The inequality (A.4) then follows from ($t\geqslant 0$)

$$\begin{aligned}1-&\sin(\alpha+\beta)\sin(\gamma+\delta)+[(S+C)^2+t]^{1/2}-[(S'+C')^2+t]^{1/2} \\ &= 1-\sin(\alpha+\beta)\sin(\gamma+\delta)+\cos(\alpha+\beta)\cos(\gamma+\delta) \\ &\quad\times\frac{S+C+S'+C'}{[(S+C)^2+t]^{1/2}+[(S'+C')^2+t]^{1/2}}\geqslant 0.\end{aligned}$$

Inequalities (A.5) and (A.6) follow from similar arguments.

To calculate ψ we need the following two lemmas (Wu and Lin 1975).

Lemma 2. For complex constants A and B

$$\int_{-\pi}^{\pi} \mathrm{d}\theta\ \ln|A\mathrm{e}^{\mathrm{i}\theta}+B| = 2\pi\ \ln\max\{|A|,|B|\}. \tag{A.7}$$

Lemma 3. For complex constants A, B and C

$$\begin{aligned}\int_{-\pi}^{\pi} &\mathrm{d}\theta\ \ln|A\ \mathrm{e}^{\mathrm{i}\theta}+B+C\,\mathrm{e}^{-\mathrm{i}\theta}| \\ &= 2\pi\ \ln|C| \qquad \text{if } |z_1|,|z_2|\geqslant 1 \\ &= 2\pi\ \ln|A| \qquad \text{if } |z_1|,|z_2|\leqslant 1 \\ &= 2\pi\ \ln|Az_1| \qquad \text{if } |z_1|\geqslant 1\geqslant|z_2|\end{aligned} \tag{A.8}$$

where z_1 and z_2 are the two roots of

$$Az^2+Bz+C=0.$$

Lemma 4. Consider a, b, b', c, c', f, f', g, g' as independent and positive parameters, then $F(\theta,\phi)\neq 0$ for all θ and ϕ if one of the following conditions is satisfied:

(1) $\quad a>b+b'+c+c'+f+f'+g+g'$

(2) $\quad b+b'>a+c+c'+f+f'+g+g' \quad$ and $\quad a>2(bb')^{1/2}$

(3) $\quad c+c'>a+b+b'+f+f'+g+g' \quad$ and $\quad a>2(cc')^{1/2}$

(4) $\quad f+f'+g+g'>a+b+b'+c+c' \quad$ and $\quad a>2(ff')^{1/2}+2(gg')^{1/2}$.

Proof. In case (1) we have

$$a>b+b'+c+c'+f+f'+g+g'\geqslant|F(\theta,\phi)-a|$$

which implies $F \neq 0$. In case (2) we have

$$(\sqrt{b}-\sqrt{b'})^2 > \varepsilon^2 + c + c' + f + f' + g + g'$$

where $\varepsilon^2 = a - 2(bb')^{1/2}$. *If* $F(\theta, \phi) = 0$. then

$$\begin{aligned} -b\,\mathrm{e}^{\mathrm{i}\theta} - b'\,\mathrm{e}^{-\mathrm{i}\theta} - 2(bb')^{1/2} &\equiv -(\sqrt{b}\,\mathrm{e}^{\mathrm{i}\theta/2} + \sqrt{b'}\,\mathrm{e}^{-\mathrm{i}\theta/2})^2 \\ &= \varepsilon^2 + c\,\mathrm{e}^{\mathrm{i}\phi} + c'\,\mathrm{e}^{-\mathrm{i}\phi} - f\,\mathrm{e}^{\mathrm{i}(\theta+\phi)} - f'\,\mathrm{e}^{-\mathrm{i}(\theta+\phi)} - g\,\mathrm{e}^{\mathrm{i}(\theta-\phi)} - g'\,\mathrm{e}^{\mathrm{i}(\phi-\theta)}. \end{aligned} \tag{A.9}$$

Equation (A.9) is impossible to satisfy for any θ and ϕ since

$$\begin{aligned} |\text{left-hand side of (A.9)}| &\geq (\sqrt{b}-\sqrt{b'})^2 \\ &> \varepsilon^2 + c + c' + f + f' + g + g' \geq |\text{right-hand side of (A.9)}|. \end{aligned}$$

Case (3) can be treated in the same way. In case (4), we define

$$a = \varepsilon^2 + 2(ff')^{1/2} + 2(gg')^{1/2} \qquad b = \varepsilon_1^2 + 2(fg)^{1/2}$$

$$b' = \varepsilon_2^2 + 2(f'g')^{1/2} \qquad c = \varepsilon_3^2 + 2(fg')^{1/2} \qquad c' = \varepsilon_4^2 + 2(f'g)^{1/2}$$

$$\alpha = \sqrt{f}\,\mathrm{e}^{\mathrm{i}(\theta+\phi)/2} \qquad \alpha\beta = (ff')^{1/2} \qquad \gamma = \sqrt{g}\,\mathrm{e}^{\mathrm{i}(\theta-\phi)/2} \qquad \gamma\delta = (gg')^{1/2}$$

we have

$$\begin{aligned} f + f' + g + g' > {} & 2[(ff')^{1/2} + (gg')^{1/2} + (fg)^{1/2} + (f'g')^{1/2} + (fg')^{1/2} + (f'g)^{1/2}] \\ & + \varepsilon^2 + \varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2 + \varepsilon_4^2 \end{aligned} \tag{A.10}$$

which implies

$$(\sqrt{f}+\sqrt{f'}+\sqrt{g}-\sqrt{g'})(\sqrt{f}+\sqrt{f'}-\sqrt{g}+\sqrt{g'})(\sqrt{f}-\sqrt{f'}+\sqrt{g}+\sqrt{g'})(\sqrt{f}-\sqrt{f'}-\sqrt{g}-\sqrt{g'}) > 0. \tag{A.11}$$

Inequality (A.11) implies that $\sqrt{f}$, $\sqrt{f'}$, $\sqrt{g}$, $\sqrt{g'}$ cannot form a polygon. Without loss of generality we assume

$$\sqrt{f} > \sqrt{f'} + \sqrt{g} + \sqrt{g'}.$$

If $F(\theta, \phi) = 0$, then

$$\begin{aligned} (\sqrt{f}-\sqrt{f'}-\sqrt{g}-\sqrt{g'})^2 &\leq |(\alpha-\beta-\gamma-\delta)^2| = |F(\theta,\phi) - (\alpha-\beta-\gamma-\delta)^2| \\ &= |4(\beta\gamma + \gamma\delta + \beta\delta) + \varepsilon^2 + \varepsilon_1^2\,\mathrm{e}^{\mathrm{i}\theta} + \varepsilon_2^2\,\mathrm{e}^{-\mathrm{i}\theta} + \varepsilon_3^2\,\mathrm{e}^{\mathrm{i}\phi} + \varepsilon_4^2\,\mathrm{e}^{-\mathrm{i}\phi}| \\ &\leq 4(f'g)^{1/2} + 4(gg')^{1/2} + 4(f'g')^{1/2} + \varepsilon^2 + \varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2 + \varepsilon_4^2 \end{aligned}$$

which contradicts (A.10).

Theorem 1

If a, $b+b'$, $c+c'$, and $f+f'+g+g'$ cannot form a polygon, then $F(\theta, \phi) \neq 0$ for all θ and ϕ which implies that ψ has no singularity and

$$\begin{aligned} \psi &= \tfrac{1}{2}\ln\max\{b_1, b_2, b'_1, b'_2\} && \text{if } b+b' > a+c+c'+f+f'+g+g' && \text{(A.12)} \\ &= \tfrac{1}{2}\ln\max\{c_1, c_2, c'_1, c'_2\} && \text{if } c+c' > a+b+b'+f+f'+g+g' && \text{(A.13)} \\ &= \tfrac{1}{2}\ln\max\{f, f', g, g'\} && \text{if } f+f'+g+g' > a+b+b'+c+c' && \text{(A.14)} \\ &= \frac{1}{2\pi}\int_0^{\pi} \mathrm{d}\phi\,\ln|Az_1| && \text{if } a > b+b'+c+c'+f+f'+g+g' && \text{(A.15)} \end{aligned}$$

where $|z_1(\phi)| \geqslant |z_2(\phi)|$ and z_1, z_2 are the roots of $Az^2 + Bz^2 + C = 0$ with

$$A = b - f\,\mathrm{e}^{\mathrm{i}\phi} - g\,\mathrm{e}^{-\mathrm{i}\phi} \qquad B = a + c\,\mathrm{e}^{\mathrm{i}\phi} + c'\,\mathrm{e}^{-\mathrm{i}\phi}$$
$$C = b' - f'\,\mathrm{e}^{-\mathrm{i}\phi} - g'\,\mathrm{e}^{\mathrm{i}\phi}.$$

Proof. To evaluate ψ we use lemma 3 to carry out the θ integration. Since

$$F(\theta, \phi) = A(\phi)\,\mathrm{e}^{\mathrm{i}\theta} + B(\phi) + C(\phi)\,\mathrm{e}^{-\mathrm{i}\theta} \neq 0$$

for all θ and ϕ, it is clear that $|z_{1,2}(\phi)| \neq 1$ for all ϕ. Let us first consider (A.12). We have

$$b + b' > 2(bb')^{1/2} + f + f' + g + g' \geqslant 2(bb')^{1/2} + 2(b_1 b_2)^{1/2} + 2(b_1' b_2')^{1/2}. \tag{A.16}$$

It follows from (A.16) that

$$(\sqrt{b_1} + \sqrt{b_2} + \sqrt{b_1'} - \sqrt{b_2'})(\sqrt{b_1} + \sqrt{b_2} - \sqrt{b_1'} + \sqrt{b_2'})(\sqrt{b_1} - \sqrt{b_2} + \sqrt{b_1'} + \sqrt{b_2'})$$
$$\times(\sqrt{b_1} - \sqrt{b_2} - \sqrt{b_1'} - \sqrt{b_2'})$$
$$> 4[(b_1 b_2)^{1/2} + (b_1' b_2')^{1/2}][(\sqrt{b_1} - \sqrt{b_2})^2 + (\sqrt{b_1'} - \sqrt{b_2'})^2] \geqslant 0.$$

Therefore $\sqrt{b_1}$, $\sqrt{b_2}$, $\sqrt{b_1'}$, $\sqrt{b_2'}$ do not form a polygon. Without loss of generality we assume $\sqrt{b_1} > \sqrt{b_2} + \sqrt{b_1'} + \sqrt{b_2'}$. It is straightforward to show that

$$b - f - g > b' - f' - g' \qquad |z_{1,2}(\phi)| < 1.$$

It follows from lemma 3 that

$$\psi = \frac{1}{4\pi} \int_{-\pi}^{\pi} \mathrm{d}\phi\, \ln|A(\phi)| = \tfrac{1}{2} \ln b_1.$$

The cases (A.13) and (A.14) can be treated in the same way. The case (A.15) follows from the fact that $|z_1(\phi)| > 1 > |z_2(\phi)|$.

Theorem 2

$$\psi = \frac{1}{8\pi^2} \int_0^{2\pi} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, \ln|a - b\,\mathrm{e}^{\mathrm{i}\theta} - b'\,\mathrm{e}^{-\mathrm{i}\theta}$$
$$-2\cos\phi[(cc')^{1/2} + (fg)^{1/2}\,\mathrm{e}^{\mathrm{i}\theta} + (f'g')^{1/2}\,\mathrm{e}^{-\mathrm{i}\theta}]| \tag{A.17}$$

if $c/c' = g'/f' = f/g$ and $a > b + b' + c + c' + f + f' + g + g'$

$$= \frac{1}{8\pi^2} \int_0^{2\pi} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, \ln[a - 2(bb')^{1/2}\cos\theta - 2(cc')^{1/2}\cos\phi - 2(ff')^{1/2}\cos(\theta+\phi)$$
$$-2(gg')^{1/2}\cos(\theta - \phi)] \tag{A.18}$$

if $bcf' = b'c'f$, $bc'g' = b'cg$ and $a > b + b' + c + c' + f + f' + g + g'$.

Proof. From theorem 1 we have

$$\psi = \frac{1}{4\pi} \operatorname{Re} \int_{-\pi}^{\pi} \mathrm{d}\phi\, \ln x_1(\phi)$$

where $|x_1| \geqslant |x_2|$ and $x_{1,2}$ satisfy $x^2 + Bx + AC = 0$. To show (A.17) we define

$$c/c' = \exp(2h) \qquad cc' = c_0^2 \qquad fg = d^2 \qquad f'g' = d'^2 \qquad y = 2\cosh(h + \mathrm{i}\phi)$$

and write

$$f(e^{i\phi}) = B^2 - 4AC = (c_0^2 - 4dd')y^2 + 2(ac_0 + 2bd' + 2b'd)y + a^2 - 4bb.$$

It can be shown that all four roots of $f(e^{i\phi})$ lie on the negative real axis. The inequality $a > b + b' + c + c' + f + f' + g + g'$ ensures that two roots lie outside the unit circle and two roots lie inside such that on the real axis these two pairs are separated by the interval $(-e^{-h}, -1)$. We then move the contour of the ϕ integration from $-\pi \to \pi$ to $-\pi + ih \to \pi + ih$ and obtain (A.17). Using identical argument and defining $c/c' = \exp(2h)$, $b/b' = \exp(2v)$, it can be shown that in the second case we can move the contour of the $\phi(\theta)$ integration from $-\pi \to \pi$ to $-\pi + ih(v) \to \pi + ih(v)$ and obtain (A.18).

Theorem 3

If a, $b + b'$, $c + c'$, and $f + f' + g + g'$ form a polygon, then $F(\theta, \phi) = 0$ has either one or three solutions (θ_i, ϕ_i) such that $-\pi \leqslant \theta_i(\phi_i) \leqslant \pi (i = 1, 2, 3)$ where (θ_i, ϕ_i) and $(-\theta_i, -\phi_i)$ are considered as the same solution. In the following special case

$$bcf' = b'c'f \qquad bc'g' = b'cg \qquad bb' \geqslant cc' = 4ff' = 4gg'$$

there exists exactly one solution. When the polygon degenerates into a straight line, $F(\theta, \phi) = 0$ if and only if

$$\begin{array}{ll} \theta = \phi = \pi & \text{if } a = b + b' + c + c' + f + f' + g + g' \\ \theta = \pi, \phi = 0 & \text{if } b + b' = a + c + c' + f + f' + g + g' \\ \theta = 0, \phi = \pi & \text{if } c + c' = a + b + b' + f + f' + g + g' \\ \theta = \phi = 0 & \text{if } f + f' + g + g' = a + b + b' + c + c'. \end{array}$$

Proof. $F(\theta, \phi) = 0$ implies

$$a + (b + b')\cos\theta + (c + c')\cos\phi - (f + f')\cos(\theta + \phi) - (g + g')\cos(\theta - \phi) = 0$$
$$(b - b')\sin\theta + (c - c')\sin\phi - (f - f')\sin(\theta + \phi) - (g - g')\sin(\theta - \phi) = 0. \qquad \text{(A.19)}$$

After some algebra we find

$$f(\cos\phi) = A\cos^4\phi + B\cos^3\phi + C\cos^2\phi + D\cos\phi + E = 0 \qquad \text{(A.20)}$$

where

$$A = 16[(cf' - c'f)(c'g' - cg) - (fg - f'g')^2]$$
$$B = 8a(c + c')(fg + f'g') - 16a(cf'g + c'fg') + 16(fg - f'g')[b(f + g) - b'(f' + g')] + 8(cf' - c'f)(bc - b'c') + 8(cg - c'g')(b'c - bc')$$
$$C = 4[bc - b'c' - a(g - g')][bc' - b'c - a(f - f')] + 4[c(f' + g) - c'(f + g')]^2 - 4[b(f + g) - b'(f' + g')]^2 + 4(cf' - cg + c'g' - c'f)[a(b - b') - (c - c')(f + f' - g - g')] - 8(fg - f'g')[b^2 - b'^2 + (f - g)^2 - (f' - g')^2]$$
$$f(1) = A + B + C + D + E = (f + g - f' - g' - b + b')^2[(a + c + c')^2 - (b + b' - f - f' + g + g')^2]$$
$$f(-1) = A - B + C - D + E = (f + g - f' - g' + b - b')^2[(a - c - c')^2 - (b + b' + f + f' + g + g')^2].$$

If a, $b+b'$, $c+c'$, $f+f'+g+g'$ form a polygon, we have

$$f(1)\geqslant 0\geqslant f(-1)$$

which implies that $f(\cos\phi)=0$ has either one or three solutions. When the polygon degenerates into a straight line, $F(\theta,\phi)=0$ has only one solution. For example, if $a=b+b'+c+c'+f+f'+g+g'$, then we have

$$\begin{aligned} a &= -b\,\mathrm{e}^{\mathrm{i}\theta}-b'\,\mathrm{e}^{-\mathrm{i}\theta}-c\,\mathrm{e}^{\mathrm{i}\phi}-c'\,\mathrm{e}^{-\mathrm{i}\phi}+f\,\mathrm{e}^{\mathrm{i}(\theta+\phi)}+f'\,\mathrm{e}^{-\mathrm{i}(\theta+\phi)}+g\,\mathrm{e}^{\mathrm{i}(\theta-\phi)}+g'\,\mathrm{e}^{\mathrm{i}(\phi-\theta)} \\ &= b+b'+c+c'+f+f'+g+g' \end{aligned}$$

which implies $\mathrm{e}^{\mathrm{i}\theta}=\mathrm{e}^{\mathrm{i}\phi}=-1$. Other cases can be proved similarly. In the special case of ($bcf'=b'c'f$, $bc'g'=b'cg$, $bb'\geqslant cc'=4ff'=4gg'$), we denote

$$\begin{array}{llll} c=c_0\,\mathrm{e}^{u} & c'=c_0\,\mathrm{e}^{-u} & b=b_0\,\mathrm{e}^{-v} & b'=b_0\,\mathrm{e}^{v} \\ f=f_0\,\mathrm{e}^{u-v} & f'=f_0\,\mathrm{e}^{v-u} & g=f_0\,\mathrm{e}^{-u-v} & g'=f_0\,\mathrm{e}^{u+v}. \end{array}$$

Without loss of generality we assume $u\geqslant v\geqslant 0$. It is straightforward to show that $f''(x)<0$ for $|x|\leqslant 1$ if either $b_0\geqslant c_0=2f_0$ or $c_0\geqslant b_0=2f_0$. Therefore $f(x)$ is a monotonic function of x if $|x|\leqslant 1$ and $f(\cos\theta)$ has exactly one solution.

Theorem 4

If a, $b+b'$, $c+c'$, and $f+f'+g+g'$ form a polygon and $F(\theta,\phi)$ has only one solution, we have

$$\begin{aligned} \psi &= \frac{1}{2\pi}\int_0^{|\phi_1|}\ln|z_1(\phi)|\,\mathrm{d}\phi+\tfrac{1}{2}\ln\max\{b_1,b_2,f,g\} && \text{if } b+f+g>b'+f'+g' \\ &= \frac{1}{2\pi}\int_0^{|\phi_1|}\ln|z_2(\phi)^{-1}|\,\mathrm{d}\phi+\tfrac{1}{2}\ln\max\{b_1',b_2',f',g'\} && \text{if } b'+f'+g'>b+f+g \end{aligned} \tag{A.21}$$

where $z_{1,2}$ are defined in theorem 1.

Proof. It is simple to show that $|z_1|>1>|z_2|$ at $\phi=0$ and $|z_{1,2}|<(>)1$ at $\phi=\pi$ if $b+f+g>(<)\ b'+f'+g'$. Therefore we have

$$\begin{array}{ll} |z_1|>1>|z_2| & \text{if } 0\leqslant\phi<|\phi_1| \\ |z_{1,2}|<(>)1 & \text{if } |\phi_1|<\phi\leqslant\pi \text{ and } b+f+g>(<)b'+f'+g' \end{array}$$

since $|z_{1,2}(\phi)|\neq 1$ if $\phi\neq\pm\phi_1$. It follows from lemma 3 that

$$\begin{aligned} \psi &= \frac{1}{2\pi}\int_0^{|\phi_1|}\ln|Az_1|\,\mathrm{d}\phi+\frac{1}{2\pi}\int_{|\phi_1|}^{\pi}\ln|A|\,\mathrm{d}\phi && \text{if } b+f+g>b'+f'+g' \\ &= \frac{1}{2\pi}\int_0^{|\phi_1|}\ln|C/z_2|\,\mathrm{d}\phi+\frac{1}{2\pi}\int_{|\phi_1|}^{\pi}\ln|C|\,\mathrm{d}\phi && \text{if } b'+f'+g'>b+f+g \end{aligned}$$

which reduces to (A.21).

Note that near the critical point where the polygon almost degenerates into a straight line, $F(\theta,\phi)=0$ has only one solution and theorem 4 applies. Equation (A.21) implies that the singular part of ψ behaves as $\Delta^{3/2}$ as $\Delta\to 0^+$ where Δ is given by equation (21).

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