Journal of Statistical Physics, Vol. 26, No. 3, 1981

Rogers–Ramanujan Identities in the Hard Hexagon Model

R. J. Baxter[1,2]

Received March 27, 1981

The hard hexagon model in statistical mechanics is a special case of a solvable class of hard-square-type models, in which certain special diagonal interactions are added. The sublattice densities and order parameters of this class are obtained, and it is shown that many Rogers–Ramanujan-type identities naturally enter the working.

KEY WORDS: Statistical mechanics; lattice statistics; Rogers–Ramanujan identities; hard hexagon model; combinatorial identities; basic hypergeometric series.

1. INTRODUCTION AND SUMMARY

In an earlier paper,(1) I outlined the solution of the hard hexagon lattice model in statistical mechanics, and gave the principal results. I mentioned therein that various Rogers–Ramanujan-type identities occur naturally in the calculation of the sublattice densities and order parameters. Here I want to show how this comes about.

In Section 2 I define a generalized hard-hexagon model (namely, the hard square model with diagonal interactions), state the condition under which this has been solved, and introduce the variables x, r, w that will be used in the following sections. Then in Sections 3 and 4 I attempt to give some idea how one calculates the sublattice densities ρ_k, culminating in the formula (36). A more complete description of this working, as well as the calculation of the partition function, will be published later.(2)

Supported in part by the National Science Foundation under Grant No. PHY-79-06376A01.

[1] Department of Theoretical Physics, Research School of Physical Sciences, The Australian National University, Canberra, A.C.T., 2600, Australia.

[2] Part of this work was performed while the author was a visiting professor at the Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11794.

0022-4715/81/1100-0427$03.00/0

In Section 5 I show explicitly how the various Rogers–Ramanujan-type identities occur in the evaluation of this formula. This section needs the prior equations (15) and (28)–(38); otherwise it can be read independently of the rest of the paper.

Finally, in Section 6 I briefly mention the critical behavior of the model.

2. DEFINITIONS

Start by considering a hard square lattice gas with diagonal interactions. Let the lattice have N sites, labeled $i = 1, \ldots, N$. With each site i associate an occupation number (or "spin") σ_i, with value 0 or 1. (The value 0 corresponds to the site being empty; the value 1 to it containing a particle.) Impose the condition that if i and j are adjacent sites, then σ_i and σ_j cannot both be 1, i.e.,

$$\sigma_i \sigma_j = 0 \qquad \text{if } i \text{ and } j \text{ are nearest neighbors} \tag{1}$$

(This corresponds to the "hard square" condition that no two particles can be adjacent.)

The set $\sigma = \{\sigma_1, \ldots, \sigma_N\}$ then specifies the state of the system. The probability of a state is

$$p(\sigma) = Z^{-1} \prod_{(i,j,k,l)} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{2}$$

where the product is over all faces of the lattice, i, j, k, l being the four sites round the face, arranged as in Fig. 1. The function $W(a,b,c,d)$ is given by

$$\begin{aligned} W(a,b,c,d) &= z^{(a+b+c+d)/4} e^{Lac+Mbd} t^{-a+b-c+d} \quad \text{if } ab = bc = cd = da = 0 \\ &= 0 \qquad \text{otherwise} \end{aligned} \tag{3}$$

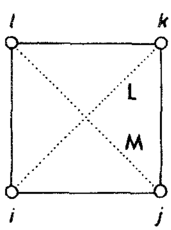

Fig. 1. A typical face of the square lattice, i, j, k, l being the surrounding sites. The diagonals associated with the interaction coefficients L, M in (3) are indicated.

This definition ensures that a state has zero probability if it violates the rule (1). The parameter t plays a trivial role in the working, since it cancels out of the expression (2) for $p(\sigma)$: even so, it simplifies some of the following discussion to include the t factor in (3).

As well as t, the numbers z, L, M (the activity and the interaction coefficients) are at our disposal: normally we require them to be real, and z to be positive. The number Z is a normalization factor (known as the partition function), which is chosen to ensure that $\sum p(\sigma) = 1$, so

$$Z = \sum_{\sigma} \prod_{(i,j,k,l)} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{4}$$

The σ sum is over all values of $\sigma_1, \ldots, \sigma_N$, subject to the condition (1), and possibly subject to the spins on the outer boundary of the lattice being given prescribed values. In this paper I am interested in calculating the average value of σ_i for some particular site i, say site 1. This is defined to be

$$\langle \sigma_1 \rangle = \sum_{\sigma} \sigma_1 p(\sigma) \tag{5}$$

From (2) and (4) we see that

$$\langle \sigma_1 \rangle = \frac{\sum_{\sigma} \sigma_1 \prod_{(i,j,k,l)} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l)}{\sum_{\sigma} \prod_{(i,j,k,l)} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l)} \tag{6}$$

(This average is the local density at site 1.)

It turns out that $\langle \sigma_1 \rangle$ can be calculated (in the limit when the site 1 is in the middle of an infinitely large lattice), provided that

$$z = (1 - e^{-L})(1 - e^{-M})/(e^{L+M} - e^{L} - e^{M}) \tag{7}$$

This restriction is satisfied automatically in the limit $L \to 0$, $M \to -\infty$. This case is of particular interest since it corresponds to no interaction along NE–SW diagonals, but complete repulsion between NW–SE diagonally adjacent particles. The model then reduces to a triangular lattice gas with nearest-neighbor exclusion, i.e., "hard hexagons."

The case $L = M = 0$ ("hard squares") does not satisfy (7) and has not been solved exactly, though approximate results are available.[3–5]

As I have indicated earlier,[1] one is led to define

$$\Delta = z^{-1/2}(1 - z e^{L+M}) \tag{8}$$

and to regard Δ as a constant, and L, M as variables satisfying the restriction (8). Eliminating z between (7) and (8) gives a symmetric biquadratic relation between e^{L} and e^{M}. This can conveniently be parametrized by introducing elliptic functions. We have to distinguish the cases $|\Delta| < \Delta_c$

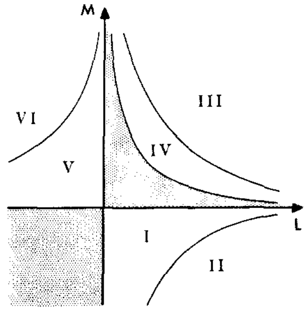

Fig. 2. The six regimes in (L, M) space. Shaded regions correspond to z in (7) being negative, so are "unphysical." The (I, II), (III, IV), and (V, VI) regime boundaries occur when $|\Delta| = \Delta_c$.

and $|\Delta| > \Delta_c$, where

$$\Delta_c^{-2} = \left[\tfrac{1}{2}(\sqrt{5} + 1) \right]^5 = \tfrac{1}{2}(11 + 5\sqrt{5}) = 11.09017 \ldots \tag{9}$$

Altogether there are six regimes in (L, M) space to consider, as indicated in Fig. 2. In regimes I, ..., VI we have $\Delta > \Delta_c$, $0 < \Delta < \Delta_c$, $-\Delta_c < \Delta < 0$, $\Delta < -\Delta_c$, $\Delta > \Delta_c$, $0 < \Delta < \Delta_c$, respectively. Regimes V and VI differ from I and II only by interchanging L and M (which is equivalent to rotating the lattice through 90°), so they will not be further considered herein.

Note that $|\Delta| = \Delta_c$ on the boundary between regimes I and II, and between III and IV. These are the "critical lines" of the model.

We parametrize L, M, t as functions of three new variables x, w, r, as follows. Define

$$g = \prod_{n=1}^{\infty} \frac{(1 - x^{5n-4})(1 - x^{5n-1})}{(1 - x^{5n-3})(1 - x^{5n-2})} \tag{10a}$$

and, for $j = 0, 1, 2, 3, 4$,

$$f_j = \prod_{n=1}^{\infty} (1 - x^{5n-5+j}w)(1 - x^{5n-j}w^{-1}) \tag{10b}$$

(Note that $f_0, \ldots, f_4$ depend on w: basically they are elliptic theta functions.) In regimes I and IV we can parametrize (7) and (8) as follows:

$$\begin{aligned} e^L &= -wf_1f_4/(xgf_0^2), \qquad e^M = f_1f_3/(gf_2^2) \\ z &= -xg^3f_0^2f_2^2/f_1^4, \qquad t = r\left[-gf_2^2/(xf_0^2)\right]^{1/4} \\ \Delta^{-2} &= -xg^5 \end{aligned} \tag{11}$$

the parameters x, w, r being real and satisfying

$$\begin{array}{lll} \text{Regime I:} & 0 > x > -1, & 1 > w > x^2 \\ \text{Regime IV:} & 0 > x > -1, & x^{-2} > w > 1 \end{array} \tag{12}$$

In regimes II and III we use the alternative parametrization:

$$\begin{aligned} e^L &= wg f_2 f_3/(xf_0^2), \qquad e^M = g f_1 f_2/(wf_4^2) \\ z &= xf_0^2 f_4^2/(g^3 f_2^4), \qquad t = r\left[f_4^2/(xg f_0^2)\right]^{1/4} \\ \Delta^{-2} &= x^{-1} g^{-5} \end{aligned} \tag{13}$$

$$\begin{array}{lll} \text{Regime II:} & 0 < x < 1, & x^{-1} > w > 1 \\ \text{Regime III:} & 0 < x < 1, & 1 > w > x \end{array} \tag{14}$$

This parametrization ensures that e^L and e^M are single-valued functions of w, while Δ is independent of w: Δ depends only on x.

As $|x| \to 1$, $|\Delta|$ tends to Δ_c and the point (L, M) approaches the I–II or III–IV inter-regime boundary in Fig. 2. These are the "critical lines" of the model.

As $x \to 0$, there are a few states σ whose probabilities $p(\sigma)$ tend to nonzero limits; the probabilities of all other states become zero. I shall call these states that survive the limit $x \to 0$ the "ground states."

In regime I and III there is just one ground state, namely, $\sigma = \{0, 0, \ldots, 0\}$, where all occupation numbers are zero (the vacuum). In regime IV there are two ground states: that shown in Fig. 3a, and the one obtainable from it by shifting all particles one site to the right. In regime II

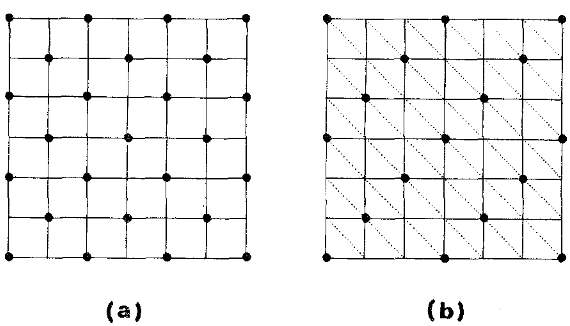

Fig. 3. Typical ground states in regimes IV and II, respectively. Solid circles denote particles ($\sigma_i = 1$), unmarked sites are empty ($\sigma_i = 0$). The other ground states can be obtained by shifting all particles one site to the right (or to the left).

there are three ground states: the one in Fig. 3b, and the two obtainable from it by shifting all particles to the right, or all to the left.

The ground states in IV are the close-packed arrangements of the hard-square lattice gas. If we add NW–SE diagonals to the square lattice, as in Fig. 3b, we transform it into the triangular lattice gas: the ground states in II can then be seen to be the close-packed arrangements of the hard-hexagon lattice gas (triangular lattice gas with nearest-neighbor exclusion). I therefore refer to the ground states in IV as "square-ordered," those in II as "triangular-ordered."

We shall find it useful to define the functions (for $|x| < 1$)

$$Q(x) = \prod_{n=1}^{\infty} (1 - x^n) \tag{15a}$$

$$P(x) = \prod_{n=1}^{\infty} (1 - x^{2n-1}) \tag{15b}$$

$$G(x) = \prod_{n=1}^{\infty} \left[(1 - x^{5n-4})(1 - x^{5n-1})\right]^{-1} \tag{15c}$$

$$H(x) = \prod_{n=1}^{\infty} \left[(1 - x^{5n-3})(1 - x^{5n-2})\right]^{-1} \tag{15d}$$

Then $g = H(x)/G(x)$, so the equations (11) and (13) for Δ can be written as

$$\begin{aligned} \Delta^{-2} &= -x\left[H(x)/G(x)\right]^5 \qquad \text{in I and IV} \\ &= x^{-1}\left[G(x)/H(x)\right]^5 \qquad \text{in II and III} \end{aligned} \tag{16}$$

The reader who is acquainted with the Rogers–Ramanujan identities should already feel he or she is entering familiar territory, even though all we have done so far is to parametrize the relations (7) and (8).

Given L, M, and t, we can regard z, Δ as defined by (7) and (8), x by (16), and w and r by (11) or (13). Alternatively, we can regard x, w, r as given, and L, M, z, t, Δ as defined by (11) or (13). From now on I shall adopt the latter viewpoint.

3. CORNER TRANSFER MATRICES (CTMs)

I calculate $\langle \sigma_1 \rangle$ by introducing "corner transfer matrices." Consider a square lattice of $m + 1$ rows and columns, as in Fig. 4a. Fix the spins on the lower and right-hand boundary sites (those denoted by crosses) to have their ground-state values. (In regimes II and IV we must specify which ground state.) Fix those on the left-hand and upper boundary sites (denoted by open circles) to have the values $\mu_1, \ldots, \mu_m$ and $\mu_1', \ldots, \mu_m'$, as

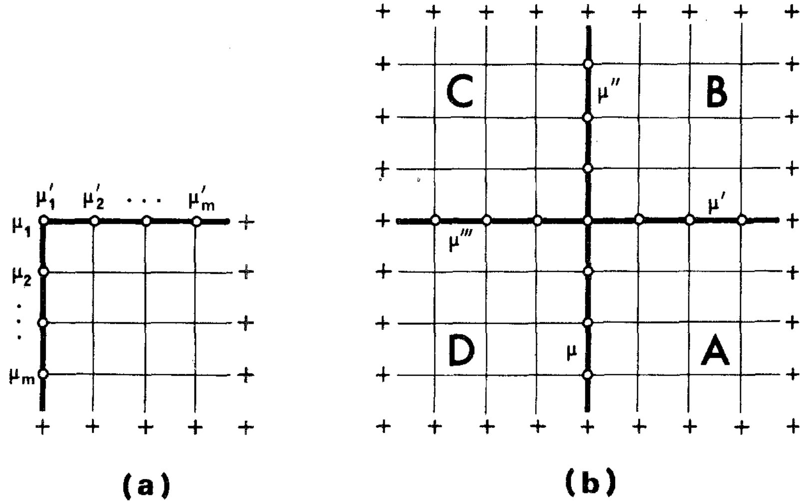

Fig. 4. The lattices whose partition functions are $A_{\mu\mu'}$, Z in (17), (18), respectively. The latter is made up of four quadrants (or "corners"), each of the same size as the former. It has $2m + 1$ rows and $2m + 1$ columns; $\sigma_1 = \mu_1$ is the center site. Spins on outer boundary sites (denoted by crosses) are fixed at their values for some particular ground state.

indicated. Since μ_1 and μ_1' are both the value of the top-left spin, we must have $\mu_1 = \mu_1'$; otherwise $\mu_1, \ldots, \mu_m$ and $\mu_1', \ldots, \mu_m'$ are at our disposal. Let us write μ for the set $\{\mu_1, \ldots, \mu_m\}$, and μ' for $\{\mu_1', \ldots, \mu_m'\}$.

The partition function is given by (4), where the sum is now only over spins on interior sites of the lattice in Fig. 4a. Plainly the partition function depends on μ and μ', so we can write it as $A_{\mu\mu'}$. It is useful to adopt the convention that μ_1 may differ from μ_1', but $A_{\mu\mu'}$ is then zero. Thus in general

$$A_{\mu\mu'} = \delta(\mu_1, \mu_1') \sum_{\sigma} \prod_{(i,j,k,l)} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{17}$$

Here $\delta(a,b) = 1$ if $a = b$; $= 0$ otherwise.

By rotating Fig. 4a anticlockwise through 90°, 180°, 270°, we can similarly define quantities $B_{\mu\mu'}$, $C_{\mu\mu'}$, $D_{\mu\mu'}$, respectively.

Now consider the lattice in Fig. 4b, with $2m + 1$ rows and columns. Divide it into four quadrants, as indicated by the heavy lines. Fix the boundary spins (on sites shown by crosses) to have their values for some particular ground state. Let $\mu_1 = \mu_1' = \mu_1'' = \mu_1'''$ be the spin at the center of the lattice; let $\mu = \{\mu_1, \ldots, \mu_m\}$ be the m spins on the lower half of the heavy vertical line (on sites marked by open circles), counting from the center downwards; let μ' be the spins on the right half of the heavy horizontal line, counting outwards; and similarly for μ'' and μ''', as indicated.

The partition function Z is given by (4): note that the summand is a product of $4m^2$ factors, one for each face. It can certainly be grouped into a product of four terms, one being the product of the factors of the faces in the lower-right quadrant, another for the upper-right quadrant, and so on. Summing over all internal spins in Fig. 4b, other than those on the heavy lines, it follows that

$$Z = \sum_{\mu} \sum_{\mu'} \sum_{\mu''} \sum_{\mu'''} A_{\mu\mu'} B_{\mu'\mu''} C_{\mu''\mu'''} D_{\mu'''\mu} \tag{18}$$

the factor $A_{\mu\mu'}$ coming from the lower-right quadrant, $B_{\mu'\mu''}$ from the upper-right quadrant, and so on, as indicated in Fig. 4b.

Strictly, the summation in (18) is subject to the restriction $\mu_1 = \mu_1' = \mu_1'' = \mu_1'''$, since each is the value of the center spin. However, the Kronecker delta in (17) ensures that the summand is zero if this condition is violated, so no harm is done by abandoning the restriction. It is then apparent that (18) may be written as

$$Z = \operatorname{Tr} ABCD \tag{19}$$

where A is the matrix with entries $A_{\mu\mu'}$ in positions (μ, μ'); and similarly for B, C, D. These matrices are known as the *corner transfer matrices*.

Now look at the expression (6), still using the lattice of Fig. 4b, and taking σ_1 to be the center spin. The denominator in (6) is just the partition function Z in (19). The numerator is similar, but contains an extra factor σ_1 in the summand. Since $\sigma_1 = \mu_1 = \mu_1' = \mu_1'' = \mu_1'''$, the numerator is given by (18), but with an extra factor μ_1 in the summand therein. It follows that (6) can be written as

$$\langle \sigma_1 \rangle = \frac{\operatorname{Tr} SABCD}{\operatorname{Tr} ABCD} \tag{20}$$

where S is the diagonal matrix with entries

$$S_{\mu\mu'} = \mu_1 \prod_{i=1}^{m} \delta(\mu_i, \mu_i') \tag{21}$$

The Kronecker delta in (17) ensures that the matrices A, B, C, D are all block-diagonal, having one block of nonzero entries with $\mu_1 = \mu_1' = 0$ and another block with $\mu_1 = \mu_1' = 1$. They therefore all commute with S.

The next step is to go to a representation in which the corner matrices are diagonal. More precisely, let λ_p be the rth largest eigenvalue of the product matrix $ABCD$, and let x_p be the corresponding eigenvector, normalized so that $x_p^T y_p = 1$. Then we can define vectors y_p, z_p, t_p, normalized so that $y_p^T y_p = z_p^T z_p = t_p^T t_p = 1$, and such that

$$\begin{aligned} Ay_p &= \alpha_p x_p, \qquad Bz_p = \beta_p y_p \\ Ct_p &= \gamma_p z_p, \qquad Dx_p = \delta_p t_p \end{aligned} \tag{22}$$

where $\alpha_p, \beta_p, \gamma_p, \delta_p$ are scalars, and $\lambda_p = \alpha_p \beta_p \gamma_p \delta_p$. We can choose the vectors x_p, y_p, z_p, t_p so that either they all have nonzero entries only for rows with $\mu_1 = 0$, or they all have nonzero entries only for rows with $\mu_1 = 1$. Setting $\zeta_p = 0$ in the former case, and $\zeta_p = 1$ in the latter, it follows that

$$\begin{aligned} Sx_p &= \zeta_p x_p, & Sy_p &= \zeta_p y_p \\ Sz_p &= \zeta_p z_p, & St_p &= \zeta_p t_p \end{aligned} \tag{23}$$

It is convenient to work with the ratios

$$\begin{aligned} a_p &= \alpha_p / \alpha_1, & b_p &= \beta_p / \beta_1 \\ c_p &= \gamma_p / \gamma_1, & d_p &= \delta_p / \delta_1 \end{aligned} \tag{24}$$

Since $\lambda_1 = \alpha_1 \beta_1 \gamma_1 \delta_1$ is the largest eigenvalue of $ABCD$, $a_p b_p c_p d_p$ cannot be greater than one.

The trace of a matrix is the sum of its eigenvalues. Dividing the numerator and denominator of (20) by $\alpha_1 \beta_1 \gamma_1 \delta_1$, it follows that

$$\langle \sigma_1 \rangle = \sum_p \zeta_p a_p b_p c_p d_p \Big/ \sum_p a_p b_p c_p d_p \tag{25}$$

This is the formula that will be used in the rest of this paper. However, before leaving the corner transfer matrices it is worth noting that they do have some symmetry properties.

From (3), the function $W(a,b,c,d)$ is unaltered by interchanging a with c, corresponding to reflecting about the NW–SE diagonal. The various possible ground states (the vacuum and those shown in Fig. 3) also have this reflection symmetry. From (17), remembering that the spins on the lower and right boundaries in Fig. 4a are fixed at their ground-state values, it follows that $A_{\mu\mu'} = A_{\mu'\mu}$, i.e., A is a symmetric matrix. Similarly from the analogs of (17) for B, C, and D, we find that

$$A^T = A, \qquad C^T = C, \qquad B^T = D \tag{26}$$

In regimes I, III, and IV there is also a reflection symmetry about the NE–SW diagonal, implying that $B^T = B$, $D^T = D$, $A^T = C$. However, this additional symmetry is violated by the ground states obtained from Fig. 3b by uniform translation, so it does not always apply in regime II.

4. EIGENVALUES OF THE CTMs

So far everything I have said has been rigorously correct: in particular, (25) is exactly true for all positive integers m. Now I assume that, for any fixed value of $p, s_p, a_p, b_p, c_p, d_p$ all tend to finite limits (in general nonzero) as $m \to \infty$. Further, if these limiting values are substituted into (25), then the resulting infinite sums are convergent, and converge to the limiting large-m values of the original sums.

This is not of course obvious, but is plausible and seems to be correct for quite general functions $W(a,b,c,d)$. One can write down equations satisfied by the CTMs, go to a representation in which A,B,C,D are diagonal, and take the limit in which the lattice is infinitely large and the matrices are of infinite dimensionality.[6] The nature of this limit has been studied for the zero-field Ising model by Tsang.[7] Numerical and series-expansion studies of the CTM equations have been made for monomer-dimers,[8] the Potts model,[9] the Ising model in a field,[10] the hard square lattice gas,[5] and hard hexagons.[11] All these calculations are fully consistent with the above assumptions: I believe them to be true.

If these assumptions are accepted (together with similar ones about the existence of limiting values of related quantities, and the interchangeability of limits), then for hard hexagons (and the eight-vertex model) the limiting values of a_p, b_p, c_p, d_p can be calculated indirectly. This is shown elsewhere.[2,12] Very briefly, the trick is to regard the matrices A,B,C,D as functions of r and w, so we can write them as $A(r,w)$, $B(r,w)$, $C(r,w)$, $D(r,w)$. [Since r enters the weight function $W(a,b,c,d)$ only via the t in (3), the r dependence is rather trivial: t cancels out of the summand in (17), except for a factor t^{μ_1} coming from the top-left site in Fig. 4a. This means that the $\mu_1 = \mu_1' = 0$ diagonal block of $A(r,w)$ is actually independent of r, while the $\mu_1 = \mu_1' = 1$ block is simply proportional to r; similarly for B^{-1}, C, D^{-1}. Even so, it is still helpful to think of r as a variable.]

Assuming that various limits can be interchanged, one can show for m large, for any numbers w, w' lying in the appropriate interval (12) or (14), and for all r, r', that

$$A(r,w)B(r',w') = k(w,w')T(r/r',w/w') \tag{27}$$

Here $k(w,w')$ is a scalar and $T(r,w)$ is a matrix whose elements are functions of r and w. [This is basically equation (4.13d) of Ref. 12, w being the exponential of a constant times u.]

Corresponding equations apply to the product of B with C, C with D, and D with A. From these it follows that the vectors x_p, y_p, z_p, t_p are independent of r and w, and that $a_p, b_p^{-1}, c_p, d_p^{-1}$ are each proportional to $r^{\zeta}w^{n}$, where ζ, n and the proportionality coefficients can depend on p and the parameter x, but not on r and w. In fact ζ is the ζ_p in (23); n is the same for a_p, b_p^{-1}, c_p and d_p^{-1}.

The proportionality coefficients can be evaluated either by considering special values of w (notably $w = 1$), or by using the inversion relation (31) in Ref. 1 (noting that A,B therein are replaced here by B,A). The exponents n (one for each value of p) can be shown to be integers. [This is basically just a corollary of the fact that $z^{1/2}$, e^{L} and e^{M}, as given by (11) or (13), are Laurent-expandable in powers of w.] Assuming that the exponents n do not change discontinuously with x inside a regime (there is no reason to suppose that they do), they must therefore be independent of x, so they can be evaluated from an appropriate small-x limit. The eigenvalues a_p, b_p, c_p, d_p are then completely determined.

When considering this small-x limit, it is necessary to take account of the boundary condition, namely, that all the spins on the boundary sites in Fig. 4b (those indicated by crosses) be fixed at the values they would have in one of the ground states. (This condition is necessary for the existence and interchangeability of the large-m limits.)

It is also convenient to have names for the corresponding ground-state values of some of the interior spins. In particular, consider the spins on the lower-half of the central vertical line in Fig. 4b, i.e., those with values $\mu = \{\mu_1, \ldots, \mu_m\}$. Let $s = \{s_1, s_2, \ldots\}$ be their values for the ground state under consideration.

In regimes I and III there is only one ground state, namely, the vacuum. Thus

$$\text{I and III:} \quad s_j = 0, \qquad \text{all integers } j \tag{28a}$$

In regime IV (square ordering) there are two ground states: that shown in Fig. 3a, and the one obtained from it by shifting all particles one site to the right. This means that

$$\text{IV:} \quad s_{2j+k} = 1, \qquad s_{2j+k+1} = 0, \qquad \text{all integers } j \tag{28b}$$

where $k = 1$ for the first ground state, $k = 2$ for the second. In regime II (triangular ordering) there are three ground states: that shown in Fig. 3b, and the two obtained from it by uniform translation of all the particles. Thus

$$\text{II:} \quad s_{3j+k} = 1, \qquad s_{3j+k\pm 1} = 0, \qquad \text{all integers } j \tag{28c}$$

where $k = 1$, 2 or 3, depending on the ground state.

When evaluating a_p, b_p, c_p, d_p, we therefore first specify the regime. Then in regimes IV and II we also specify the ground state: this can be done by giving the value of k in (28b) or (28c). Altogether there are seven cases to consider (1 + 1 + 2 + 3).

To express the results, let $\sigma = \{\sigma_1, \ldots, \sigma_m\}$ be a set of m spins, each with value 0 or 1, satisfying the constraint

$$\sigma_j \sigma_{j+1} = 0, \qquad j = 1, \ldots, m \tag{29}$$

where $\sigma_{m+1} = s_{m+1}$. Define

$$\begin{aligned} r_0^2 &= -xg^{-1}, \qquad x^{-1}g, \qquad xg, \qquad -x^{-1}g^{-1} \\ w_0 &= -x^3, \qquad x^{-3/2}, \qquad x, \qquad x^{-2} \end{aligned} \tag{30}$$

in regimes I, II, III, IV, respectively. Set

$$n(\sigma) = \sum_{j=1}^{m-1} j(\sigma_{j+1} - s_{j+1}) \qquad \text{in I and IV}$$
$$= \sum_{j=1}^{m} j(\sigma_{j+1} - \sigma_j\sigma_{j+2} - s_{j+1} + s_js_{j+2}) \qquad \text{in II and III} \tag{31}$$

where

$$\sigma_{m+1} = s_{m+1} \quad \text{and} \quad \sigma_{m+2} = s_{m+2} \tag{32}$$

Here $s_1, s_2, \ldots$ are the ground-state spin values in (28). In regimes II and IV they depend on the value of k in (28c) and (28d), so $n(\sigma)$ therefore also depends on k. [The explicit dependence on s in (31) is rather trivial, merely contributing an additive constant to $n(\sigma)$: it is the boundary condition (32) that is important.]

Using these definitions, it turns out that $\zeta_p, a_p, b_p, c_p, d_p$ are

$$\begin{aligned} \zeta_p &= \sigma_1 \\ a_p &= c_p = r^{\sigma_1 - s_1} w^{n(\sigma)} \\ b_p &= d_p = (r_0/r)^{\sigma_1 - s_1}(w_0/w)^{n(\sigma)} \end{aligned} \tag{33}$$

where now it is natural to label the eigenvalues by the spin-set σ, rather than the integer p: put another way, we can construct a one-to-one correspondence between positive integers p and spin-sets σ satisfying (29). (Remember that p is the position of the eigenvalue product $a_pb_pc_pd_p$ in a decreasing sequence.) It is always true that $p = 1$ corresponds to $\sigma = s$. Further, for any value of p, there exists an integer l (independent of m) such that if $m > l$, then $\sigma_j = s_j$ for $j = l + 1, \ldots, m$.

Substituting the expressions (32) into (25), it follows that

$$\langle \sigma_1 \rangle = \sum_\sigma \sigma_1 r_0^{2\sigma_1} w_0^{2n(\sigma)} \Big/ \sum_\sigma r_0^{2\sigma_1} w_0^{2n(\sigma)} \tag{34}$$

where the sums are over all values of $\sigma = \{\sigma_1, \ldots, \sigma_m\}$ satisfying (29). Note that r and w have cancelled out of this expression. (This is to be expected because two models with different L, M, t, but the same Δ, have row-to-row transfer matrices that commute. Their eigenvectors ψ therefore depend only on Δ, i.e., on x. Since $\langle \sigma_1 \rangle = \psi^T \sigma_1 \psi$, where ψ is the maximal eigenvector of the transfer matrix, it therefore depends only on x.)

The results (33) and (34) are only true in the limit $m \to \infty$ (p fixed). However, it is convenient here to regard m as large but finite, and to defer explicitly taking the $m \to \infty$ limit until later.

Apart from boundary conditions, the model is translation invariant. If we consider a finite number of sites i near the center of the lattice, and then let the lattice become infinite in both directions ($m \to \infty$ in Fig. 4b), we might expect the disturbing effect of the boundary conditions to disappear, and the sites to become equivalent.

In regimes I and III (the disordered regimes), exactly this happens. The local density $\langle \sigma_i \rangle$ is the same for all sites i, so $\langle \sigma_1 \rangle = \rho$, where ρ is the mean density of particles.

In regime IV (square ordering) it does not happen, and translation invariance is said to be "spontaneously broken." In this case $\langle \sigma_i \rangle$ has one value if i lies on the sublattice of solid circles in Fig. 3a, another value if it lies on the other sublattice. These two values are the sublattice densities ρ_1 and ρ_2, respectively. The total mean density is $\rho = \frac{1}{2}(\rho_1 + \rho_2)$.

Regime II (triangular ordering) is similar except that now there are three sublattices: the sublattice of solid circles in Fig. 3b, the sublattice of sites that are one space to the right of a solid circle, and the sublattice of sites that are one space to the left of a solid circle. Then $\langle \sigma_i \rangle$ has one value if i lies on the first sublattice, another value for the second sublattice, and another value for the third. These values are the three sublattice densities ρ_1, ρ_2, ρ_3, and the total mean density is $\rho = (\rho_1 + \rho_2 + \rho_3)/3$. Here we arrange the boundary conditions so that sublattice 1 is occupied preferentially: it is still true that sublattices 2 and 3 are equivalent, and hence that $\rho_2 = \rho_3$.

In our calculation we have considered a fixed site (site 1 at the center of Fig. 4b), but can vary the preferred sublattice by varying the boundary conditions. This is done by changing k in (28b) or (28c). In all cases it is true that

$$\rho_k = \langle \sigma_1 \rangle \tag{35}$$

the suffix k being redundant in regimes I and III.

Using the expression (34) for $\langle \sigma_1 \rangle$, singling out the σ_1 summations for special attention, we obtain

$$\rho_k = r_0^2 F_k(1) / \left[F_k(0) + r_0^2 F_k(1) \right] \tag{36}$$

where

$$F_k(\sigma_1) = \sum_{\sigma_2, \ldots, \sigma_m} w_0^{2n(\sigma)} \tag{37}$$

the summation being over all values (0 or 1) of $\sigma_2, \ldots, \sigma_m$, subject to the constraint (29).

We are interested in the extent to which the translation invariance is spontaneously broken. In both regimes II and IV this is measured by the "order parameter"

$$R = \rho_1 - \rho_2 \tag{38}$$

5. EXPLICIT FORMULAS FOR THE VARIOUS CASES

I have now set the stage to the point where I can begin to show how Rogers–Ramanujan-type identities occur in this model. Before doing so, I should recapitulate the results that will be needed.

There are four distinct regimes to consider: I, II, III, and IV. There is an independent real variable x, which lies in the interval $(-1, 0)$ in regimes I and IV, and in the interval $(0, 1)$ in regimes II and III. There is a set of integers $s_1, s_2, s_3, \ldots$ defined by (28); in regimes II and IV this set depends on an integer k which can take the values 1, 2, or 3 in regime II, and values 1 or 2 in regime IV.

The number g is defined by (10a), and the functions $Q(x)$, $P(x)$, $G(x)$, $H(x)$ by (15). Comparing these, it is apparent that

$$g = H(x)/G(x) \tag{39}$$

The numbers r_0, w_0 are defined by (30), and the function $n(\sigma)$ by (31) and (32), where m is a positive integer that is at our disposal, but which we ultimately intend to become infinitely large. The function $F_k(\sigma_1)$ is defined by (37), where the summation is over all values (0 or 1) of $\sigma_2, \ldots, \sigma_m$ that satisfy (29). The sublattice densities ρ_k are then given by (36). We expect them to tend to finite limits (between 0 and 1) as $m \to \infty$. We want to obtain tractable expressions for these limiting values, and for the order parameter R in (38).

The suffix k is redundant in regimes I and III: I shall omit it therein. From now on I shall adopt the convention that

$$\sum_{(l, m)} \tag{40}$$

denotes a summation over $\sigma_l, \ldots, \sigma_m$ (each with value 0 or 1), *subject to the constraint* (29). Note that this constraint automatically induces a dependence on σ_{l-1}, and on the boundary value s_{m+1} of the spin σ_{m+1}. I shall also use the standard notation[13]

$$(a; q)_n = \prod_{j=0}^{n-1} (1 - aq^j) \tag{41}$$

$$(q)_n = (q; q)_n = \prod_{j=1}^{n} (1 - q^j) \tag{42}$$

5.1. Regime I

From (30), (39) and (12):

$$w_0 = -x^3, \qquad r_0^2 = -xG(x)/H(x) \tag{43}$$

where $-1 < x < 0$. From (28a), (31), and (37),

$$F(\sigma_1) = \sum_{(2,m)} q^{\sigma_2+2\sigma_3+3\sigma_4+\cdots+(m-1)\sigma_m} \tag{44}$$

where $q = x^6$. There is only one ground state (the vacuum), so the suffix k in (37) is redundant.

Define, for $l = 1, \ldots, m-1$,

$$G_l(\sigma_l) = \sum_{(l+1,m)} q^{\sum i\sigma_{i+1}} \tag{45}$$

where the inner sum is over $i = l, \ldots, m-1$. Considering explicitly the contributions from $\sigma_{l+1} = 0$ and $\sigma_{l+1} = 1$, it is easily seen that

$$\begin{aligned} G_l(0) &= G_{l+1}(0) + q^l G_{l+1}(1) \\ G_l(1) &= G_{l+1}(0) \end{aligned} \tag{46}$$

for $l = 1, \ldots, m-1$ [taking $G_m(0) = G_m(1) = 1$].

We can immediately take the limit $m \to \infty$. We still have (46), for all positive integers l, together with the "boundary condition"

$$G_l(0), \quad G_l(1) \to 1 \qquad \text{as } l \to \infty \tag{47}$$

We can expand $G_l(0)$ and $G_l(1)$ in increasing powers of q^l, with coefficients that depend on q but are independent of l. Substituting the expansions into (44), the coefficients can be obtained recursively, giving

$$\begin{aligned} G_l(0) &= \sum_{r=0}^{\infty} q^{rl+r(r-1)}/(q)_n \\ G_l(1) &= \sum_{r=0}^{\infty} q^{rl+r^2}/(q)_n \end{aligned} \tag{48}$$

It is evident from (44) and (45) that $F(\sigma_1) = G_1(\sigma_1)$, so

$$\begin{aligned} F(0) &= \sum_{r=0}^{\infty} q^{r^2}/(q)_n \\ F(1) &= \sum_{r=0}^{\infty} q^{r(r+1)}/(q)_n \end{aligned} \tag{49}$$

Also, taking ratios of the two equations (46), it is readily seen that $F(1)/F(0)$ [and $F(0)$ and $F(1)$ enter (36) only via this ratio] is the simple continued fraction

$$F(1)/F(0) = 1/\big(1 + q/\big(1 + q^2/\big(1 + q^3/(1 + \cdots)\big)\big)\big) \tag{50}$$

The series on the right of (49) are very well known in the mathematical theory of partitions.[14] Rogers[15] proved that

$$F(0) = G(q), \qquad F(1) = H(q) \tag{51}$$

where $G(q)$ and $H(q)$ are the functions defined in (15). These identities were rediscovered by Ramanujan,[16] and are known as the Rogers–Ramanujan identities.

The functions G and H therefore occur not only in our formulas (16) and (43) for Δ and r_0, but also in our results for $F(0)$ and $F(1)$. It is intriguing that this should be so. It is also very useful: in statistical mechanics we are particularly interested in the critical behavior, which in this case is the behavior of ρ near $x = -1$ and $q = 1$. The series (49) are quite tricky to analyze near $q = 1$, but the products (15) are basically elliptic theta functions, and can readily be handled by going to the conjugate modulus.

The simplifications do not stop at (51). Substituting these results into (36), using (43), and remembering that $q = x^6$, we obtain

$$\rho = -xG(x)H(x^6)/\left[H(x)G(x^6) - xG(x)H(x^6)\right] \tag{52}$$

Ramanujan stated [Eq. (8) of Ref. 17], and Rogers[18] proved that

$$H(x)G(x^6) - xG(x)H(x^6) = P(x)/P(x^3) \tag{53}$$

where $P(x)$ is defined in (15). The denominator in (52) therefore simplifies dramatically, and we finally obtain

$$\rho = -xG(x)H(x^6)P(x^3)/P(x) \tag{54}$$

5.2. Regime II

Regime I is the easiest case to discuss; this is the hardest. The function $n(\sigma)$ is more complicated and there are three cases to consider, corresponding to $k = 1, 2, 3$ in (28c).

From (30), (39) and (14) we have

$$w_0 = x^{-3/2}, \qquad r_0^2 = x^{-1}H(x)/G(x) \tag{55}$$

where $0 < x < 1$. From (28c), (31), and (37), we have

$$F_k(\sigma_1) = \sum_{(2,m)} q^{\sum i(\sigma_i\sigma_{i+2} - \sigma_{i+1} + s_{i+1})} \tag{56}$$

where $q = x^3$ and the inner summation is over $i = 1, \ldots, m$. The k dependence enters via (28c) and the boundary condition (32).

We can set up recurrence relations to evaluate $F_k(\sigma_1)$. They are similar to (46), but more complicated because of the $\sigma_i\sigma_{i+2}$ term in (56). Set

$$G_l(\sigma_l, \sigma_{l+1}) = \sum_{(l+2,m)} q^{\sum i(\sigma_i\sigma_{i+2} - \sigma_{i+1} + s_{i+1})} \tag{57}$$

where now the inner summation is from $i = l$ to m, and the k dependence is implicit. Then by considering the sum over σ_{l+2}, it is readily verified that

$$\begin{aligned} G_l(0,0) &= \beta_l\left[G_{l+1}(0,0) + G_{l+1}(0,1)\right] \\ G_l(0,1) &= \beta_l q^{-l} G_{l+1}(1,0) \\ G_l(1,0) &= \beta_l\left[G_{l+1}(0,0) + q^l G_{l+1}(0,1)\right] \end{aligned} \tag{58a}$$

where $\beta_l = q^{s_{l+1}}$, i.e.,

$$\begin{aligned} \beta_l &= q^l \qquad \text{if } l = k-1 \pmod 3 \\ &= 1 \qquad \text{otherwise} \end{aligned} \tag{58b}$$

Comparing (56) and (57), we see that

$$\begin{aligned} F_k(0) &= G_0(0,0) = G_0(1,0) \\ F_k(1) &= G_0(0,1) \end{aligned} \tag{59}$$

Each $G_l(\sigma, \sigma')$ tends to a limit as $m \to \infty$. If we take this limit first, and then consider the large-l behavior, we find that

$$\begin{aligned} G_l(0,0) &= (1-q)^{-1} + \mathcal{O}(q^l) \\ G_l(0,1) &= q\left[(1-q)(1-q^2)\right]^{-1} + \mathcal{O}(q^l) \\ G_l(1,0) &= 1 + \mathcal{O}(q^l) \end{aligned} \tag{60}$$

provided that $(l-k)/3$ is an integer.

The recurrence relations (58), together with the boundary conditions (60), define the $G_l(\sigma, \sigma')$ in the $m \to \infty$ limit. Unfortunately the method used in the other three regimes (namely, to expand in powers of q^l) becomes rather difficult here, the coefficients not being simple products like (41) or (42).

However, Andrews[19] has used other methods (he defers taking the $m \to \infty$ limit until later, which enables him to combine regime II with III, and IV with I), and has obtained series expansions of $F_k(0)$ and $F_k(1)$. Define, for non-negative integers j,

$$u_j = \sum_r q^{-r} / \left[(q^2)_r (q)_{j-2r} \right] \tag{61a}$$

$$v_j = \sum_r q^{r} / \left[(q^2)_r (q)_{j-2r} \right] \tag{61b}$$

where the summations are over all integers r such that $0 \leqslant r \leqslant \frac{1}{2}j$. Then Andrews[19] finds that, in the limit $m \to \infty$,

$$\begin{aligned} F_1(0) &= \sum q^{3n(n+1)/2} u_{3n+1} \\ F_1(1) &= \sum q^{3n(n+1)/2} u_{3n} \\ F_2(0) &= \sum{}' q^{n(3n-1)/2} u_{3n-1} \\ F_2(1) &= \sum q^{(n+1)(3n+2)/2} u_{3n+1} \\ F_3(0) &= \sum q^{n(3n+1)/2} u_{3n} \\ F_3(1) &= \sum{}' q^{n(3n+1)/2} u_{3n-1} \end{aligned} \tag{62}$$

where the sums are from $n = 0$ to $n = \infty$; except for the primed sums, which are from $n = 1$ to $n = \infty$.

[Given these results, it is possible to guess and to verify the solution of (58); in particular,

$$\begin{aligned} G_l(0,0) &= \sum q^{nl + n(3n+1)/2} v_{3n+1} \\ G_l(0,1) &= \sum{}' q^{(n-1)l + n(3n+1)/2} u_{3n-1} \\ G_l(1,0) &= \sum q^{nl + n(3n+1)/2} u_{3n} \end{aligned} \tag{63}$$

provided that $(l - k)/3$ is an integer.]

Just as each of the Rogers–Ramanujan identities expresses a series as a product, so has Andrews[19] shown that each of the series in (62) can be written as the sum of at most two products:

$$F_1(0) = \left[E(q^4, q^{15}) + qE(q, q^{15}) \right] / Q(q) \tag{64a}$$

$$F_1(1) = \left[E(q^7, q^{15}) - qE(q^2, q^{15}) \right] / Q(q) \tag{64b}$$

$$F_2(0) = F_3(0) = E(q^6, q^{15}) / Q(q) \tag{64c}$$

$$F_2(1) = F_3(1) = qE(q^3, q^{15}) / Q(q) \tag{64d}$$

where the function $E(z, q)$ is defined by

$$E(z,q) = \prod_{n=1}^{\infty} (1 - q^{n-1}z)(1 - q^n z^{-1})(1 - q^n) \tag{65}$$

I originally conjectured the results (64) from truncated series expansions, but without deriving (62). As I remarked in the paragraph before the one containing (35), the sublattices 2 and 3 are equivalent, so it is to be expected that $F_2(\sigma_1) = F_3(\sigma_1)$; however, this is far from obvious in the intermediate equations (56)–(62).

First consider the cases $k = 2$ and $k = 3$. Using the definitions (15) of the functions G, H, Q, we can write (64c) and (64d) as

$$\begin{aligned} F_2(0) = F_3(0) &= Q(q^{15})/[\,Q(q)H(q^3)] \\ F_2(1) = F_3(1) &= qQ(q^{15})/[\,Q(q)G(q^3)] \end{aligned} \tag{66}$$

Substituting these expressions into (36), using (55), and remembering that $q = x^3$, we obtain

$$\rho_2 = \rho_3 = x^2H(x)H(x^9)/[\,G(x)G(x^9) + x^2H(x)H(x^9)] \tag{67}$$

Now we consult the "sums of products" Rogers–Ramanujan-type identities listed by Birch,[17] and find from Eq. (6) therein that

$$G(x)G(x^9) + x^2H(x)H(x^9) = [\,Q(x^3)]^2/[\,Q(x)Q(x^9)] \tag{68}$$

so (67) simplifies to

$$\rho_2 = \rho_3 = x^2H(x)H(x^9)\,Q(x)\,Q(x^9)/[\,Q(x^3)]^2 \tag{69}$$

The case $k = 1$ is more complicated. We use the standard elliptic function identity (implied by Sections 8.181 and 8.192 of Ref. 20)

$$E(z,q) = \sum_{n=0}^{\infty}(-1)^n q^{n(n+1)/2}(z^{-n} - z^{n+1}) \tag{70}$$

to write (64a) and (64b) as

$$\begin{aligned} F_1(0) &= [\,G(x^9)Q(x^9) - H(x)Q(x)]/[\,xQ(x^3)] \\ F_1(1) &= [\,G(x)Q(x) + x^2H(x^9)Q(x^9)]/Q(x^3) \end{aligned} \tag{71}$$

[We do this by noting that $G(q)Q(q)$ and $H(q)Q(q)$ are of the form (65), using (70) to series-expand the numerators in (64a), (64b), and (71), and equating the series term-by-term. Note that it follows that each right-hand side in (71) can be expanded in integer powers of x^3: something that is far from obvious.]

Substituting these expressions for $F_1(0)$ and $F_1(1)$ into (36), we obtain

$$\rho_1 = \frac{H(x)[\,G(x)Q(x) + x^2H(x^9)Q(x^9)]}{\{\,Q(x^9)[\,G(x)G(x^9) + x^2H(x)H(x^9)]\}} \tag{72}$$

Again we can use the identity (68) to simplify the denominator, giving

$$\rho_1 = H(x)\,Q(x)[\,G(x)Q(x) + x^2H(x^9)Q(x^9)]/[\,Q(x^3)]^2 \tag{73}$$

From (69) and (73), the order parameter is therefore

$$R = \rho_1 - \rho_2 = G(x)H(x)\left[Q(x)/Q(x^3)\right]^2$$
$$= Q(x)\,Q(x^5)/\left[Q(x^3)\right]^2$$
$$= \prod_{n=1}^{\infty} (1 - x^n)(1 - x^{5n})/(1 - x^{3n})^2 \tag{74}$$

which is a particularly simple result.

[This expression has a similar form to that for the order parameter M of the eight-vertex model, given in Ref. 21 and in Eq. (4.42) of Ref. 12.]

5.3. Regime III

In this case the analogs of (43) and (44) are

$$w_0 = x, \qquad r_0^2 = xH(x)/G(x) \tag{75}$$

$$F(\sigma_1) = \sum_{(2,m)} q^{\sum i(\sigma_{i+1} - \sigma_i\sigma_{i+2})} \tag{76}$$

where $0 < x < 1$, $q = x^2$, the inner sum is over $i = 1, \ldots, m$, and $\sigma_{m+1} = \sigma_{m+2} = 0$. The suffix k in (37) is redundant.

The expression (75) is the same as (56), except that q is inverted and the s_i are zero. We can therefore evaluate $F(0)$ and $F(1)$ by using the recursion relations (58a), with q inverted and $\beta_l = 1$, together with (59). Again we let $m \to \infty$. The boundary conditions are then that for l large

$$\begin{aligned} G_l(0,0) &= 1 + \mathcal{O}(q^l) \\ G_l(0,1) &= \mathcal{O}(q^l) \\ G_l(1,0) &= (1-q)^{-1} + \mathcal{O}(q^l) \end{aligned} \tag{77}$$

We can expand the G_l in powers of q^l, and systematically evaluate the coefficients from (58a) (with q replaced by q^{-1}). Doing this, we find that

$$\begin{aligned} G_l(0,0) &= \sum_{n=0}^{\infty} q^{nl+n(3n-1)/2}/\left[(q)_n(q;q^2)_n\right] \\ G_l(0,1) &= \sum_{n=1}^{\infty} q^{nl+3n(n-1)/2}/\left[(q)_{n-1}(q;q^2)_n\right] \\ G_l(1,0) &= \sum_{n=0}^{\infty} q^{nl+n(3n+1)/2}/\left[(q)_n(q;q^2)_{n+1}\right] \end{aligned} \tag{78}$$

From (59), it follows that

$$
\begin{aligned}
F(0) &= \sum_{n=0}^{\infty} q^{n(3n-1)/2} / \left[(q)_n (q; q^2)_n \right] \\
F(1) &= \sum_{n=0}^{\infty} q^{3n(n+1)/2} / \left[(q)_n (q; q^2)_{n+1} \right]
\end{aligned}
\tag{79}
$$

Just as the regime I series (49) could be simplified by using the Rogers–Ramanujan identities, so can (79) be simplified by using the further identities (46) and (44) in the list compiled by Slater.[22] These give

$$
\begin{aligned}
F(0) &= G(q^2) Q(q^2) / Q(q) \\
F(1) &= H(q^2) Q(q^2) / Q(q)
\end{aligned}
\tag{80}
$$

From (36) and (75), it follows that

$$
\rho = xH(x)H(x^4) / \left[G(x)G(x^4) + xH(x)H(x^4) \right] \tag{81}
$$

Now we look again at the list of Rogers–Ramanujan "sums-of-products" identities given by Birch,[17] and find from Eq. (2) therein the relation

$$
G(x)G(x^4) + xH(x)H(x^4) = \left[P(-x) \right]^2 \tag{82}
$$

which was proved by Rogers.[18] Thus (81) simplifies to

$$
\rho = xH(x)H(x^4) / \left[P(-x) \right]^2 \tag{83}
$$

5.4. Regime IV

This regime has two ground states and we have to distinguish the cases $k = 1$ and $k = 2$ in (28b). From (30), (39), (37), and (12), we have

$$
w_0 = x^{-2}, \qquad r_0^2 = -x^{-1} G(x) / H(x) \tag{84}
$$

$$
F_k(\sigma_1) = \sum_{(2,m)} q^{\sum i(s_{i+1} - \sigma_{i+1})} \tag{85}
$$

where $-1 < x < 0$, $q = x^4$ and the inner sum is over $i = 1, \ldots, m-1$.

The expression (85) is the same as that in (44), except that q is inverted and the s_i are not all zero. We can proceed as in (45) and (46). Define

$$
G_l(\sigma_l) = \sum_{(l+1,m)} q^{\sum i(s_{i+1} - \sigma_{i+1})} \tag{86}
$$

where the inner sum is now over $i = l, \ldots, m-1$. Considering explicitly the contributions from $\sigma_{l+1} = 0$ and $\sigma_{l+1} = 1$, we obtain

$$
\begin{aligned}
G_l(0) &= \beta_l \left[G_{l+1}(0) + q^{-l} G_{l+1}(1) \right] \\
G_l(1) &= \beta_l G_{l+1}(0)
\end{aligned}
\tag{87a}
$$

where

$$\begin{aligned} \beta_l &= 1 \qquad \text{if } l-k \text{ is even} \\ &= q^l \qquad \text{if } l-k \text{ is odd} \end{aligned} \tag{87b}$$

Clearly

$$F_k(0) = G_1(0), \qquad F_k(1) = G_1(1) \tag{88}$$

Each $G_l(0)$ and $G_l(1)$ tends to a limit as $m \to \infty$, and these limiting values satisfy the boundary condition

$$G_l(0) \to (1-q)^{-1}, \qquad G_l(1) \to 1 \text{ as } l \to \infty \tag{89}$$

provided $l-k$ is even.

We can expand $G_l(0)$ and $G_l(1)$ in powers of q^l. Substituting the expansions into (87) and equating coefficients, we find that, for $l-k$ even,

$$\begin{aligned} G_l(0) &= \sum_{n=0}^{\infty} q^{nl+n^2}/(q)_{2n+1} \\ G_l(1) &= \sum_{n=0}^{\infty} q^{nl+n^2}/(q)_{2n} \end{aligned} \tag{90}$$

The values for $l-k$ odd can be readily obtained from (87). From (88) it follows that

$$\begin{aligned} F_1(0) &= \sum_{n=0}^{\infty} q^{n(n+1)}/(q)_{2n+1} \\ F_1(1) &= \sum_{n=0}^{\infty} q^{n(n+1)}/(q)_{2n} \\ F_2(0) &= \sum_{n=0}^{\infty} q^{n^2}/(q)_{2n} \\ F_2(1) &= \sum_{n=1}^{\infty} q^{n^2}/(q)_{2n-1} \end{aligned} \tag{91}$$

Again we look at the list of Rogers–Ramanujan-type identities compiled by Slater.[22] From her equations (94), (99), (98), and (96) we obtain

$$\begin{aligned} F_1(0) &= H(-q)/P(q) \\ F_1(1) &= G(-q)/P(q) \\ F_2(0) &= G(q^4)/P(q) \\ F_2(1) &= qH(q^4)/P(q) \end{aligned} \tag{92}$$

where again the functions Q, P, G, H are those defined in (15).

Substituting these results into (36), using (84) and $q = x^4$ we obtain

$$\begin{aligned} \rho_1 &= G(x)G(-x^4)/\left[G(x)G(-x^4) - xH(x)H(-x^4)\right] \\ \rho_2 &= -x^3G(x)H(x^{16})/\left[H(x)G(x^{16}) - x^3G(x)H(x^{16})\right] \end{aligned} \tag{93}$$

The first of these denominators does not appear to be explicitly mentioned in the literature, but Ramanujan did state, and Watson[23] proved, that

$$G(x)H(-x) + G(-x)H(x) = 2/\left[P(x^2)\right]^2 \tag{94}$$

[this is Eq. (23) of Birch[17]]. Further, Rogers[15] proved that

$$G(-x^4) = Q(x^2)\left[H(x) + H(-x)\right]/\left[2Q(x^8)\right] \tag{95a}$$

$$H(-x^4) = Q(x^2)\left[G(x) - G(-x)\right]/\left[2xQ(x^8)\right] \tag{95b}$$

$$H(x^{16}) = Q(x^2)\left[H(x) - H(-x)\right]/\left[2x^3Q(x^8)\right] \tag{95c}$$

From (94), (95a), and (95b), it follows that

$$G(x)G(-x^4) - xH(x)H(-x^4) = P(-x^2) \tag{96}$$

Also, Ramanujan stated [Eq. (5) of Birch[17]], and Rogers[18] proved, that

$$H(x)G(x^{16}) - x^3G(x)H(x^{16}) = P(-x^2) \tag{97}$$

Both denominators in (93) can therefore be simplified (in fact they are equal), giving

$$\begin{aligned} \rho_1 &= G(x)G(-x^4)/P(-x^2) \\ \rho_2 &= -x^3G(x)H(x^{16})/P(-x^2) \end{aligned} \tag{98}$$

Using the identities (95a) and (95c), it follows that the mean total density is

$$\rho = \tfrac{1}{2}(\rho_1 + \rho_2) = \tfrac{1}{2}G(x)H(-x)\left[P(x^2)\right]^2 \tag{99}$$

and the order parameter is

$$\begin{aligned} R = \rho_1 - \rho_2 &= G(x)H(x)\left[P(x^2)\right]^2 \\ &= \left[Q(x^2)\right]^2 Q(x^5)/\left\{Q(x)\left[Q(x^4)\right]^2\right\} \\ &= \prod_{n=1}^{\infty} (1 - x^{2n})^2(1 - x^{5n})/\left\{(1 - x^n)(1 - x^{4n})^2\right\} \end{aligned} \tag{100}$$

This has a similar form to the order parameter (74) in regime II, and to the eight-vertex model order parameter M_0 [Eq. (15) of Ref. 21, Eq. (4.42) of Ref. 12], being a ratio of products of Q functions.

5.5. Comments

This completes the derivation of the sublattice densities and order parameters of the generalized hard hexagon model. I have discussed the four regimes separately, but we can now see many common features. We can write down recursion relations defining $F_k(0)$ and $F_k(1)$. Using these, or using finite-m expressions,[19] $F_k(0)$ and $F_k(1)$ can be written as infinite series. In every case there then exists a Rogers–Ramanujan-type identity by which the series can be written as an infinite product, or at worst the sum of two such products. (In regimes I, III, and IV these identities are included in the list compiled by Slater[22]; in regime II we need the new identities obtained by Andrews.[19])

Further, when we substitute the results into (36), we always find that the denominator can be written as a single product by using the "sums-of-products" Rogers–Ramanujan identities listed by Birch.[17] Finally, in regimes II and IV the order parameter $R = \rho_1 - \rho_2$ is found to be a simple ratio of products of Q functions.

It is fascinating that these Rogers–Ramanujan-type identities occur so frequently in the working. With the benefit of hindsight, we can see that this must in some way be connected with the apparently uninteresting relations (7) and (8), and our desire to parametrize these so as to make e^L and e^M single-valued functions of a parameter w, Δ being independent of w. This led automatically to an elliptic function parametrization where the one-fifth period plays a special role, and to the relation (16) involving the functions $G(x)$ and $H(x)$.

6. CRITICAL BEHAVIOR

The behavior of the functions $Q(x)$, $P(x)$, $G(x)$, $H(x)$ near $x = \pm 1$ can be studied by using the conjugate modulus relations for elliptic theta functions, e.g.,

$$\begin{aligned} Q(e^{-\lambda}) &= (2\pi/\lambda)^{1/2} \exp\left[\frac{\lambda}{24} - \frac{\pi^2}{6\lambda}\right] Q(e^{-4\pi^2/\lambda}) \\ Q(-e^{-\lambda}) &= (\pi/\lambda)^{1/2} \exp\left[\frac{\lambda}{24} - \frac{\pi^2}{24\lambda}\right] Q(-e^{-\pi^2/\lambda}) \end{aligned} \tag{101}$$

for $\lambda > 0$. Doing this, we are led to define parameters ϵ and p by

$$\begin{aligned} &\text{I and IV:} \quad x = -e^{-\pi^2/5\epsilon}, \qquad p = -e^{-\epsilon} \\ &\text{II and III:} \quad x = e^{-4\pi^2/5\epsilon}, \qquad p = e^{-\epsilon} \end{aligned} \tag{102}$$

Then in all regimes it is true that

$$|\Delta| = \Delta_c \prod_{n=1} \left[\frac{1 + \frac{1}{2}(1 - \sqrt{5})p^n + p^{2n}}{1 + \frac{1}{2}(1 + \sqrt{5})p^n + p^{2n}} \right]^{5/2} \tag{103}$$

where Δ_c is the "critical" value of Δ defined by (9).

Thus p is zero when $|\Delta| = \Delta_c$. This occurs on the (I, II) and (III, IV) regime boundaries. Further, p vanishes linearly with $\Delta^2 - \Delta_c^2$.

On these boundaries the sublattice densities are all equal to the critical mean density

$$\rho_c = (5 - \sqrt{5})/10 = 0.27639 \ldots \tag{104}$$

Near the boundaries we find that the mean density ρ and the order parameter R behave as

$$\begin{aligned} &\text{I:} \quad \rho = \rho_c - 5^{-1/2}(-p)^{2/3} + \mathcal{O}(p) \\ &\text{II:} \quad \rho = \rho_c + 5^{-1/2}p^{2/3} + \mathcal{O}(p) \\ &\text{III:} \quad \rho = \rho_c - 5^{-1/2}p^{1/4} + \mathcal{O}(p) \\ &\text{IV:} \quad \rho = \rho_c + 5^{1/2}(-p) + \mathcal{O}(p^4) \\ &\text{II:} \quad R = (3/\sqrt{5})p^{1/9}\left[1 - p + 2p^{5/3} + \mathcal{O}(p^2)\right] \\ &\text{IV:} \quad R = (2/\sqrt{5})(-p)^{1/4}\left[1 - p + \mathcal{O}(p^2)\right] \end{aligned} \tag{105}$$

In particular, the fifth of these equations implies that the original hard hexagon model (where $L \to 0$ and $M \to -\infty$) has a critical exponent $\beta = 1/9$ (as well as $\alpha = 1/3$), as reported earlier.

ACKNOWLEDGMENTS

I had enormous help in locating the various Rogers–Ramanujan-type identities that occur, notably from George E. Andrews [who proved (62) and (64)], Richard Askey and David Bressoud [who showed that (96) is a consequence of (94) and (95), and carefully guided me through the relevant identities in Ref. 17], as well as from Mike Hirschhorn and Geoff Joyce. I am extremely grateful for their encouragement and assistance.

REFERENCES

1. R. J. Baxter, *J. Phys. A: Math. Gen.* **13**:L61 (1980).
2. R. J. Baxter, *Exactly Solved Models in Statistical Mechanics*, Chap. 14, (to be published by Academic, London, 1981/2).
3. D. S. Gaunt and M. E. Fisher, *J. Chem. Phys.* **43**:2840 (1965).
4. L. K. Runnels and L. L. Combs, *J. Chem. Phys.* **45**:2482 (1966).
5. R. J. Baxter, I. G. Enting, and S. K. Tsang, *J. Stat. Phys.* **22**:465 (1980).
6. R. J. Baxter, *J. Stat. Phys.* **19**:461 (1978); *Physica* **106A**:18 (1981).
7. S. K. Tsang, *J. Stat. Phys.* **20**:95 (1979).
8. R. J. Baxter, *J. Math. Phys.* **9**:650 (1968).
9. S. B. Kelland, *Can. J. Phys.* **54**:1621 (1976).
10. R. J. Baxter and I. G. Enting, *J. Stat. Phys.* **21**:103 (1979).
11. R. J. Baxter and S. K. Tsang, *J. Phys. A: Math. Gen.* **13**:1023 (1980).
12. R. J. Baxter, Exactly Solved Models, in *Fundamental Problems in Statistical Mechanics V*, E. G. D. Cohen, ed. (North-Holland, Amsterdam, 1980).
13. L. J. Slater, *Generalized Hypergeometric Functions* (Cambridge University Press, Cambridge, 1966).
14. G. E. Andrews, *The Theory of Partitions*, Chap. 7 (Addison-Wesley, Reading, Massachusetts, 1976).
15. L. J. Rogers, *Proc. London Math. Soc.* (1), **25**:318 (1894).
16. S. Ramanujan, *Proc. Cambridge Philos. Soc.* **19**:214 (1919).
17. B. J. Birch, *Math. Proc. Cambridge Philos. Soc.* **78**:73 (1975).
18. L. J. Rogers, *Proc. London Math. Soc.* (2), **19**:387 (1921).
19. G. E. Andrews, The Hard-Hexagon Model and New Rogers–Ramanujan Type Identities, Dept. Math. Research Report 8167, Pennsylvania State University (1981).
20. I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1965).
21. M. N. Barber and R. J. Baxter, *J. Phys. C: Solid State Phys.* **6**:2913 (1973).
22. L. J. Slater, *Proc. London Math. Soc.* (2), **54**:147 (1951).
23. G. N. Watson, *J. Indian Math. Soc.* **20**:57 (1933).