Journal of Statistical Physics, Vol. 44, Nos. 5/6, 1986

Lattice Gas Generalization of the Hard Hexagon Model. II. The Local Densities as Elliptic Functions

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Received April 24, 1986

In a previous paper we considered an extension of the hard hexagon model to a solvable two-dimensional lattice gas with at most two particles per pair of adjacent sites. Here we use various mathematical identities (in particular Gordon's generalization of the Rogers–Ramanujan relations) to express the local densities in terms of elliptic functions. The critical behavior is then readily obtained.

KEY WORDS: Statistical mechanics; lattice statistics; number theory; hard hexagon model; Rogers–Ramanujan identities.

1. INTRODUCTION

This is a continuation of an earlier paper,[1] hereinafter referred to as I. There we remarked that the solution[2] of the hard hexagon model involved the well-known Rogers–Ramanujan identities,[3,4] and that this suggested the existence of solvable square-lattice statistical mechanical models corresponding to Gordon's[5] generalized identities. Such models would have at most $n-1$ particles per pair of adjacent sites ($n=2$ corresponding to the original hard hexagon model). Their Boltzmann weights would satisfy the "star-triangle" relations.

We went on to obtain the $n=3$ solution of the star-triangle relations, and to use corner transfer matrices to write the local densities as multiple

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0022-4715/86/0900-0713$05.00/0 © 1986 Plenum Publishing Corporation

822/44/5-6-1

sums (similar to one-dimensional partition functions). Kuniba, Akutsu, and Wadati[6] have independently obtained the $n=3, 4$, and 5 solutions. Partly guided by their $n=4$ result, we conjectured in I the arbitrary-n multiple sum expressions for the local densities.

Another generalization of the $n=2$ hard hexagon model is the restricted eight vertex solid-on-solid (8VSOS) model.[7] In that case the multiple sums could be expressed in terms of Gaussian polynomials, which are q-series analogues of binomial coefficients that occur in the theory of partitions.[8] For our $n=3$ model we have found that the sums can be expressed in terms of q-series trinomial coefficients. We give the details of these fascinating identities in a separate publication; here we quote the relevant large-lattice results and use them to express the local densities and order parameters in terms of elliptic functions. The critical behavior is then readily obtained.

2. THE MULTIPLE-SUM EXPRESSIONS

The elliptic θ functions of argument u and nome $p^{1/2}$ (where $|p|<1$) are

$$\theta_1(u, p) = 2p^{1/8} \sin u \prod_{j=1}^{\infty} (1 - 2p^j \cos 2u + p^{2j})(1 - p^j) \tag{2.1a}$$

$$\theta_4(u, p) = \prod_{j=1}^{\infty} (1 - 2p^{(2j-1)/2} \cos 2u + p^{2j-1})(1 - p^j) \tag{2.1b}$$

$$\theta_2(u, p) = \theta_1\left(u + \frac{\pi}{2}, p\right), \qquad \theta_3(u, p) = \theta_4\left(u + \frac{\pi}{2}, p\right) \tag{2.1c}$$

In equation (4.1) of I we express the Boltzmann weights of the $n=3$ model in terms of θ_1 functions, all of nome $p^{1/2}$, and with arguments depending on a variable u which is restricted to the interval $-(5\pi/14) < u < \pi/7$. We define an integer t by

$$\begin{aligned} t &= 2 \qquad \text{if} \quad 0 < u < \pi/7 \\ &= -5 \qquad \text{if} \quad -(5\pi/14) < u < 0 \end{aligned} \tag{2.2}$$

There are then four separate cases, or regimes, to consider

$$\begin{aligned} &\text{I: } p<0, &&t=-5 \\ &\text{II: } p>0, &&t=-5 \\ &\text{III: } p>0, &&t=2 \\ &\text{IV: } p<0, &&t=2 \end{aligned} \tag{2.3}$$

The parameter p is at our disposal, and we can introduce a related parameter s by

$$|p| = e^{-2\pi s} \tag{2.4}$$

Limiting special cases occur when $|p| = 1$ (which is complete order or disorder) and when $p = 0$ (when the system is critical).

As in (5.16) of I, for integer values of a, b, c we define a function $H(a, b, c)$ by

$$\begin{aligned} p > 0\colon H(a, b, c) &= -|a-c|/2 \qquad &&\text{if } a+c \text{ is even} \\ &= -(a+c+1)/2 \qquad &&\text{if } a+c \text{ is odd} \end{aligned} \tag{2.5a}$$

$$p < 0\colon H(a, b, c) = b \tag{2.5b}$$

We further define (for $1 \leqslant a, b, c \leqslant 3$, $b + c \geqslant 4$ and $q \in \mathbb{C}$) the function

$$X_m(a, b, c; q) = \sum_{\sigma_2} \cdots \sum_{\sigma_m} q^{\sum jH(\sigma_j, \sigma_{j+1}, \sigma_{j+2})} \tag{2.6}$$

where the inner summation is from $j = 1$ to $j = m$ and the outer sum is over all integer values of $\sigma_2, \ldots, \sigma_m$ satisfying

$$\begin{aligned} &0 \leqslant \sigma_j, \qquad 0 \leqslant \sigma_j + \sigma_{j+1} \leqslant 2, \qquad 1 \leqslant j \leqslant m+1 \\ &\sigma_1 = 3 - a, \qquad \sigma_{m+1} = 3 - b, \qquad \sigma_{m+2} = 3 - c \end{aligned} \tag{2.7}$$

Now we take

$$q = e^{\pi t/7s} \tag{2.8}$$

and set

$$F(a) = \theta_1(\pi a/7, p)\, q^{(3-a)(4-a)/14} X_m(a, b, c; q) \tag{2.9}$$

where we have dropped the explicit dependence in m, b, and c. Then the probability that a site deep inside the lattice contains $3 - a$ particles (with $a = 1, 2,$ or 3) is

$$P(a) = F(a)/[F(1) + F(2) + F(3)] \tag{2.10}$$

Thus we can regard $F(a)$ as an unnormalized probability.

We have changed notation slightly from I: the integer arguments of X_m, F, P are now a, b, c rather than σ_1, σ_{m+1}, σ_{m+2}. The old and new arguments are related by (2.7).

As defined, $P(a)$ has an implicit dependence on m, b, and c (and of course on p, or equivalently, s). In the large-lattice limit we let m become large. We find that $P(a)$ then tends to a limit, except that in regimes III and IV the limit may depend on whether it is taken through even or odd values of m. In regime II it depends on whether it is taken through values equal to 0, 1, 2, 3, or 4, modulo 5.

This alternation of the limit reflects the fact that the system is then in an ordered phase. For instance, in regime III there is a phase with a ground state in which alternate sites have 0 and 2 particles. We can regard σ_{m+1} and σ_{m+2} as occupation numbers of boundary sites, and these should be fixed at the appropriate ground state values. If the ground state is kept fixed (relative to the center site 1 with occupation number σ_1), then as m increases through integer values the boundary sites move, so σ_{m+1} and σ_{m+2} should alternately take the values 0 and 2, i.e., b and c should alternately equal 3 and 1. If one thus makes b and c dependent on m, then $P(a)$ tends to a limit through *all* values of m. Alternatively, if one fixes b and c, then site 1 moves relative to the ground state, and so $P(a)$ alternates as m increases.

If the system is disordered, then $P(a)$ should tend to a limit as m becomes large, and this limit should be independent of b and c. This occurs in regime I.

From (2.5) and (2.6), for finite m each $X_m(a, b, c; q)$ is a polynomial in q (in regimes II and III actually a polynomial in q^2), possibly multiplied by a negative integer power. As we remarked above we have expressed these polynomials in terms of q-series trinomial coefficients, and give the details elsewhere. In the next section we give the large-m limiting behavior from which the ordered phases can be deduced.

From (2.3) and (2.8), note that $0<q<1$ in regimes I and II while $q>1$ in regimes III and IV.

We need to use the functions (defined for $|x|<1$, $r>0$)

$$Q(x)=\prod_{j=1}^{\infty}(1-x^j) \tag{2.11}$$

$$R(x)=\prod_{j=1}^{\infty}(1-x^{2j-1}) \tag{2.12}$$

$$\{r, s, t; x\}=\sum_{j=-\infty}^{\infty} x^{(rj^2+sj+t)/2} \tag{2.13}$$

$$\{r, s, t; x\}_-=\sum_{j=-\infty}^{\infty}(-1)^j x^{(rj^2+sj+t)/2} \tag{2.14}$$

$$=x^{t/2}\prod_{j=1}^{\infty}(1-x^{rj-(r-s)/2})(1-x^{rj-(r+s)/2})(1-x^{rj}) \tag{2.15}$$

They satisfy the conjugate modulus relations[9] true for all ε, r, s, t provided $\varepsilon > 0$ and $r > 0$

$$Q(e^{-2\pi\varepsilon}) = \varepsilon^{-1/2} \exp[\pi(\varepsilon - \varepsilon^{-1})/12]\, Q(e^{-2\pi/\varepsilon}) \tag{2.16}$$

$$R(e^{-2\pi\varepsilon}) = 2^{1/2} \exp[-\pi(2\varepsilon + \varepsilon^{-1})/24]/R(e^{-\pi/\varepsilon}) \tag{2.17}$$

$$R(-e^{-\pi\varepsilon}) = \exp[\pi(\varepsilon^{-1} - \varepsilon)/24]\, R(-e^{-\pi/\varepsilon}) \tag{2.18}$$

$$\{r, s, t; e^{-2\pi\varepsilon}\} = (r\varepsilon)^{-1/2}\, e^{-(t - s^2/4r)\pi\varepsilon}\theta_3(\pi s/2r, e^{-2\pi/r\varepsilon}) \tag{2.19}$$

$$\{r, s, t; e^{-2\pi\varepsilon}\}_- = (r\varepsilon)^{-1/2}\, e^{-(t - s^2/4r)\pi\varepsilon}\theta_2(\pi s/2r, e^{-2\pi/r\varepsilon}) \tag{2.20}$$

3. LARGE-m LIMITING VALUES

Regime I. We have discussed this case in I, remarking how the limiting value of X_m can immediately be obtained from Gordon's identity

$$\lim_{m \to \infty} q^{(b-3)m} X_m(a, b, c; q) = \prod_{\substack{j=1 \\ j \neq 0, \pm a \ (\mathrm{mod}\ 7)}}^{\infty} (1 - q^j)^{-1}$$
$$= \{7, 7 - 2a, 0; q\}_-/Q(q) \tag{3.1}$$

Using (2.9) and (2.20), ignoring a-independent factors that cancel out of (2.10), it follows that

$$F(a) = \theta_1(\pi a/7, -e^{-2\pi s})\, \theta_1(\pi a/7, e^{-4\pi s/5}) \tag{3.2}$$

Regime II. For finite m, the polynomials of this model are very different from those of the 8VSOS model.[7] Even so, in the limit of large m, it turns out that in regime II (and in regime I) we regain basically the 8VSOS results. Let $x_m(a, b, c; q)$ be the function defined (for $r = 7$) in (2.6.1) of Ref. 7. Then we find, for m large and $a = 1, 2, 3$, that

$$X_m(a, 1, 3; q) = q^{-m(m+1)} x_{2m}(\tau_a, 1, 2; q^2) \tag{3.3}$$

where $\tau_1, \tau_2, \tau_3 = 1, 5, 3$. When we say that an equation is true "for m large," we mean that the ratio of the LHS to the RHS tends to unity as $m \to \infty$.

Also, by considering the recursion relations between X_m and X_{m-1}, we can verify that for m large

$$X_m(a, b, c; q) = q^{-[3m^2 + \alpha(b,c)m + \beta(b)]/5} S_{m + \alpha(b,c)}(a; q) \tag{3.4}$$

where $1 \leqslant a,\ b,\ c \leqslant 3$ and

$$\begin{gathered}\alpha(1,3), \alpha(3,3), \alpha(2,3), \alpha(2,2), \alpha(3,2), \alpha(3,1) = 0, 1, 2, 3, 4, 6 \\ \beta(1), \beta(2), \beta(3) = 3, 5, 6\end{gathered} \tag{3.5}$$

$$S_{m+5}(a; q) = S_m(a; q) \tag{3.6}$$

The function S contains an overall multiplicative fractional power of q, but is otherwise Taylor-expandable in powers of q^2.

We can use (3.3) and (3.4) to express S in terms of x. Taking $\hat{x}_m(a, b, c; q)$ to be the function defined in (2.6.52) of Ref. 7, we find that

$$S_m(a; q) = \hat{x}_{2m}(\tau_a, 1, 2; q^2) \tag{3.7}$$

Hence, from (2.6.53) of Ref. 7 (with $r = 7$)

$$S_m(a; q) = q^{a(7-a)/10} \hat{\eta}_{\tau_a, m + (\tau_a - 1)/2} \tag{3.8}$$

the function $\hat{\eta}_{a,j}$ being defined as in Section 2.6 of Ref. 7, but with q therein replaced by q^2. We have used the fact that $\tau_a(7-\tau_a) = a(7-a)$.

From (2.9), (3.4), and (3.8), we can now express $F(a)$ in terms of $\hat{\eta}$. The next step is to use (3.3.7) of Ref. 7, which is effectively a "conjugate modulus" identity; unfortunately it contains an error: $(r-a)^2$ should be replaced by $(r-2a)^2$. Doing this, noting that r, ε in Ref. 7 now becomes 7, $2\pi s$, and ignoring a-independent factors of $F(a)$ that cancel out of (2.10), we obtain

$$F(a) = \theta_1(\pi\tau_a/7, e^{-2\pi s})\, \lambda_{\tau_a, m + \alpha(b,c) + (\tau_a - 1)/2} \tag{3.9}$$

[We have used the fact that $\theta_1(\pi a/7, x) = \theta_1(\pi\tau_a/7, x)$.]

From (3.3.10) through (3.3.12) of Ref. 7, for general integer values of r, we can regard the $\lambda_{a,j}$ as defined by the periodicity condition

$$\lambda_{a, j+r-2} = \lambda_{a,j} \tag{3.10}$$

together with the identity (true for all complex numbers u and all integers a)

$$\begin{aligned}&\frac{Q(t)^3\, \theta_1(\pi a/r, t)\, \theta_4(ru, t^r)}{2t^{1/8} Q(t^r)^2\, \theta_4(u, t)\, \theta_4(u + \pi a/r, t)} \\ &\quad = \frac{r}{4(r-2)} \sum_{j=0}^{r-3} \lambda_{a,j} \theta_4\left[u + \frac{\pi(r-1)}{2r-4} + \frac{\pi j}{r-2} - \frac{\pi a}{r(r-2)}, t^{1/(r-2)}\right]\end{aligned} \tag{3.11}$$

where $t = e^{-2\pi s/(r-2)}$. In our case we have $r = 7$.

Note that m still enters (3.9), but because of (3.10) it only enters via its value to modulo 5. Thus $P(a)$ tends to a limit if m is taken to infinity through values differing by integer multiples of 5.

Regime III. In regime III, and also in regime IV, we find that the large-m results for $X_m(a, b, c; q)$ take the form

$$X_m(a, b, c; q) = (-1)^a[\tilde{G}_m(2a, b, c; q^{-1}) - \tilde{G}_m(7-2a, b, c; q^{-1})] \tag{3.12}$$

where $\tilde{G}_m$ is a sum of modular forms. Note that $t=2$ in regimes III and IV, so from (2.8) we see that the argument q of $X_m(a, b, c; q)$ is greater than 1.

Since $a=1$, 2, or 3, the function $\tilde{G}_m(j, b, c; q^{-1})$ is needed for $j=1, 2,..., 6$. Setting

$$D_1,..., D_6 = 0, 1, 3, 7, 13, 20 \tag{3.13}$$

we also find it convenient to introduce a function $G_m(j, b, c; q)$ by

$$\tilde{G}_m(j, b, c; q) = q^{D_j} G_m(j, b, c; q) \tag{3.14}$$

Using (2.9), together with the properties $\theta_1(-u, p) = -\theta_1(u, p) = \theta_1(u+\pi, p)$, we find that (for $a=1, 2, 3$)

$$F(a) = \sum_{j=2a,7-2a} \theta_1(4\pi j/7, p)\, q^{-(6j-8)(j-1)/7} G_m(j, b, c; q^{-1}) \tag{3.15}$$

the sum being over only two values: $j=2a$ and $j=7-2a$.

Specializing to regime III, we find that in the limit of m large, for $j=1,..., 6$

$$G_m(j, 2, 2; q) = \{35, 20j-7, 2j^2-1; q^2\}/[R(q^2)\, Q(q^2)] \tag{3.16a}$$

$$G_m(j, 3, 3; q) = \{35, 20j-21, 2(j-1)^2; q^2\}/[R(q^2)\, Q(q^2)] \tag{3.16b}$$

for $(b, c) = (3, 2)$ or $(2, 3)$

$$\begin{aligned} G_m(j, b, c; q) = [&R(-q)\{35, 20j-14, 2j^2-2j; q^2\} + \operatorname{sign}(b-c)(-1)^m R(q) \\ &\times \{35, 20j-14, 2j^2-2j; q^2\}_-]/[2Q(q^2)] \end{aligned} \tag{3.16c}$$

and for $(b, c) = (3, 1)$ or $(1, 3)$

$$\begin{aligned} G_m&(j, b, c; q) \\ &= [R(-q)\{35, 20j-28, 2j^2-6j+4; q^2\} \\ &\quad + \operatorname{sign}(b-c)(-1)^m R(q)\{35, 20j-28, 2j^2-6j+4; q^2\}_-]/[2Q(q^2)] \end{aligned} \tag{3.16d}$$

The functions $\{r, s, t; x\}$, $\{r, s, t; x\}_-$ are defined in (2.13), (2.14). Define $\alpha(b, c)$ by

$$\alpha(2,2)=1, \qquad \alpha(2,3)=\alpha(3,2)=2, \qquad \alpha(3,3)=3$$
$$\alpha(1,3)=\alpha(3,1)=4 \tag{3.17}$$

Then by using the conjugate modulus transformations (2.16)–(2.20), ignoring a-independent factors that cancel out of (2.10), from (3.15) we find that, for m large, $1 \leqslant a, b, c \leqslant 3$, $b+c \geqslant 4$

$$F(a) = \sum_{j=2a,7-2a} \theta_1\left(\frac{4\pi j}{7}, e^{-2\pi s}\right)\left\{\theta_3\left[\frac{2\pi j}{7} - \frac{\pi\alpha(b,c)}{10}, e^{-\pi s/5}\right]\right.$$
$$\left. + \operatorname{sign}(b-c)(-1)^m\, \xi(s)\, \theta_2\left[\frac{2\pi j}{7} - \frac{\pi\alpha(b,c)}{10}, e^{-\pi s/5}\right]\right\} \tag{3.18}$$

where we take $\operatorname{sign}(0)=0$, and

$$\begin{aligned}\xi(s) &= R(e^{-2\pi/7s})/R(-e^{-2\pi/7s}) \\ &= 2^{1/2} e^{-7\pi s/16}/[R(e^{-7\pi s})\, R(-e^{-7\pi s/2})] \\ &= \theta_1(\pi/4, e^{-7\pi s/2})/\theta_4(\pi/4, e^{-7\pi s/2}) \\ &= k^{1/4}\end{aligned} \tag{3.19}$$

k being the elliptic modulus with nome $e^{-7\pi s/2}$ (Eq. 8.197.3 of Ref. 10).

Regime IV. As in regime III, we find that the large-m results take the form (3.12)–(3.15), where $G_m(j, b, c; q)$ is expressible in terms of the modular functions (2.11)–(2.15). Since $H(a, b, c)$ is now given by (2.5b), $X_m(a, b, c; q)$, and hence $G_m(j, b, c; q)$ is independent of c. We find, for m large and $j = 1,..., 6$, that

$$\begin{aligned}G_{m-1}(j, 1, c; q) &= G_m(j, 3, c; q) \\ &= q^{-m^2/2}[R(-q^{1/2})\{21, 12j-14, 0; q\} \\ &\quad + (-1)^m R(q^{1/2})\{21, 12j-14, 0; q\}_-]/[2Q(q)]\end{aligned} \tag{3.20a}$$

$$G_m(j, 2, c; q) = q^{-m(m+1)/2}\{21, 12j-7, 2j-2; q\}/[R(q)\, Q(q)] \tag{3.20b}$$

We have actually obtained the large-m behavior of $X_m(a, b, c; q)$ by two rather different routes. One gives (3.20), the other replaces (3.20a) by

$$G_{2m-1}(j,1,c;q)=G_{2m}(j,3,c;q)$$
$$=q^{-2m^2}[\{84,48j-49,6(j-1)^2;q^2\}$$
$$+\{84,48j-7,6j^2-1;q^2\}]/Q(q) \tag{3.21a}$$
$$G_{2m}(j,1,c;q)=G_{2m+1}(j,3,c;q)$$
$$=q^{-2m(m+1)}[\{84,48j-35,6j^2-8j+2;q^2\}$$
$$+\{84,48j-77,6j^2-20j+16;q^2\}]/Q(q) \tag{3.21b}$$

The expressions (3.21) need not be the same as (3.20a), but on substitution into (3.15) they must yield the same results for $F(a)$. We have been able to verify this directly.

Substituting the results (3.20) into (3.15) and applying the conjugate modulus transformations (2.16)–(2.20) (ignoring a-independent factors that cancel out of (2.10)), we find for m large and $a, b=1, 2, 3$ that

$$F(a)=\sum_{j=2a,7-2a}\theta_1\left(\frac{4\pi j}{7}, -e^{-2\pi s}\right)\left[\theta_3\left(\frac{2\pi j}{7}-\frac{\pi d(b)}{6}, e^{-2\pi s/3}\right)\right.$$
$$\left.+(-1)^m(b-2)\,\xi(2s)\,\theta_2\left(\frac{2\pi j}{7}-\frac{\pi d(b)}{6}, e^{-2\pi s/3}\right)\right] \tag{3.22}$$

where

$$d(1), d(2), d(3)=2, 1, 2 \tag{3.23}$$

and the function $\xi(s)$ is defined in (3.19).

If we use the alternative expressions (3.21), then for $b=1$ or 3 we find that

$$F(a)=\eta(s)\sum_{j=2a,7-2a}\theta_1\left(\frac{4\pi j}{7}, -e^{-2\pi s}\right)\left[\theta_3\left(\frac{2\pi j}{7}-\gamma_m(b), e^{-\pi s/12}\right)\right.$$
$$\left.+\theta_3\left(\frac{2\pi j}{7}-\gamma_m(b)-\frac{\pi}{4}, e^{-\pi s/12}\right)\right] \tag{3.24}$$

where

$$\eta(s)=2^{-1/2}e^{-7\pi s/24}/R(-e^{-7\pi s}) \tag{3.25}$$

$$\begin{aligned}\gamma_m(b)&=\pi/24 \qquad \text{if} \quad m+(3-b)/2 \text{ is even}\\ &=5\pi/24 \qquad \text{if} \quad m+(3-b)/2 \text{ is odd}\end{aligned} \tag{3.26}$$

The factor $\eta(s)$ remains if we discard only the a-independent factors that we discarded in (3.22). Thus for $b=1$ or 3 the expressions (3.22) and (3.24) must be precisely the same; again, we have been able to verify this directly.

4. "SUMS-OF-PRODUCTS" IDENTITIES

We now have expressions for the unnormalized probabilities $F(a)$ in each regime. The next step is to determine the normalized probabilities $P(a)$ from (2.10), which means evaluating the sum

$$M = F(1) + F(2) + F(3) \tag{4.1}$$

In regimes III and IV we see from (3.18) and (3.22) that

$$F(a) = L(2a) + L(7-2a) \tag{4.2}$$

where $L(j)$ is the summand on the RHS of the respective equation. It has the property that $L(7) = 0$, so (4.1) can be written as

$$M = \sum_{j=1}^{7} L(j) \tag{4.3}$$

Since $L(j)$ is periodic of period 7, the sum (4.3) is over a full period.

We should note that $F(a)$ may depend on b and c (which determine the occupancy of the boundary sites) and may have a residual dependence (modulo 2 or 5) on m. When evaluating (4.1) or (4.3), b, c, and m must be kept fixed.

In each regime, $F(a)$ or $L(j)$ is a sum of products of elliptic functions with different nomes. As in the hard-hexagon[2] and 8VSOS[7] models, there exist mathematical identities that enable us to write M as a simple product of elliptic functions.

The normalized probability $P(a)$ is then given by

$$P(a) = F(a)/M \tag{4.4}$$

$F(a)$ being defined by (3.2), (3.9), (3.18), or (3.22).

Regimes I and II. In these regimes we can immediately use the corresponding identity of the 8VSOS model. These are (3.2.25) and (3.2.27) of Ref. 7. Here we use the conjugate modulus form of these identities, which can be readily obtained from (3.3.18) and (3.1.9) of Ref. 7, together with the convention given after (3.1.2). The identities are given in Ref. 7 for all positive values (even or odd) of an integer r; here we quote them for the case when r is odd, i.e.

$$r = 2n + 1$$

where n is any positive integer. Then the identities can be written as

$$\sum_{a=1}^{n} \theta_1\left(\frac{\pi a}{r}, -t^{r-2}\right)\theta_1\left(\frac{\pi a}{r}, t^2\right) = (r/2)\,\theta_3(0, t^{2r(r-2)})\,\theta_2(0, -t^r) \tag{4.5}$$

$$\sum_{\substack{1\leqslant\tau\leqslant r-2\\ \tau\ \text{odd}}} \theta_1\left(\frac{\pi\tau}{r}, t^{r-2}\right)\lambda_{\tau,(\tau+j)/2} = 2t^{(r-2)/8}Q(t^r) \tag{4.6}$$

where $|t|<1$, j is any odd integer, and the $\lambda_{a,j}$ are defined as functions of t and the integers a, j by (3.10) and (3.11). (We need only (4.6) as written, but it is also true if j is even and the summation is taken through even values of τ from 2 to $r-1$.)

For regimes I and II, $F(a)$ is given by (3.2) and (3.9), where τ_a is defined following (3.3)

$$\tau_1,\ \tau_2,\ \tau_3 = 1, 5, 3 \tag{4.7}$$

Substituting these expressions into (4.1) (and for regime II replacing the a-summation by a sum over τ_a), we obtain precisely the LHS of (4.5) and (4.6), with $r=7$ and $t=\exp(-2\pi s/5)$. Thus

$$M = 7\theta_3(0, e^{-28\pi s})\,\theta_2(0, -e^{-14\pi s/5}) \qquad \text{for regime I} \tag{4.8}$$

$$= 2e^{-\pi s/4}Q(e^{-14\pi s/5}) \qquad \text{for regime II} \tag{4.9}$$

Regime III. Since the summation identities needed for regimes I and II are the same as those of the 8VSOS model, it is natural to see if this is also true in regime III. The corresponding 8VSOS identity can be obtained from (3.3.18c) and (3.1.9) of Ref. 7, correcting the definition (3.3.16) to $s=p^{1/(4r-4)}$. Writing r in Ref. 7 as r_1, we find that we need to take $r_1 = 7/2$, which is not allowed as r_1 must be an integer.

We need to extend the 8VSOS identity to half-integer values of r_1, i.e., to $r_1 = r/2$ where r is an odd integer. This can be done (in some ways it is easier than for integer values). We obtain two relevant identities, true for all odd integers $r\geqslant 3$ and for all complex numbers u, t such that $|t|<1$

$$\sum_{j=1}^{r} \theta_1\left(\frac{4\pi j}{r}, t^{2r-4}\right)\theta_3\left(\frac{2\pi j}{r}-u, t\right) = r\theta_1(2u, t^{2r})\,\theta_4[(r-2)u, t^{r(r-2)}] \tag{4.10a}$$

$$\sum_{j=1}^{r} \theta_1\left(\frac{4\pi j}{r}, t^{2r-4}\right)\theta_2\left(\frac{2\pi j}{r}-u, t\right) = -r\theta_4(2u, t^{2r})\,\theta_1[(r-2)u, t^{r(r-2)}] \tag{4.10b}$$

(These identities can be obtained fairly straightforwardly by using the series expansions of the theta functions: eq. 8.192 of Ref. 10.)

The sum M is given by (4.3), where $L(j)$ is the summand in (3.18). We see that we can evaluate M by using (4.10) with $r=7$, $t=\exp(-\pi s/5)$, $u=\pi\alpha(b, c)/10$. This gives

$$M=7\theta_1\left[\frac{\pi\alpha(b, c)}{5}, e^{-14\pi s/5}\right]\theta_4\left[\frac{\pi\alpha(b, c)}{2}, e^{-7\pi s}\right] \tag{4.11}$$

(From (3.18), $L(j)$ is the sum of two terms, the second containing a factor sign $(b-c)$. From (4.10b), the sum of these terms contains a factor $\theta_1[\pi\alpha(b, c)/2, e^{-7\pi s}]$. Since $\alpha(b, c)$ is even if $b \neq c$, it follows that the sum of the second terms is always zero.)

Regime IV. This case is very similar to regime III. If r_1 is the r of Ref. 7, we find that our results (3.22) look like the 8VSOS ones with $r_1=7/2$. Thus we need to extend the 8VSOS identities to half-integer values of r_1.

We find, for all odd integers $r \geqslant 3$ and all complex numbers u, t with $|t|<1$, that

$$\sum_{j=1}^{r} \theta_1\left(\frac{4\pi j}{r}, -t^{r-4}\right)\theta_3\left(\frac{2\pi j}{r}-u, t\right) = r\theta_1(2u, -t^r)\,\theta_4[(r-4)u, t^{r(r-4)}] \tag{4.12a}$$

$$\sum_{j=1}^{r} \theta_1\left(\frac{4\pi j}{r}, -t^{r-4}\right)\theta_2\left(\frac{2\pi j}{r}-u, t\right) = r\theta_2(2u, -t^r)\,\theta_1[(r-4)u, t^{r(r-4)}] \tag{4.12b}$$

(Again, these identities can be proved using the series expansions of the theta functions.)

The function $L(j)$ is now the summand of (3.22), so we can evaluate M by using (4.12) with $r=7$, $t=\exp(-2\pi s/3)$, and $u=\pi d(b)/6$. As in regime III, the second term in $L(j)$, proportional to $(b-2)\,\xi(s)$, gives zero contribution to M, either because $b=2$ or because (4.12b) gives a result proportional to $\theta_1(\pi)$. Thus

$$M=7\theta_1\left[\frac{\pi d(b)}{3}, -e^{-14\pi s/3}\right]\theta_4\left[\frac{\pi d(b)}{2}, e^{-14\pi s}\right] \tag{4.13}$$

5. PHASES

The local probabilities $P(a)$ are given by (4.4), where for regimes I,..., IV, respectively, $F(a)$ is given by (3.2), (3.9), (3.18), and (3.22), and M is given by (4.8), (4.9), (4.11), (4.13).

As we remarked in Section 2, $P(a)$ may have an implicit dependence on m and on b and c (which determine the occupancy of the boundary sites). From the above results we find no such dependence in regime I, which implies that the system is then in a disordered phase. In regime II, $P(a)$ depends on m, b, c via the integer $m+\alpha(b, c)$ and only on this to modulo 5. The ground states are therefore those in which $m+\alpha(b, c)$ remains constant as m increases, taking $b=3-\sigma_{m+1}$ and $c=3-\sigma_{m+2}$ to depend on m. From (3.4), it follows that in the ground state the occupation numbers $\sigma_1,..., \sigma_{m+2}$ form a sequence that repeats modulo 5

$$\cdots 0\ 1\ 1\ 0\ 2\ 0\ 1\ 1\ 0\ 2\ 0 \cdots \tag{5.1}$$

Thus there are five phases, corresponding to where this sequence begins: these in turn correspond to the five distinct values of $m+\alpha(b, c)$ in (3.9). In some sense there is an element of disorder in regime II, in that fixing $b, c=3, 3$ (i.e., $\sigma_{m+1}, \sigma_{m+2}=0, 0$) gives the same function $P(a)$ as taking $b, c=3, 1$ ($\sigma_{m+1}, \sigma_{m+2}=0, 2$).

In regime III, we see from (3.18) that if $b=c=2$ or 3, then there is no dependence on m: these correspond to the two uniform ground states $\cdots 1\ 1\ 1\ 1 \cdots$ and $\cdots 0\ 0\ 0\ 0 \cdots$. Otherwise $F(a)$ remains constant if b and c alternate as m increases. Thus the ground states are $\cdots 0\ 1\ 0\ 1\ 0\ 1 \cdots$ and $\cdots 0\ 2\ 0\ 2\ 0\ 2 \cdots$: in each case there are two ways of starting the sequence, so in regime III there are two uniform phases and four alternating phases.

In regime IV we find from (3.22) that there is one uniform phase ($b=2$) and two alternating phases ($b=1, 3$), with ground-state sequences

$$1\ 1\ 1\ 1\ 1 \cdots \qquad 0\ 2\ 0\ 2\ 0 \cdots \qquad 2\ 0\ 2\ 0\ 2 \cdots \tag{5.2}$$

6. CRITICAL BEHAVIOR

The Boltzmann weights, and hence the probability $P(a)$ that the center site has $3-a$ particles, are functions of the parameter p. When $p \to 0$, we find in each regime that $P(a) \to P_0(a)$, where for $a=1, 2, 3$

$$P_0(a)=(4/7) \sin^2(\pi a/7) \tag{6.1}$$

This is independent of m, b, c so is the same for all phases. All order parameters (which measure the difference between phases) therefore vanish, suggesting the system is critical at $p=0$.

The Boltzmann weights are given by eq. (4.1) of I and are analytic functions of p that approach their $p=0$ values linearly. We can therefore regard p as a "deviation from criticality" variable, similar to $(T-T_c)/T_c$. Expanding our results for $P(a)$ in powers of p to leading order we find for the four regimes that

$$\text{I} \qquad P(a)/P_0(a) = 1 - (-p)^{2/5}[1 + 2\cos(2\pi a/7)] + O(p, p^{6/5}) \tag{6.2a}$$

$$\text{II} \qquad P(a)/P_0(a) = 1 + 4p^{2/25}\cos(\pi\tau_a/7)\cos\{2\pi[m + \alpha(b, c)]/5\} + O(p^{3/25}) \tag{6.2b}$$

$$\text{III} \qquad P(a)/P_0(a) = 1 - 4p^{3/20}\cos(\pi a/7)\cos[\pi\alpha(b, c)/5] + O(p^{2/5}) + \operatorname{sign}(b-c)(-1)^m\{2^{-3/2}p^{9/160}\sec(4\pi a/7) \times \sec[\pi\alpha(b, c)/10] + O(p^{5/32})\} \tag{6.2c}$$

$$\text{IV} \qquad P(a)/P_0(a) = 1 - 4(-p)^{1/2}\cos(\pi a/7)\cos[\pi d(b)/3] + O(p, p^{4/3}) + (-1)^m(b-2)\{2^{-3/2}(-p)^{5/16}\sec(4\pi a/7) \times \sec[\pi d(b)/6] + O(p^{31/48})\} \tag{6.2d}$$

As in the 8VSOS model,[11] we can define various order parameters, each with its own critical exponent. For regimes II, III, IV, the leading deviations from criticality are proportional to the differences between the $P(a)$ for different phases and have exponents

$$\begin{aligned} \beta &= 2/25 \\ &= 9/160 \\ &= 5/16 \end{aligned} \tag{6.3}$$

for regimes II, III, IV, respectively.

The probabilities $P(a)$ are in general local properties of the model: they depend on the site whose occupation number is taken to be σ_1. For definiteness we have up to now taken this to be the center site, but it could be any site deep within the lattice.

Thus we can fix the boundary conditions (the values of $b=3-\sigma_{m+1}$ and $c=3-\sigma_{m+2}$) and define an average value $\bar{P}(a)$ of $P(a)$ by averaging over central site locations. The effect of this is to average (6.2) over m. In regimes I, III, IV we can immediately obtain the results by simply deleting the terms containing a factor $(-1)^m$. For regime II we have to go to higher order: the calculation is given in Ref. 7, and from (3.3.24) we obtain for regime II

$$\bar{P}(a)/P_0(a) = 1 + p^{2/5}[1 + 2\cos(2\pi\tau_a/7)] + \cdots \tag{6.4}$$

(Note that this differs from the regime I result (6.2a) only by sign factors.)

For regimes I and II the averaged $\bar{P}(a)$ is independent of b and c, i.e., of boundary conditions, so it is natural to treat $\bar{P}(a)$ as a lattice gas density, with critical exponent

$$1 - \alpha = \tfrac{2}{5} \tag{6.5}$$

For regimes III and IV, $\bar{P}(a)$ still depends (via $\alpha(b, c)$ and $d(b)$) on the boundary conditions, so their leading deviations from criticality are order parameters. (In fact, for nonzero p the model lies on a first-order coexistence surface in an extended parameter space, just as the regime III hard-hexagon model does.[12,13] The differences in $\bar{P}(a)$ for different boundary conditions are the discontinuities that occur as this coexistence curve is crossed.) From (6.2c) and (6.2d), the corresponding critical exponents are

$$\begin{aligned} \bar{\beta} &= \tfrac{3}{20} \\ &= \tfrac{1}{2} \end{aligned} \tag{6.6}$$

for regimes III and IV, respectively.

7. SUMMARY

For the three-state model defined in I, we have obtained the local probability $P(a) = F(a)/M$ that a site contains $3 - a$ particles. For the four regimes I,..., IV the results for $F(a)$ are given in (3.2), (3.9), (3.18), (3.22), respectively, and for M in (4.8), (4.9), (4.11) and (4.13).

It would be of interest to extend these calculations to the general n-state model of this type using the $n = 4$ and 5 solutions for w given by Kuniba, Akutsu, and Wadati[6] and our general n-conjectures for the multiple-sum expressions for the polynomials $X_m(a, b, c; q)$. (These conjectures are given in I: $X_m(a, b, c; q)$ is still given by (2.5) and (2.6), but now 2 and 3 in (2.7) are replaced by $n - 1$ and n.) For regime III with $n = 4$ we do have some indications that the $X_m(a, b, c; q)$ may be modular functions, in particular that

$$X_m(4, 4, 4; q) = \{9, 1, 0; q\}_{-} \{5, 1, 0; q^3\}_{-} / Q(q)^2 \tag{7.1}$$

This preliminary result is a conjecture based on the first 125 terms of the series expansion in powers of q. We emphasize that the $n=3$ results (3.1), (3.4)–(3.8), (3.16), (3.20) are *not* such conjectures, but have been rigorously obtained from (2.6). Their proof will be given elsewhere.

Relation to the 8VSOS Model

Part of the motivation for this work was to find a model corresponding to Gordon's generalization of the Rogers–Ramanujan identities, we having come to feel that the 8VSOS model did not fill this role. Certainly this model is quite different from the 8VSOS model, and for finite m the polynomials $X_m(a, b, c; q)$ are *not* those of the 8VSOS model.

It is therefore remarkable that when we take the limit $m \to \infty$ we regain, in regimes I and II, precisely the 8VSOS model results for $P(\tau_a)$ with $r=7$. Also, in regimes III and IV our results are *not* the $r=7$ results of the 8VSOS model, but they *are* very similar to the $r=7/2$ results. In fact, $\bar{P}(a)$ of this paper is the same as $P(a)$ of eqs. (3.3.18c) and (3.3.18d) of Ref. 7, provided r, a, $\theta_4(0,...)$ therein are first replaced by $7/2$, $4a$, $2\theta_4(\pi d,...)$; and d is then taken to be $\alpha(b, c)/2$ in regime III, $d(b)/2$ in regime IV. It will be interesting to see if there are analogous relations for the general n-state model (and to reconcile them for the hard hexagon $n=2$ case, when the lattice gas and 8VSOS models are equivalent).

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