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LETTER TO THE EDITOR

Equation of state and isothermal compressibility for the hard hexagon model in the disordered regime

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Abstract. The equation of state for the hard hexagon model in the disordered regime is computed. The isothermal compressibility is given as a rational function of κ and ρ.

The hard hexagon model is a lattice gas on a triangular lattice with the rule that if a site is occupied, then the six neighbouring sites are necessarily vacant. Baxter (1980, 1981) has shown that this model is exactly solvable by the method of commuting transfer matrices (Baxter 1972, 1982). In the disordered regime, Baxter's exact results are

$$\kappa = \prod_{n=1}^{\infty} \left(\frac{1-x^{5n}}{1-x^{6n}}\right)^2 \frac{(1-x^{5n-1})^2(1-x^{5n-4})^2(1-x^{6n-3})^2(1-x^{6n-2})(1-x^{6n-4})}{(1-x^{5n-2})^3(1-x^{5n-3})^3(1-x^{6n-1})(1-x^{6n-5})} \tag{1}$$

$$\rho = -\prod_{n=1}^{\infty} \frac{(1-x^{6n-3})}{(1-x^{2n-1})(1-x^{5n-1})(1-x^{5n-4})(1-x^{30n-12})(1-x^{30n-18})} \tag{2}$$

$$z = x \prod_{n=1}^{\infty} \left(\frac{(1-x^{5n-1})(1-x^{5n-4})}{(1-x^{5n-2})(1-x^{5n-3})}\right)^5 \tag{3}$$

where κ is the partition function per site in the thermodynamic limit (so $p\beta = \ln \kappa$), ρ is the density, and z is the activity.

It is the purpose of this letter to compute the equation of state in the disordered regime. We find it is of the form

$$P(\kappa, \rho) = 0 \tag{4}$$

where P is a polynomial of degree eight in κ and degree 22 in ρ (see (19) and (20) below). Since the reduced isothermal compressibility, $\chi = k_B T\rho K_T$, $K_T = -(1/V)(\partial V/\partial p)_T$, can also be written as $\chi = \kappa/(\mathrm{d}\kappa/\mathrm{d}\rho)$, we conclude from (4) that

$$\chi = -\kappa \frac{(\partial P/\partial \kappa)}{(\partial P/\partial \rho)} \tag{5}$$

that is, χ is expressed as a rational function of κ and ρ with κ and ρ satisfying (4).

The critical point (Baxter 1980, 1981) of the hard hexagon model

$$\kappa_c = [(27/250)(25+11\sqrt{5})]^{1/2} \qquad \rho_c = (5-\sqrt{5})/10 \tag{6}$$

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is a singular point of the algebraic curve (4). Explicitly, the point (κ_c, ρ_c) is a cusp with tangent line $\kappa - \kappa_c = 0$. Due to the special form of (4) (see (20) below), P, as a polynomial in κ, is solvable by radicals.

From either Baxter's results (1) and (2) or from (4) and (5) one can prove that as $\rho \to \rho_c^-$

$$\chi(\rho) = (\rho_c - \rho)^{-1/2} \sum_{n=0}^{\infty} c_n(\rho_c - \rho)^{n/2} \tag{7}$$

of which the first few terms are

$$\chi(\rho) = [(5+\sqrt{5})/75]t^{-1/2}[1 - 2t^{1/2} + \tfrac{1}{8}(1+4\sqrt{5})t + O(t^{3/2})]$$

with $t = \sqrt{5}(\rho_c - \rho)$. Using (19) and (5), χ is plotted as a function of ρ in figure 1.

A trivial example of our mathematical problem is the problem of going from $x = \cos\theta$, $y = \sin\theta$ to $x^2 + y^2 = 1$. Just as the trigonometric functions are invariant under certain symmetry groups, so are the functions appearing in (1)-(3). If we let $x = e^{2\pi i\tau}$ and define

$$\Gamma_1[N] = \{A \in SL(2, \mathbb{Z}) | A \equiv \pm\left(\begin{smallmatrix}1 & * \\ 0 & 1\end{smallmatrix}\right) \bmod N\}$$

then we have the following theorem as proved by Tracy *et al* (1987).

Theorem. In the disordered regime, $\chi(\tau)$ is a modular function with respect to the group $\Gamma_1[5]$, and $\kappa(\tau)$ and $\rho(\tau)$ are modular functions with respect to the group Γ_1 [30].

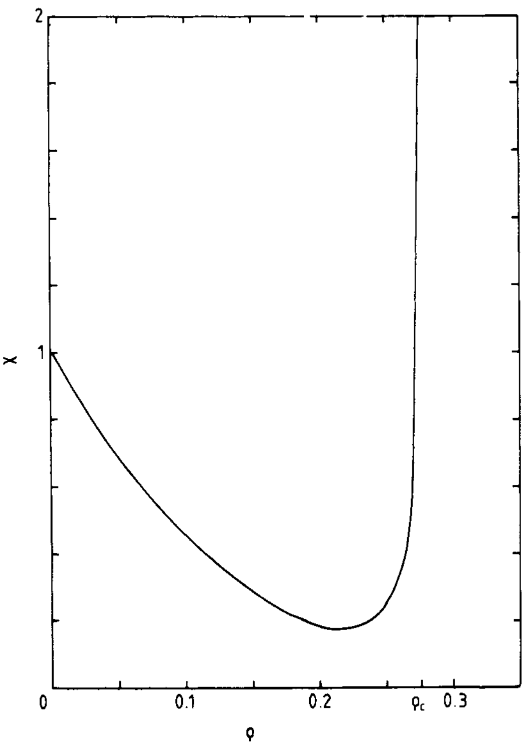

Figure 1. The reduced isothermal compressibility χ as a function of density ρ.

It was also shown that the valence of $\kappa(\tau)$ is 22 and the valence of $\rho(\tau)$ is eight. Modular function theory (Lehner 1964) now tells us there exists a polynomial relation of the form stated above. It is quite important for our method to know both the existence of this polynomial P and to have bounds on its degree.

Before describing the details of our calculation, we stress that the general method has wider applicability, not only to other polynomial relations in the hard hexagon model (for example, there exists a polynomial relation between κ in the disordered regime and κ in the ordered regime) but also to other solvable models. This will be pursued in later work.

The group Γ_1 [30] has 32 inequivalent cusps. One complete set of inequivalent cusps is $\{i\infty, 0, \frac{1}{2}, \frac{1}{3}, \frac{2}{3}, \frac{1}{4}, \frac{1}{5}, \frac{2}{5}, \frac{3}{5}, \frac{4}{5}, \frac{1}{6}, \frac{5}{6}, \frac{1}{7}, \frac{1}{8}, \frac{1}{9}, \frac{2}{9}, \frac{1}{10}, \frac{3}{10}, \frac{7}{10}, \frac{9}{10}, \frac{1}{11}, \frac{1}{12}, \frac{5}{12}, \frac{1}{13}, \frac{1}{14}, \frac{1}{15}, \frac{2}{15}, \frac{4}{15}, \frac{7}{15}, \frac{7}{30}, \frac{11}{30}, \frac{13}{30}\}$. At each of these cusps a local uniforming variable x is introduced and local expansions of κ and ρ are computed. Perhaps the easiest way to see that such expansions exist is to rewrite (1) and (2) in terms of the Dedekind eta function and the generalised Dedekind eta function (see Schoeneberg 1974) and then to appeal to their known transformation properties under $SL(2, \mathbb{Z})$. The details of this can be found in Tracy *et al* (1987); in particular, tables 2, 4 and 5. All the arguments which follow refer to these three tables.

We first show that only even powers of κ appear in (4). Pick $\gamma \in SL(2, \mathbb{Z})$ such that $\gamma(i\infty) = \frac{11}{30}$. For this γ, κ is sent to $-\kappa$ and ρ is sent to itself as seen from tables 4 and 5. Hence

$$P(\kappa, \rho) = 0 = \gamma(P(\kappa, \rho)) = P(\gamma(\kappa), \gamma(\rho)) = P(-\kappa, \rho).$$

We therefore write

$$P(\kappa, \rho) = \sum_{\substack{0 \leq i \leq 22 \\ 0 \leq j \leq 4}} c_{ij} \rho^i \kappa^{2j}. \tag{8}$$

For notational convenience we set $k = \kappa^2$. We now present an algorithm to determine the coefficients c_{ij}.

Step 1. To leading order, at the cusps $\frac{5}{6}$ and $\frac{1}{12}$, we have $k = k_1 x^{-10}$ and $k = k_2 x^{-10}$ with $k_1 = -c_1^2/100$, $k_2 = -c_2^2/100$, $c_1 = \sin^2(\pi/5) \sin^3(2\pi/5)$ and $c_2 = \sin^2(2\pi/5)/\sin^3(\pi/5)$, respectively. The density, to leading order, is $\rho = \rho_0 x^{-1}$ at the cusp $\frac{5}{6}$ and $\rho = -\rho_0 x^{-1}$ at the cusp $\frac{1}{12}$ with $\rho_0 = [4 \sin(\pi/5) \sin(2\pi/5)]^{-1}$. As always, the x refers to the local uniformising variable at the cusp. At either of these cusps, since $P \equiv 0$, we can eliminate terms which contribute poles. The highest-order pole ($=62$) comes from the single term $\rho^{22} k^4$ implying that $c_{22,4} = 0$. Setting $c_{22,4} = 0$ in (8), we look at the coefficient of the next highest pole ($=61$) which must be zero. In this way $c_{j,4} = 0$ for $j = 22, 21, \ldots, 13$. For a pole of order 52, two different terms contribute: $c_{12,4}\rho^{12}k^4 + c_{22,3}\rho^{22}k^3$. Considering the leading behaviour of this expression at both cusps $\frac{5}{6}$ and $\frac{1}{12}$ leads to a system of linear equations

$$A\begin{pmatrix} c_{12,4} \\ c_{22,3} \end{pmatrix} = \begin{pmatrix} \rho_0^{12} k_1^4 & \rho_0^{22} k_1^3 \\ \rho_0^{12} k_2^4 & \rho_0^{22} k_2^3 \end{pmatrix} \begin{pmatrix} c_{12,4} \\ c_{22,3} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{9}$$

which has the unique solution $c_{12,4} = c_{22,3} = 0$. Once we know these coefficients are zero, the next-highest pole is of order 51, resulting in the system

$$A\begin{pmatrix} c_{11,4} \\ c_{21,3} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} c_{11,4} \\ c_{21,3} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{10}$$

Repeating this argument we obtain

$$\begin{pmatrix} c_{j,4} \\ c_{10+j,3} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad \text{for } j = 10, 9, \ldots, 3 \tag{11}$$

corresponding to pole orders 50, 49, . . . , 43, respectively. For a pole of order 42 there are three terms contributing; namely,

$$c_{2,4}\rho^2 k^4 + c_{12,3}\rho^{12}k^3 + c_{22\,2}\rho^{22}k^2. \tag{12}$$

Since there are a pair of cusps and three unknowns, we cannot from this determine the coefficients. However, (12) will give an internal check later.

Step 2. Consider the cusp $\frac{7}{30}$. Here the leading order behaviour is $k = x^{-2}$ and $\rho = 1$. At this cusp, $P(\kappa, \rho)$ will have a pole of order eight coming from terms with a κ^8 $(= k^4)$. In view of step 1, these terms are

$$c_{2,4}\rho^2 k^4 + c_{1,4}\rho k^4 + c_{0,4}k^4.$$

Considering the leading coefficient, this gives

$$c_{2,4} + c_{1,4} + c_{0,4} = 0.$$

Since $P(\kappa, \rho)$ is only defined up to an overall multiplicative factor, one coefficient is arbitrary. We can therefore take

$$c_{0,4} = 1. \tag{13}$$

Set $c_{1,4} = z$, so that $c_{2,4} = -1 - z$.

Step 3. Next consider the cusps $\mathrm{i}\infty$, $\frac{3}{5}$, $\frac{7}{10}$ and $\frac{7}{15}$. Write $k = \sum_{n=0}^{\infty} k_{jn}x^n$ for $j = 1, 2, 3$ and 4 corresponding to cusps $\mathrm{i}\infty$, $\frac{3}{5}$, $\frac{7}{10}$ and $\frac{7}{15}$, respectively (as seen from table 4 each of these points is a holomorphic point of k) where $k_{10} = 1$, $k_{20} = -432$, $k_{30} = -27$, and $k_{40} = 16$. From table 5, the small x expansions of ρ at $\mathrm{i}\infty$ and $\frac{3}{5}$ are identical as are the expansions of ρ at $\frac{7}{10}$ and $\frac{7}{15}$. At each of these four cusps ρ has a simple zero. Write $\rho = \sum_{n=0}^{\infty} \rho_{1n}x^n$ at cusps $\mathrm{i}\infty$ and $\frac{3}{5}$ and write $\rho = \sum_{n=0}^{\infty} \rho_{2n}x^n$ at cusps $\frac{7}{10}$ and $\frac{7}{15}$, and find from table 5 that $\rho_{11} = -1$ and $\rho_{21} = 1$. For notational convenience write

$$P(\kappa, \rho) = \sum_{i=0}^{22} \rho^i q_i \qquad q_i = \sum_{j=0}^{4} c_{ij}k^j \tag{14}$$

and let $P(n) = \sum_{i=0}^{n} \rho^i q_i$. At these four cusps, the x^0 term of the x expansion of P comes from q_0, thus giving

$$c_{00} + c_{01}k_{j0} + c_{02}(k_{j0})^2 + c_{03}(k_{j0})^3 + c_{04}(k_{j0})^4 = 0 \tag{15}$$

where, as before, $j = 1, 2, 3, 4$ corresponds to cusps $\mathrm{i}\infty$, $\frac{3}{5}$, $\frac{7}{10}$ and $\frac{7}{15}$, respectively. This leads to the system of equations

$$B\begin{pmatrix} c_{00} \\ c_{01} \\ c_{02} \\ c_{03} \end{pmatrix} = \begin{pmatrix} 1 & k_{10} & k_{10}^2 & k_{10}^3 \\ 1 & k_{20} & k_{20}^2 & k_{20}^3 \\ 1 & k_{30} & k_{30}^2 & k_{30}^3 \\ 1 & k_{40} & k_{40}^2 & k_{40}^3 \end{pmatrix}\begin{pmatrix} c_{00} \\ c_{01} \\ c_{02} \\ c_{03} \end{pmatrix} = -\begin{pmatrix} k_{10}^4 \\ k_{20}^4 \\ k_{30}^4 \\ k_{40}^4 \end{pmatrix}. \tag{16}$$

Since B is invertible, the coefficients c_{0j}, $j = 0, 1, 2, 3$, are now uniquely determined and hence q_0 is now determined.

The coefficient of x^1 in P is completely determined by $P(1)$. If $f(x)=\Sigma\, a_n x^n$ is a cusp expansion at cusp p/q, denote by $\mathrm{coef}(f, x^n, p/q)$ the coefficient a_n. Then extracting the coefficient of x^1 from $P(1)$ we obtain the system

$$B\begin{pmatrix} c_{10} \\ c_{11} \\ c_{13} \\ c_{14} \end{pmatrix} = -z\begin{pmatrix} k_{10}^4 \\ k_{20}^4 \\ k_{30}^4 \\ k_{40}^4 \end{pmatrix} + \begin{pmatrix} \mathrm{coef}(q_0, x, i\infty) \\ \mathrm{coef}(q_0, x, \frac{3}{5}) \\ -\mathrm{coef}(q_0, x, \frac{7}{10}) \\ -\mathrm{coef}(q_0, x, \frac{7}{15}) \end{pmatrix}. \tag{17}$$

Thus c_{ij}, $j=0, 1, 2, 3$ and q_1 are determined in terms of $z=c_{14}$. We may repeat this process for each of the coefficients $x^2, x^3, \ldots, x^{13}$, obtaining equations of similar structure to (17). In each case we can determine c_{i0}, c_{i1}, c_{i2}, and c_{i3}, $i=3, 4, \ldots, 13$ as a function of z. At the $i=13$ stage, however, we already know from (11) that $c_{13,3}=0$. This condition determines z. Now the above process can be repeated for x^{14}, $x^{15}, \ldots, x^{22}$ terms. This determines all the coefficients c_{ij} in (8).

The above algorithm was implemented on a SUN 3/50 workstation using the computer algebra software SMP. The results are more easily displayed if we first make the change of variable

$$y = \rho - 1. \tag{18}$$

We denote by $P(k, y)$ the function $P(\sqrt{k}, y+1)$ defined by (8). This should not cause any confusion. Write

$$P(k, y) = \sum_{i=0}^{4} g_i k^i \tag{19a}$$

then

$$\begin{aligned} g_0 &= 432^2 y^{22} \qquad g_1 = -432 y^{10} g_3 \\ g_2 &= 16y^4 + 192y^5 + 645y^6 - 516y^7 - 5826y^8 - 4116y^9 \\ &\quad + 9349y^{10} - 11400y^{11} - 42672y^{12} - 9800y^{13} \\ &\quad + 7350y^{14} - 4500y^{15} + 1750y^{16} + 3125y^{22} \\ g_3 &= -1 - 12y - 48y^2 - 56y^3 + 42y^4 + 12y^5 - 100y^6 + 132y^7 + 625y^{12} \\ g_4 &= y^2. \end{aligned} \tag{19b}$$

Equation (19) can be rewritten as

$$y^2(432y^{10} - k^2 - kg_3/2y^2)^2 - (k^2/4y^2)M = 0 \tag{20a}$$

where

$$\begin{aligned} M = {} & (1+5y+5y^2)^3(1+y+y^2)(1+4y-5y^2-10y^3 \\ & +44y^4 - 88y^5 + 121y^6 - 110y^7 + 55y^8)^2. \end{aligned} \tag{20b}$$

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