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LETTER TO THE EDITOR

Exact results for the activity and isothermal compressibility of the hard-hexagon model

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Abstract. The Klein and Fricke theory of modular functions is used to derive closed-form algebraic expressions for the activity $z(\rho)$ and isothermal compressibility $\kappa_T(\rho)$ of the hard-hexagon lattice gas model in the disordered regime, where ρ is the dimensionless number density. Similar results which are valid in the ordered regime are also presented.

The hard-hexagon lattice gas model (Gaunt and Fisher 1965, Runnels and Combs 1966, Gaunt 1967) was solved exactly by Baxter (1980, 1981) using the method of corner transfer matrices (Baxter 1972, 1982). In particular, in the disordered regime Baxter obtained the basic results

$$\Xi = \frac{H^3(x)}{G^2(x)} \prod_{n=1}^{\infty} \frac{(1-x^{6n-4})(1-x^{6n-3})^2(1-x^{6n-2})(1-x^{5n})^2}{(1-x^{6n-5})(1-x^{6n-1})(1-x^{6n})^2} \tag{1}$$

$$\rho = -xG(x)H(x^6)P(x^3)/P(x) \tag{2}$$

$$z = -x[H(x)/G(x)]^5 \tag{3}$$

where Ξ is the grand partition function per site in the thermodynamic limit, ρ is the dimensionless number density, z is the activity of the gas,

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

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

$$P(x) = \prod_{n=1}^{\infty} (1-x^{2n-1}) \tag{6}$$

and x is a non-physical parameter with $-1 < x \leqslant 0$. When $x \to -1+$ the model exhibits an order–disorder phase transition with critical values for ρ and z given by

$$\rho_c = \tfrac{1}{10}(5-\sqrt{5}) \tag{7}$$

and

$$z_c = \tfrac{1}{2}(11+5\sqrt{5}) \tag{8}$$

respectively. Baxter also derived similar results in the ordered regime $z_c < z < \infty$.

Recently Tracy *et al* (1987) have proved that if we write

$$x = \exp(2\pi i \tau) \tag{9}$$

where τ is a complex variable in the upper half-plane, then the quantities (1)–(3) are modular functions of τ with respect to certain congruence subgroups of the modular group (Schoeneberg 1974). From this result and standard theorems in modular function theory it is possible to establish the existence of various polynomial equations which are satisfied by the functions $\Xi(\tau)$, $\rho(\tau)$ and $z(\tau)$. In particular, Richey and Tracy (1987) have shown that $\Xi(\tau)$ and $\rho(\tau)$ satisfy a polynomial relation of the type

$$\sum_{i=0}^{22}\sum_{j=0}^{4} c_{ij}\rho^i\Xi^{2j}=0 \tag{10}$$

where the coefficients c_{ij} are real constants. The basic equation of state (10) was used by Richey and Tracy to express the isothermal compressibility $\kappa_T(\rho)$ in the disordered regime as a rational function of Ξ and ρ.

The main aim in this letter is to demonstrate that the polynomial equation for the modular functions $\rho(\tau)$ and $z(\tau)$ can be obtained *directly* from the classic work of Klein and Fricke (1892). This polynomial relation will then be used to derive *explicit* closed-form expressions for the functions $z(\rho)$ and $\kappa_T(\rho)$ in the disordered regime. Similar formulae which are valid in the *ordered* regime will also be given.

We begin by applying the Ramanujan identity

$$P(x^3)/P(x)=[H(x)G(x^6)-xG(x)H(x^6)]^{-1} \tag{11}$$

to (2). The result (11) was stated by Ramanujan in an unpublished manuscript (see Birch 1975) and proved by Rogers (1921). Hence we find that

$$x[H(x^6)/G(x^6)]=-[H(x)/G(x)][\rho/(1-\rho)]. \tag{12}$$

Next we express (3) and (12) in terms of the icosahedral function (Klein and Fricke 1892, p 383)

$$\zeta(\tau)=x^{1/5}[H(x)/G(x)] \tag{13}$$

where $x=\exp(2\pi i\tau)$. In this manner we obtain the basic equations

$$\zeta^5(\tau)=-z(\tau) \tag{14}$$

and

$$\zeta(6\tau)=-\zeta(\tau)\rho(\tau)/[1-\rho(\tau)]. \tag{15}$$

The function $\zeta(\tau)$ is a univalent modular function (or hauptmodul) for the principal congruence subgroup $\Gamma(5)$, and is of special interest since every modular function associated with $\Gamma(5)$ can be expressed as a rational function of $\zeta(\tau)$. It is also known that the two functions $\zeta(\tau)$ and $\zeta(n\tau)$, where $n=2,3,4,\ldots$, must satisfy a polynomial modular equation (see Klein and Fricke 1892, Mordell 1922). For the case $n=6$ the detailed structure of this modular equation can be determined from the work of Klein and Fricke (1892, pp 137-9, 150-1). It is found that

$$\begin{aligned}187[&42\zeta_1^5\zeta_6^5(\zeta_1+\zeta_6)-42(\zeta_1+\zeta_6)+(\zeta_1^6+\zeta_6^6)+36\zeta_1\zeta_6(\zeta_1^4+\zeta_6^4)\\
&+225\zeta_1^2\zeta_6^2(\zeta_1^2+\zeta_6^2)+400\zeta_1^3\zeta_6^3]^2\\
&-882(\zeta_6-\zeta_1)^2\{374(\zeta_1^{10}\zeta_6^{10}+1)-66(\zeta_1^5\zeta_6^5-1)[21(\zeta_1^5+\zeta_6^5)\\
&+175\zeta_1\zeta_6(\zeta_1^3+\zeta_6^3)+450\zeta_1^2\zeta_6^2(\zeta_1+\zeta_6)]+(\zeta_1^{10}+\zeta_6^{10})\\
&+100\zeta_1\zeta_6(\zeta_1^8+\zeta_6^8)+2025\zeta_1^2\zeta_6^2(\zeta_1^6+\zeta_6^6)+14\,400\zeta_1^3\zeta_6^3(\zeta_1^4+\zeta_6^4)\\
&+44\,100\zeta_1^4\zeta_6^4(\zeta_1^2+\zeta_6^2)+63\,504\zeta_1^5\zeta_6^5\}\\
&+1936(\zeta_6-\zeta_1)^6[42\zeta_1^5\zeta_6^5(\zeta_1+\zeta_6)-42(\zeta_1+\zeta_6)+(\zeta_1^6+\zeta_6^6)\\
&+36\zeta_1\zeta_6(\zeta_1^4+\zeta_6^4)+225\zeta_1^2\zeta_6^2(\zeta_1^2+\zeta_6^2)+400\zeta_1^3\zeta_6^3]\\
&-1241(\zeta_6-\zeta_1)^{12}=0\end{aligned} \tag{16}$$

where $\zeta_1 \equiv \zeta(\tau)$ and $\zeta_6 \equiv \zeta(6\tau)$. If (14) and (15) are substituted in this result we obtain the required polynomial relation:

$$\rho(1-\rho)^{11}-(1-\rho)^5 P_1(\rho)z+\rho^2(1-\rho)^2 P_2(\rho)z^2-\rho^5 P_1(\rho)z^3+\rho^{11}(1-\rho)z^4=0 \tag{17}$$

where

$$P_1(\rho)=(1-13\rho+66\rho^2-165\rho^3+220\rho^4-165\rho^5+77\rho^6-22\rho^7) \tag{18}$$

$$P_2(\rho)=(1-13\rho+63\rho^2-125\rho^3+6\rho^4+401\rho^5-689\rho^6+476\rho^7-119\rho^8). \tag{19}$$

Equation (17) was first derived by the present author several years ago in unpublished work, and was used to investigate the singularity structure of the virial series for the hard-hexagon model (see Gaunt and Joyce 1980).

Next we establish a closed-form expression for the physical branch of the algebraic function $z=z(\rho)$ by solving the quartic equation (17). The final result is

$$\begin{aligned}4\rho^6(1-\rho)z(\rho)&=(1-5\rho+5\rho^2)^2\sqrt{Q_1(\rho)}+Q_2(\rho)\\&\quad-(1-5\rho+5\rho^2)[2Q_3(\rho)+2Q_2(\rho)\sqrt{Q_1(\rho)}]^{1/2}\end{aligned} \tag{20}$$

where

$$Q_1(\rho)=(1-\rho+\rho^2)(1-5\rho+5\rho^2) \tag{21}$$

$$Q_2(\rho)=(1-2\rho)(1-11\rho+44\rho^2-77\rho^3+66\rho^4-33\rho^5+11\rho^6) \tag{22}$$

$$\begin{aligned}Q_3(\rho)=(1&-16\rho+106\rho^2-378\rho^3+803\rho^4-1080\rho^5+962\rho^6\\&-576\rho^7+219\rho^8-50\rho^9+10\rho^{10}).\end{aligned} \tag{23}$$

The physical branch $z(\rho)$ has a Taylor series representation about $\rho=0$ with a radius of convergence

$$\rho_r=\tfrac{1}{10}\sqrt{5}[(4\sqrt{10}-5\sqrt{5}+5)-\sqrt{10}(4\sqrt{10}-5\sqrt{5}-4\sqrt{2}+7)^{1/2}]^{1/2} \tag{24}$$

which is *less than* ρ_c (see Joyce 1988), whereas the critical behaviour of $z(\rho)$ as $\rho \to \rho_c-$ is described by the Puiseux expansion (see Hille 1973):

$$\begin{aligned}z/z_c=1-5^{3/2}y^3[1&+\tfrac{3}{2}y+\tfrac{21}{8}y^2-\tfrac{1}{2}(-6+5\sqrt{5})y^3-\tfrac{3}{128}(-77+320\sqrt{5})y^4\\&-\tfrac{3}{4}(9+25\sqrt{5})y^5-\tfrac{1}{1024}(10\,739+35\,520\sqrt{5})y^6-\tfrac{15}{4}(-1+13\sqrt{5})y^7\\&+\tfrac{3}{32\,768}(1138\,969-209\,280\sqrt{5})y^8+3(131+45\sqrt{5})y^9\\&+\tfrac{3}{262\,144}(91\,333\,921+51\,570\,560\sqrt{5})y^{10}+\ldots]\end{aligned} \tag{25}$$

where

$$y=[\sqrt{5}(\rho_c-\rho)]^{1/2}. \tag{26}$$

It can be shown that the radius of convergence of this expansion is

$$y_r=\tfrac{1}{2}\sqrt{2}[(4\sqrt{10}-5\sqrt{5}+1)-\sqrt{2}(4\sqrt{10}-5\sqrt{5}-4\sqrt{2}+7)^{1/2}]^{1/4}. \tag{27}$$

We now determine the isothermal compressibility κ_T in the disordered regime by using formula (20) to evaluate the thermodynamic relation

$$\kappa_T^* \equiv k_B T\rho\kappa_T=(z/\rho)(dz/d\rho)^{-1}. \tag{28}$$

In this manner we obtain

$$\frac{2(1-\rho)}{\kappa_T^*}=-5+\frac{[R_1(\rho)+R_2(\rho)(1-\rho+\rho^2)^{-1}\sqrt{Q_1(\rho)}]}{[2Q_3(\rho)+2Q_2(\rho)\sqrt{Q_1(\rho)}]^{1/2}} \tag{29}$$

where

$$R_1(\rho)=(7-44\rho+99\rho^2-110\rho^3+55\rho^4) \tag{30}$$

$$R_2(\rho)=(1-2\rho)(7-16\rho+21\rho^2-10\rho^3+5\rho^4) \tag{31}$$

and $0\leqslant\rho\leqslant\rho_c$. It follows from the closed-form expression (29) that the reduced isothermal compressibility κ_T^* satisfies the polynomial equation

$$\begin{aligned}(1-\rho)^4(1-\rho+\rho^2)^2S_1(\rho)+10(1-\rho)^3(1-\rho+\rho^2)^2S_1(\rho)\kappa_T^*\\ +(1-\rho)^2(1-\rho+\rho^2)S_2(\rho)(\kappa_T^*)^2-210\rho(1-\rho)^2Q_1(\rho)(\kappa_T^*)^3\\ -36(1-5\rho+5\rho^2)(\kappa_T^*)^4=0\end{aligned} \tag{32}$$

where

$$S_1(\rho)=(1-10\rho+33\rho^2-36\rho^3+18\rho^4-70\rho^5+140\rho^6-100\rho^7+25\rho^8) \tag{33}$$

$$\begin{aligned}S_2(\rho)=(25-317\rho+1352\rho^2-2395\rho^3+2385\rho^4-3100\rho^5+5700\rho^6-7750\rho^7\\ +6625\rho^8-3125\rho^9+625\rho^{10})\end{aligned} \tag{34}$$

and $0\leqslant\rho<\rho_c$.

The quartic equation (32) can be used to expand κ_T^* in the form

$$\kappa_T^*=\sum_{l=0}^{\infty}k_l\rho^l \qquad |\rho|<\rho_r \tag{35}$$

where ρ_r is defined in (24). A list of the coefficients k_l is given in table 1 for $l\leqslant 24$. The coefficients k_l for $l\leqslant 7$ were calculated by Gaunt (1967) using diagrammatic

Table 1. Coefficients k_l in the expansion (35).

l	k_l
0	1
1	−7
2	18
3	−24
4	24
5	6
6	66
7	258
8	1 014
9	3 906
10	14 760
11	54 696
12	198 510
13	704 010
14	2 431 110
15	8 130 096
16	26 103 624
17	79 292 226
18	221 534 442
19	532 863 372
20	870 102 906
21	−842 584 128
22	−17 420 140 980
23	−111 985 825 752
24	−559 952 980 782

methods. It is found from formula (29) that the function $\kappa_T^*(\rho)$ exhibits two non-physical branch point singularities on the circle of convergence $|\rho| = \rho_r$ at

$$\rho_0^{\pm} = \tfrac{1}{2} - \tfrac{1}{20}\sqrt{10}[(4\sqrt{10} - 5\sqrt{5} - 4\sqrt{2} + 7)^{1/2} \pm i(4\sqrt{10} - 5\sqrt{5} + 4\sqrt{2} - 7)^{1/2}]. \tag{36}$$

These singularities give rise to an interesting periodic variation in the sign of the coefficient k_l as $l \to \infty$. The critical behaviour of κ_T^* as $\rho \to \rho_c-$ may also be determined from (32) by applying the Puiseux expansion method to the singular point ρ_c. This procedure yields

$$\begin{aligned}\kappa_T^* = \tfrac{1}{75}(5+\sqrt{5})y^{-1}[1 &- 2y + \tfrac{1}{8}(1+4\sqrt{5})y^2 + \tfrac{1}{2}(5-2\sqrt{5})y^3 \\ &+ \tfrac{1}{128}(479+40\sqrt{5})y^4 + \tfrac{1}{4}(29+3\sqrt{5})y^5 \\ &+ \tfrac{1}{1024}(13\,889+2076\sqrt{5})y^6 + \tfrac{1}{2}(45+8\sqrt{5})y^7 \\ &+ \tfrac{1}{32\,768}(1031\,867+255\,440\sqrt{5})y^8 + \tfrac{1}{4}(99+53\sqrt{5})y^9 \\ &+ \tfrac{7}{262\,144}(-1616\,383+735\,604\sqrt{5})y^{10} + \ldots]\end{aligned} \tag{37}$$

where the variable y is defined in (26) and $|y| < y_r$.

In principle the grand partition function per site $\Xi(\rho)$ in the disordered regime can be determined from formula (29) by using the relation

$$\ln\Xi(\rho) = \int [\kappa_T^*(\rho)]^{-1}\, d\rho + C_1 \tag{38}$$

where C_1 is a constant of integration. It is clear, however, that the *direct* evaluation of the integral (38) is a difficult task. It is fortunate, therefore, that a closed-form expression for $\Xi(\rho)$ may be readily obtained by solving the implicit equation of state (10) established by Richey and Tracy (1987). The final result is

$$\begin{aligned}4u^2\Xi^2 = T_1(u) &- (1+u+u^2)^{1/2}(1+5u+5u^2)^{3/2}T_2(u) \\ &+ [2T_3(u) - 2(1+u+u^2)^{1/2}(1+5u+5u^2)^{3/2}T_1(u)T_2(u)]^{1/2}\end{aligned} \tag{39}$$

where

$$T_1(u) = (1 + 12u + 48u^2 + 56u^3 - 42u^4 - 12u^5 + 100u^6 - 132u^7 - 625u^{12}) \tag{40}$$

$$T_2(u) = (1 + 4u - 5u^2 - 10u^3 + 44u^4 - 88u^5 + 121u^6 - 110u^7 + 55u^8) \tag{41}$$

$$\begin{aligned}T_3(u) = (1 &+ 24u + 240u^2 + 1264u^3 + 3564u^4 + 4344u^5 - 1016u^6 - 4104u^7 \\ &+ 5562u^8 + 568u^9 - 11\,388u^{10} + 16\,920u^{11} - 6780u^{12} - 18\,600u^{13} \\ &+ 44\,496u^{14} - 50\,400u^{15} + 37\,800u^{16} + 24\,000u^{17} \\ &- 128\,500u^{18} + 165\,000u^{19} + 384\,375u^{24})\end{aligned} \tag{42}$$

$$u = \rho - 1 \tag{43}$$

and $0 \leq \rho \leq \rho_c$.

If the expansion (35) is substituted in (38) we can construct the virial series for the reduced pressure of the gas

$$pa_0/k_B T = \ln\Xi(\rho) = \sum_{l=1}^{\infty} B_l \rho^l \qquad |\rho| < \rho_r \tag{44}$$

where a_0 is the area of a unit cell in the lattice. The values of the virial coefficients B_l have already been given by Gaunt and Joyce (1980) for $l \leqslant 24$. In a similar manner the Puiseux expansion (37) may be used to determine the critical behaviour of $p(\rho)$ as $\rho \to \rho_c-$. We find that

$$\begin{aligned}(p_c - p)a_0/k_B T = \tfrac{5}{2}(\sqrt{5}-1)y^3[1 + \tfrac{3}{2}y + \tfrac{3}{40}(31 - 4\sqrt{5})y^2 \\ + \tfrac{1}{2}(5-\sqrt{5})y^3 - \tfrac{3}{128}(-37+40\sqrt{5})y^4 - \tfrac{9}{8}(7+\sqrt{5})y^5 \\ - \tfrac{11}{3072}(8943 + 196\sqrt{5})y^6 - \tfrac{9}{10}(97 - 3\sqrt{5})y^7 \\ - \tfrac{3}{32\,768}(2049\,079 - 139\,952\sqrt{5})y^8 - \tfrac{3}{2}(213 - 25\sqrt{5})y^9 \\ - \tfrac{9}{262\,144}(10\,051\,017 - 2469\,676\sqrt{5})y^{10} + \ldots]\end{aligned} \qquad (45)$$

where

$$p_c a_0/k_B T = \tfrac{1}{2}\ln[\tfrac{27}{250}(25 + 11\sqrt{5})] \qquad (46)$$

and the variable y is defined in (26).

Finally, we note that modular function theory also enables one to derive closed-form expressions for $z(\rho)$, $\kappa_T^*(\rho)$ and $\Xi(\rho)$ which are valid in the *ordered* regime $\rho_c < \rho < \tfrac{1}{3}$. In particular, we have

$$\begin{aligned}[z(\rho)]^{-1} = -\tfrac{1}{2}(2-3\rho)^{-1}(1-\rho)^{-3}[(1 - 12\rho + 45\rho^2 - 66\rho^3 + 33\rho^4) \\ + (-1 + 5\rho - 5\rho^2)^{3/2}(-1 + 9\rho - 9\rho^2)^{1/2}]\end{aligned} \qquad (47)$$

and

$$\begin{aligned}[\kappa_T^*(\rho)]^{-1} = 3(1-3\rho)^{-1}(2-3\rho)^{-1}(1-\rho)^{-1}[(-1+5\rho-5\rho^2) \\ + (1-2\rho)(-1+5\rho-5\rho^2)^{1/2}(-1+9\rho-9\rho^2)^{-1/2}].\end{aligned} \qquad (48)$$

A more detailed discussion and analysis of these results is given elsewhere (Joyce 1988).

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