On the Dhar directed-site animals-enumeration problem for the simple cubic lattice

1989 J. Phys. A: Math. Gen. 22 L919

(http://iopscience.iop.org/0305-4470/22/19/001)

J. Phys. A: Math. Gen. 22 (1989) L919–L924. Printed in the UK

LETTER TO THE EDITOR

On the Dhar directed-site animals-enumeration problem for the simple cubic lattice

G S Joyce
Wheatstone Physics Laboratory, King's College, Strand, London WC2R 2LS, UK

Received 22 June 1989

Abstract. It is proved that the generating function $A(y)$ for the Dhar directed-site animals-enumeration problem on the simple cubic lattice is an *algebraic* function. This result is used to analyse the detailed critical behaviour of $A(y)$ as $y \to y_c-$, where $y_c = \frac{1}{22}(-9+5\sqrt{5})$. Next an asymptotic expansion for the total number A_n of directed lattice animals with n sites is derived. Finally, an exact closed-form expression for the generating function $A(y)$ is given.

Dhar (1983) has obtained an exact solution for a directed-site animals-enumeration problem (Stanley *et al* 1982) on the simple cubic lattice with nearest-neighbour and next-nearest-neighbour connections. In particular, it was shown that the generating function for the problem

$$A(y) = \sum_{n=1}^{\infty} A_n y^n \tag{1}$$

where A_n is the total number of directed lattice animals with n sites, can be expressed in the form

$$A(y) = -\rho(z) \tag{2}$$

with

$$z = -y/(1+y) \tag{3}$$

where $\rho(z)$ is the mean density function for the hard-hexagon lattice-gas model in the disordered regime (Gaunt and Fisher 1965, Gaunt 1967) and z is the activity parameter for the lattice gas. The application of known exact results for the hard-hexagon model (Baxter 1980, 1981) to the basic relation (2) enabled Dhar to prove that

$$A_n \sim a_0 \lambda^n n^{-5/6}[1 + a_1 n^{-5/6} + \mathrm{O}(1/n)] \tag{4}$$

as $n \to \infty$, where

$$\lambda = \tfrac{1}{2}(9+5\sqrt{5}) \tag{5}$$

and a_0, a_1 are constants.

The main purpose of this letter is to demonstrate that the theory of modular functions (Klein and Fricke 1892, Schoeneberg 1974) can be used to determine the

0305-4470/89/190919+06$02.50

detailed mathematical properties of the generating function $A(y)$. We begin by considering the following parametric representation for the mean density function in the disordered regime (Baxter 1981):

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

$$z(x) = -x(H(x)/G(x))^5 \tag{7}$$

where

$$G(x) = \prod_{n=1}^{\infty} [(1-x^{5n-4})(1-x^{5n-1})]^{-1} \tag{8}$$

$$H(x) = \prod_{n=1}^{\infty} [(1-x^{5n-3})(1-x^{5n-2})]^{-1} \tag{9}$$

and x is a non-physical parameter with $-1 < x < 1$. Next we write equations (6) and (7) in the alternative τ-parametric form

$$\rho(\tau) = (1 - \{\zeta(\tau)/\zeta(6\tau)\})^{-1} \tag{10}$$

$$z(\tau) = -\zeta^5(\tau) \tag{11}$$

where

$$\zeta(\tau) = x^{1/5}(H(x)/G(x)) \tag{12}$$

is the icosahedral function (Klein and Fricke 1892, p 383),

$$x = \exp(2\pi i \tau) \tag{13}$$

and the parameter τ lies in the upper half of the complex τ-plane with $\mathrm{Re}(\tau) = 0$ or $\frac{1}{2}$.

The function $\zeta(\tau)$ is a univalent modular function (or hauptmodul) for the principal congruence subgroup $\Gamma(5)$, and is of particular importance because every modular function associated with $\Gamma(5)$ can be expressed as a rational function of $\zeta(\tau)$. It can also be shown 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 $n = 6$ this modular equation has the form

$$\begin{aligned}\zeta_6^{11}\zeta_1^{11} &+ (\zeta_6^{12}\zeta_1^5 + \zeta_6^5\zeta_1^{12}) + 6(\zeta_6^{11}\zeta_1^6 + \zeta_6^6\zeta_1^{11}) + 9(\zeta_6^{10}\zeta_1^7 + \zeta_6^7\zeta_1^{10}) - 5(\zeta_6^9\zeta_1^8 + \zeta_6^8\zeta_1^9)\\ &- (\zeta_6^{10}\zeta_1^2 + \zeta_6^2\zeta_1^{10}) - 5(\zeta_6^9\zeta_1^3 + \zeta_6^3\zeta_1^9)\\ &+ 36(\zeta_6^7\zeta_1^5 + \zeta_6^5\zeta_1^7) + 59\zeta_6^6\zeta_1^6 - (\zeta_6^7 + \zeta_1^7) - 6(\zeta_6^6\zeta_1 + \zeta_6\zeta_1^6)\\ &- 9(\zeta_6^5\zeta_1^2 + \zeta_6^2\zeta_1^5) + 5(\zeta_6^4\zeta_1^3 + \zeta_6^3\zeta_1^4) + \zeta_6\zeta_1 = 0\end{aligned} \tag{14}$$

where $\zeta_1 \equiv \zeta(\tau)$ and $\zeta_6 \equiv \zeta(6\tau)$. We can now use equations (10) and (11) to eliminate ζ_1 and ζ_6 from the modular equation (14). This procedure yields the further polynomial equation

$$\sum_{i=0}^{12} \sum_{j=0}^{4} \rho^i(z) b_{ij} z^j = 0 \tag{15}$$

where the coefficients b_{ij} are integral constants. (The numerical values of the integers b_{ij} are readily obtained from the work of Joyce (1988).) If we apply equations (2) and

(3) to this result we find that the generating function $A(y)$ is an *algebraic* function which satisfies a polynomial equation of the type

$$f(A, y) \equiv \sum_{i=0}^{12} \sum_{j=0}^{4} A^i(y) c_{ij} y^j = 0. \tag{16}$$

The numerical values of the coefficients c_{ij} are listed in table 1.

Next we use the Sylvester determinant to eliminate $A(y)$ from the equations $f(A, y) = 0$ and $\partial f(A, y)/\partial A = 0$, (Goursat 1959, Bliss 1966). This procedure yields the resultant polynomial

$$\mathrm{Res}(f, \partial f/\partial A; A) \equiv 2^8 \times 3^9 y^{22}(y+1)^{22}(11y^2+9y-1)^{24}. \tag{17}$$

It follows from the zeros of the resultant (17) that the 12-branched algebraic function $A(y)$ has singular points in the finite y-plane at $y = 0$, -1, y_c and $-(11y_c)^{-1}$, where

$$y_c = \tfrac{1}{22}(-9 + 5\surd 5). \tag{18}$$

The *physical* branch $A(y)$ is clearly analytic at $y = 0$ and has a Taylor series representation (1) with a radius of convergence y_c. We can determine the Taylor series coefficients A_n by using the Newton–Raphson iteration method to obtain a symbolic solution of (16). In table 2 we list the numerical values of A_n for $n \leqslant 24$.

The behaviour of the generating function $A(y)$ in the neighbourhood of the branch-point y_c can also be found by applying the Newton–Raphson method to (16) provided that suitable local transformations are made to the variables A and y. In this manner we obtain the Puiseux expansion (see Hille 1973):

$$A(y) = (u\surd 5)^{-1}\left(1 + \sum_{n=1}^{\infty} d_n u^n\right) \tag{19}$$

where

$$u = \xi^{1/6}[1 - (y/y_c)]^{1/6} \tag{20}$$

$$\xi = \tfrac{1}{50}(-25 + 13\surd 5). \tag{21}$$

A list of the non-zero coefficients d_n is given in table 3 for $n \leqslant 24$. (It should be noted that the coefficient d_n is zero for $n = 2$, 3, 4, 8, 9 and 14.) We can now establish the

Table 1. Coefficients c_{ij} in the polynomial equation (16).

i	$j=0$	$j=1$	$j=2$	$j=3$	$j=4$
0	0	1	3	3	1
1	−1	14	48	50	17
2	−11	97	358	381	131
3	−55	415	1 590	1 715	595
4	−165	1 180	4 620	5 040	1 765
5	−330	2 321	9 207	10 130	3 574
6	−462	3 247	12 832	14 062	4 939
7	−462	3 300	12 408	13 002	4 356
8	−330	2 475	7 920	6 930	1 815
9	−165	1 375	2 860	715	−605
10	−55	550	220	−1 595	−1 210
11	−11	143	−219	−988	−616
12	−1	18	−59	−198	−121

Table 2. Coefficients A_n in the series expansion (1)

n	A_n
1	1
2	6
3	45
4	365
5	3 101
6	27 144
7	242 636
8	2 202 873
9	20 241 055
10	187 766 940
11	1 755 409 652
12	16 517 284 570
13	156 265 005 369
14	1 485 269 469 971
15	14 174 126 304 850
16	135 741 870 538 293
17	1 303 996 171 096 108
18	12 561 249 340 326 373
19	121 298 814 197 201 725
20	1 173 923 653 088 144 637
21	11 383 888 351 299 784 090
22	110 593 459 758 405 535 558
23	1 076 185 941 425 661 372 698
24	10 488 271 889 303 327 382 712

Table 3. Non-zero coefficients d_n in the Puiseux expansion (19).

n	d_n
1	$-\frac{1}{2}(1+\sqrt{5})$
5	2
6	$-\frac{1}{66}(123+5\sqrt{5})$
7	-1
10	3
11	$\frac{2}{33}(81+10\sqrt{5})$
12	$-\frac{1}{4356}(38\,861+3075\sqrt{5})$
13	$-\frac{1}{11}(57+5\sqrt{5})$
15	4
16	$\frac{3}{22}(149+15\sqrt{5})$
17	$\frac{2}{1089}(13\,636+2025\sqrt{5})$
18	$-\frac{1}{39\,204}(2445\,813+289\,895\sqrt{5})$
19	$-\frac{6}{121}(764+95\sqrt{5})$
20	6
21	$\frac{4}{33}(366+35\sqrt{5})$
22	$\frac{3}{484}(25\,811+3725\sqrt{5})$
23	$\frac{16}{107\,811}(1073\,331+198\,290\sqrt{5})$
24	$-\frac{1}{5174\,928}(2639\,186\,447+409\,253\,835\sqrt{5})$

asymptotic behaviour of the coefficient A_n as $n \to \infty$ by applying the method of Darboux (1878) to the singular part of the expansion (19). The final result is

$$A_n \sim a_0 \lambda^n n^{-5/6} \sum_{m=1}^{5} (-1)^{m-1} [\Gamma(\tfrac{1}{6})/\Gamma(\tfrac{m}{6})](\xi/n)^{\frac{5}{6}(m-1)} S_m(n) \tag{22}$$

as $n \to \infty$, where

$$a_0 = [\sqrt{5}\Gamma(\tfrac{1}{6})\xi^{1/6}]^{-1} \tag{23}$$

$$\begin{aligned} S_1(n) = [1 &+ \tfrac{1}{360}(-275 + 134\sqrt{5})n^{-1} - \tfrac{11}{259\,200}(168\,433 - 75\,260\sqrt{5})n^{-2} \\ &- \tfrac{187}{1399\,680\,000}(1070\,424\,025 - 478\,699\,214\sqrt{5})n^{-3} \\ &+ \tfrac{313\,973}{2015\,539\,200\,000}(-28\,868\,526\,247 + 12\,910\,400\,040\sqrt{5})n^{-4} + \ldots] \end{aligned} \tag{24}$$

$$\begin{aligned} S_2(n) = \tfrac{4}{3}[1 &+ \tfrac{1}{90}(175 - 73\sqrt{5})n^{-1} - \tfrac{2}{2025}(-25\,754 + 11\,555\sqrt{5})n^{-2} \\ &- \tfrac{11}{1366\,875}(-73\,873\,975 + 33\,041\,201\sqrt{5})n^{-3} + \ldots] \end{aligned} \tag{25}$$

$$S_3(n) = \tfrac{9}{4}[1 + \tfrac{1}{40}(325 - 142\sqrt{5})n^{-1} - \tfrac{7}{3200}(-99\,283 + 44\,460\sqrt{5})n^{-2} + \ldots] \tag{26}$$

$$S_4(n) = \tfrac{112}{27}[1 + \tfrac{1}{45}(800 - 353\sqrt{5})n^{-1} + \ldots] \tag{27}$$

$$S_5(n) = \tfrac{1729}{216}[1 + \ldots] \tag{28}$$

and $\Gamma(x)$ denotes the gamma function. This asymptotic representation gives an accurate approximation for A_n when n is *small.* For example, if the asymptotic value for A_n is rounded to the nearest integer one obtains the exact value for A_n, provided $n \leq 7$! When $n = 24$ the representation (22) gives

$$A_{24} \simeq 1.048\,827\,1833 \times 10^{22} \tag{29}$$

which is in excellent agreement with the exact value in table 2.

It can be shown by using the work of Forsyth (1902) that the algebraic generating function $A(y)$ satisfies a homogeneous linear differential equation of 12th order with polynomial coefficients in y. From this result and the Taylor series (1) it follows that the coefficient A_n satisfies a finite linear recurrence relation of the type proposed by Guttmann and Joyce (1972). It is also possible to derive a closed-form expression for $A(y)$ by applying modular function theory to (10). The final result is

$$[A(y)]^{-1} = y^{1/5}(1+y)^{-1/5}\Theta - 1 \tag{30}$$

where

$$\begin{aligned} 4\zeta_2^3\Theta = 1 &+ [(1 - 8\zeta_2^5) - 4\zeta_2^5(\zeta_2^{-5} - 11 - \zeta_2^5)^{1/3}]^{1/2} + \{2(1 - 8\zeta_2^5) + 4\zeta_2^5(\zeta_2^{-5} - 11 - \zeta_2^5)^{1/3} \\ &+ 2[(1 - 8\zeta_2^5) - 4\zeta_2^5(\zeta_2^{-5} - 11 - \zeta_2^5)^{1/3}]^{1/2} \\ &+ 8\zeta_2^5[5 - 2(\zeta_2^{-5} - 11 - \zeta_2^5)^{1/3} + (\zeta_2^{-5} - 11 - \zeta_2^5)^{2/3}]^{1/2}\}^{1/2} \end{aligned} \tag{31}$$

$$\zeta_2 = \tfrac{1}{3}y^{2/5}(1+y)^{-2/5}[-1 + 2y^{-1/2}(3+4y)^{1/2}\sin\varphi] \tag{32}$$

$$\varphi = \tfrac{1}{3}\sin^{-1}[y^{1/2}(18+19y)(3+4y)^{-3/2}] \tag{33}$$

and $0 < y < y_c$. The transcendental functions in (32) and (33) are associated with the solution of a cubic *algebraic* equation which has three real roots (the irreducible case).

References

Baxter R J 1980 *J. Phys. A: Math. Gen.* **13** L61–70
——1981 *J. Stat. Phys.* **26** 427–52
Bliss G A 1966 *Algebraic Functions* (New York: Dover)
Darboux M G 1878 *J. Math.* **4** 5–56, 377–416
Dhar D 1983 *Phys. Rev. Lett.* **51** 853–6
Forsyth A R 1902 *Theory of Differential Equations* vol 4 (Cambridge: Cambridge University Press) p 44
Gaunt D S 1967 *J. Chem. Phys.* **46** 3237–59
Gaunt D S and Fisher M E 1965 *J. Chem. Phys.* **43** 2840–63
Goursat E 1959 *Functions of a Complex Variable* (*A Course in Mathematical Analysis* vol 2, part 1) (New York: Dover).
Guttmann A J and Joyce G S 1972 *J. Phys. A: Math. Gen.* **5** L81–4
Hille E 1973 *Analytic Function Theory* vol 2 (New York: Chelsea) p 105
Joyce G S 1988 *Phil. Trans. R. Soc.* A **325** 643–702
Klein F and Fricke R 1892 *Vorlesungen über die Theorie der elliptischen Modulfunktionen* vol 2 (Leipzig: Teubner)
Mordell L J 1922 *Proc. Lond. Math. Soc.* (2) **20** 408–16
Schoeneberg B 1974 *Elliptic Modular Functions* (Berlin: Springer)
Stanley H E, Redner S and Yang Z-R 1982 *J. Phys. A: Math. Gen.* **15** L569–73