RAPID COMMUNICATIONS

PHYSICAL REVIEW E VOLUME 47, NUMBER 4 APRIL 1993

Staircase polygons, elliptic integrals, Heun functions, and lattice Green functions

A. J. Guttmann*
Department of Theoretical Physics, Oxford University, 1 Keble Road, Oxford OX1 3NP, United Kingdom

T. Prellberg
Department of Mathematics, The University of Melbourne, Parkville, Victoria 3052, Australia
(Received 21 October 1992)

We show that the generating function for d-dimensional staircase polygons (by perimeter) can be expressed in terms of the generating function for the square of d-dimensional multinomial coefficients. This latter generating function is found to satisfy a linear, homogeneous differential equation of order $d-1$. This equation is solved for $d \leq 4$. For $d=3$ and $d=4$ the solution is obtained in terms of Heun functions, which are then shown to be expressible in terms of the complete elliptic integral of the first kind. The solutions are also shown to be related to lattice Green functions on three-dimensional lattices. The critical behavior of this model is determined exactly in all dimensions.

PACS number(s): 64.60.Ak, 36.20.Ey, 75.40.Cx

In recent years there has been renewed interest in a number of two-dimensional polygon problems [1–3]. In particular, the generating function by perimeter of pyramid polygons, bar-graph polygons, staircase polygons, convex polygons, row-convex polygons, and almost convex polygons [4] have all been obtained, while for self-avoiding polygons on the square lattice, enumerations to 70 steps are now known [5]. As well as their intrinsic combinatorial interest, and as models of phase transitions, these exactly solved models will, it is hoped, shed light on the solution of the unsolved self-avoiding polygon problem. Additionally, they are of some interest in a computer science setting [2, 3], as manifestations of certain grammars.

In dimension $d > 2$, however, essentially nothing is known. In this Rapid Communication we study d-dimensional staircase polygons, and show that their perimeter generating function can be expressed as the square of the d-dimensional multinomial coefficient. We then find that this generating function satisfies a Fuchsian differential equation of order $(d-1)$. We solve these ordinary differential equations for $d=3$ and $d=4$ in terms of Heun functions, which we show can then be transformed into lattice Green functions and hence [6] expressed in terms of complete elliptic integrals of the first kind. We also obtain the exact critical point, critical exponent, and amplitude for the generating function (free-energy analogue) of the model in all dimensions. This is the first nontrivial polygon problem to be completely solved in dimensions 3 and 4.

Any d-dimensional staircase polygon of perimeter $2n$ may be considered as made up of two paths, each of length n, with common origin and end point, and with successive steps joining neighboring points on the lattice $\mathbf{Z}^d$. The two paths are constrained to have no point in common other than the origin and the end point, and successive steps must be in the positive direction in all d coordinates.

We denote the generating function of staircase polygons in d dimensions by $G(x_1, x_2, \ldots, x_d)$. If there are k_i steps in direction i, then the number of distinct paths is clearly given by the multinomial coefficient $\binom{k_1+k_2+\cdots+k_d}{k_1,k_2,\ldots,k_d}$. Relaxing for the moment the condition that the two paths do not intersect, the number of two such paths with common origin and end point at $(k_1, k_2, \ldots, k_d)$ is given by the square of the above multinomial coefficient, and the corresponding generating function $Z(x_1, x_2, \ldots, x_d)$, including a walk of zero length for later convenience, is

$$Z(x_1, x_2, \ldots, x_d) = \sum_{k_1,k_2,\ldots,k_d=0}^{\infty} \binom{k_1+k_2+\cdots+k_d}{k_1,k_2,\ldots,k_d}^2 x_1^{2k_1} x_2^{2k_2} \cdots x_d^{2k_d} . \quad (1)$$

This generating function produces a chain of staircase polygons (Fig. 1), each link of which comprises either a staircase polygon or a double bond. Let $H(x_1, x_2, \ldots, x_d)$ be the generating function for a link, that is, for a single staircase polygon or double bond

$$H(x_1, x_2, \ldots, x_d) = \sum_{i=1}^{d} x_i^2 + 2G(x_1, x_2, \ldots, x_d) \quad (2)$$

[due to the orientability of walks, each staircase polygon is produced twice in the definition of $H(x_1, x_2, \ldots, x_d)$].

We see in Fig. 1 that the chains consist of polygons generated by H, or H^2, or H^3, etc., whence

$$Z = 1 + H + H^2 + H^3 + \cdots = \frac{1}{1-H} \quad (3)$$

(where the arguments of Z and H have been suppressed). Combining (3) with (2) we get

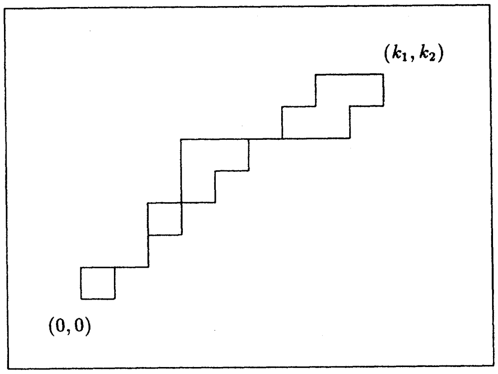

FIG. 1. Two directed walks with common start and end points forming a loop in two dimensions. This can be interpreted as a chain consisting of staircase polygons and double bonds. The picture is readily generalizable to higher dimensions.

$$G = \frac{1}{2}\left(H - \sum_{i=1}^{d} x_i^2\right) = \frac{1}{2}\left(1 - \sum_{i=1}^{d} x_i^2 - Z^{-1}\right) . \qquad (4)$$

Setting $x_1 = x_2 = \cdots = x_d = x$ and writing $G(\underbrace{x, x, \ldots, x}_{d}) = G_d(x^2)$ $[Z(\underbrace{x, x, \ldots, x}_{d}) = Z_d(x^2)]$, we have

$$G_d(x^2) = \frac{1}{2}\left(1 - dx^2 - \frac{1}{Z_d(x^2)}\right), \qquad (5)$$

where

$$Z_d(x^2) = \sum_{k_1,k_2,\ldots,k_d=0}^{\infty} \binom{k_1 + k_2 + \cdots + k_d}{k_1, k_2, \ldots, k_d}^2 x^{2(k_1+k_2+\cdots+k_d)} \qquad (6)$$

and, respectively,

$$G_d(x^2) = \frac{1}{2}\left\{1 - dx^2 - \left(\sum_{n=0}^{\infty} S_n^{(d)} x^{2n}\right)^{-1}\right\}, \qquad (7)$$

with

$$S_n^{(d)} = \sum_{k_1+\cdots+k_d=n} \binom{n}{k_1, k_2, \ldots, k_d}^2 . \qquad (8)$$

For $d = 1$ this last sum is just $S_n^{(1)} = 1$, hence $G_1(x^2) = 0$. For $d = 2$ the multinomial is a binomial and from the identity $\sum_{k=0}^{n} \binom{n}{k}^2 = \binom{2n}{n}$ we find

$$G_2(x^2) = \frac{1}{2}(1 - 2x^2 - \sqrt{1 - 4x^2}) . \qquad (9)$$

For $d > 2$ no expression is known for the generating function of the square of the multinomial coefficient. We observe the simple recursion

$$S_n^{(d)} = \sum_{m=0}^{n} \binom{n}{m}^2 S_m^{(d-1)}, \qquad (10)$$

but that does not help in simplifying the generating function.

However, if we simply generate the coefficients of the generating function $Z_d(x^2)$ from the definition, inspection of the coefficients (aided by computer algebra) reveals a simple recurrence relation among the coefficients. Such recurrences abound in exactly solvable models in statistical mechanics, and their identification and analysis are standard tools [7]. In particular, we get

$$nS_n^{(2)} = 2(2n-1)S_{n-1}^{(2)}, \qquad (11a)$$

$$n^2 S_n^{(3)} = (10n^2 - 10n + 3)S_{n-1}^{(3)} - 9(n-1)^2 S_{n-2}^{(3)}, \qquad (11b)$$

$$n^3 S_n^{(4)} = 2(2n-1)(5n^2 - 5n + 2)S_{n-1}^{(4)} - 64(n-1)^3 S_{n-2}^{(4)}, \qquad (11c)$$

$$n^4 S_n^{(5)} = (35n^4 - 70n^3 + 63n^2 - 28n + 5)S_{n-1}^{(5)} - (259n^2 - 518n + 285)(n-1)^2 S_{n-2}^{(5)} + 225(n-1)^2(n-2)^2 S_{n-3}^{(5)}, \qquad (11d)$$

$$n^5 S_n^{(6)} = 2(2n-1)(14n^4 - 28n^3 + 28n^2 - 14n + 3)S_{n-1}^{(6)} - 4(196n^2 - 392n + 255)(n-1)^3 S_{n-2}^{(6)} + 1152(2n-3)(n-1)^2(n-2)^2 S_{n-3}^{(6)} . \qquad (11e)$$

These recurrences can be reexpressed as differential equations. In this way we find the following differential equations for $Z_d(x)$:

$$Z_2'(x) - \frac{2}{1-4x} Z_2(x) = 0, \qquad (12a)$$

$$Z_3''(x) + \frac{1 - 20x + 27x^2}{x(1-x)(1-9x)} Z_3'(x) - \frac{3(1-3x)}{x(1-x)(1-9x)} Z_3(x) = 0, \qquad (12b)$$

$$Z_4'''(x) + \frac{3(1 - 30x + 128x^2)}{x(1-4x)(1-16x)} Z_4''(x) + \frac{1 - 68x + 448x^2}{x^2(1-4x)(1-16x)} Z_4'(x) - \frac{4}{x^2(1-4x)} Z_4(x) = 0, \qquad (12c)$$

$$Z_5^{(4)}(x) + \frac{2(3 - 140x + 1295x^2 - 1350x^3)}{x(1-x)(1-9x)(1-25x)} Z_5'''(x) + \frac{7 - 518x + 6501x^2 - 8550x^3}{x^2(1-x)(1-9x)(1-25x)} Z_5''(x) + \frac{1 - 196x + 3963x^2 - 7200x^3}{x^3(1-x)(1-9x)(1-25x)} Z_5'(x) - \frac{5(1 - 57x + 180x^2)}{x^3(1-x)(1-9x)(1-25x)} Z_5(x) = 0, \qquad (12d)$$

$$Z_6^{(5)}(x) + \frac{10(1-70x+1176x^2-4032x^3)}{x(1-4x)(1-16x)(1-36x)} Z_6^{(4)}(x) + \frac{25-2408x+51196x^2-211968x^3}{x^2(1-4x)(1-16x)(1-36x)} Z_6'''(x)$$
$$+ \frac{3(5-812x+23992x^2-126720x^3)}{x^3(1-4x)(1-16x)(1-36x)} Z_6''(x) + \frac{1-516x+25956x^2-193536x^3}{x^4(1-4x)(1-16x)(1-36x)} Z_6'(x)$$
$$- \frac{6(1-170x+2304x^2)}{x^4(1-4x)(1-16x)(1-36x)} Z_6(x) = 0 \,. \quad (12e)$$

These differential equations are all Fuchsian, with regular singular points at the origin, at infinity, and at $x = 1/d^2, 1/(d-2)^2, 1/(d-4)^2, \ldots$, the sequence of singular points terminating at $x=1$ (d odd) or $x = \frac{1}{4}$ (d even). Moreover, the solutions that are regular in the neighborhood of $x = 0$ have singularities with exponents $\frac{d-3}{2}$ at the other regular singular points, so that, in particular, the dominant singular behavior is given by

$$Z_d(x^2) \sim \begin{cases} B_d(1-d^2x^2)^{(d-3)/2} & d \text{ even} \\ B_d(1-d^2x^2)^{(d-3)/2}\ln(1-d^2x^2) & d \text{ odd.} \end{cases} \quad (13)$$

Further analysis of the coefficients $S_n^{(d)}$ shows that the asymptotic behavior is

$$S_n^{(d)} = \binom{2n}{\frac{2n}{d}, \ldots, \frac{2n}{d}} [1+O(n^{-1})]$$
$$= \frac{d^{2n+d/2}}{(4\pi n)^{\frac{d-1}{2}}} [1+O(n^{-1})] \,. \quad (14)$$

From this the amplitudes B_d in (13) can be readily calculated. Furthermore, denoting the number of d-dimensional staircase polygons with perimeter $2n$ as $T_n^{(d)}$, we get for large n

$$\frac{T_n^{(d)}}{S_n^{(d)}} \sim \begin{cases} 1/4n, & d=2 \\ 1/\ln(n)^2, & d=3 \\ C_d > 1/2, & d>3 \end{cases} \quad (15)$$

with $C_d \to 1/2$ for $d \to \infty$. It follows that the probability of self-intersection of a d-dimensional directed random loop (given by $\lim_{n\to\infty} 1 - 2T_n^{(d)}/S_n^{(d)}$) equals 1 for $d \le 3$. However, for $d > 3$ it is strictly smaller than 1 and approaches zero for $d \to \infty$. Therefore $d = 3$ can be seen as an upper critical dimension for this problem.

For $d = 2$ the solution can clearly be expressed as a ${}_2F_1$ hypergeometric function, but we have already given the solution in terms of simpler algebraic functions.

For $d = 3$ the differential equation can be rewritten as Heun's equation [8], a generalization of the ${}_2F_1$ hypergeometric equation to the case of four, rather than three, regular singular points. The definitive work on Heun functions is by Snow [9], but further and more recent applications can be found in [10]. We denote the solution as

$$Z_3(x^2) = F(\tfrac{1}{9}, -\tfrac{1}{3}; 1,1,1,1; x^2) \quad (16)$$

in the notation of Snow. (This notation becomes transparent if compared to the Riemannian representation of the differential equation, and is an obvious generalization of the hypergeometric notation.) The singularities are all logarithmic.

In $d = 4$, the differential equation can be rewritten as

$$Z'''(x) + 3f(x)Z''(x) + [2f(x)^2 + f'(x) + 4g(x)]Z'(x)$$
$$+ [4f(x)g(x) + 2g'(x)]Z(x) = 0, \quad (17)$$

with

$$f(x) = \frac{1-30x+128x^2}{x(1-4x)(1-16x)},$$
$$g(x) = \frac{-2(1-8x)}{x(1-4x)(1-16x)}, \quad (18)$$

and hence [11] its solution can be expressed in terms of the two linearly independent solutions Y_1, Y_2 of the second-order differential equation

$$Y''(x) + f(x)Y'(x) + g(x)Y(x) = 0 \quad (19)$$

as $Z = AY_1^2 + BY_1Y_2 + CY_2^2$. This second-order differential equation can also be written as the Heun differential equation, and so, after matching the arbitrary constants A, B, C to the boundary conditions, given by the first terms of the generating function, we find

$$Z_4(x^2) = [F(\tfrac{1}{4}, -\tfrac{1}{8}; \tfrac{1}{2}, \tfrac{1}{2}, 1, \tfrac{1}{2}; 4x^2)]^2, \quad (20)$$

and that the singularities at all four regular singular points are square-root branch points.

To proceed further, we note from Snow (Eq. VII.15) that the Heun functions can be analytically continued, so that

$$Z_3(w^2) = F(\tfrac{1}{9}, -\tfrac{1}{3}; 1,1,1,1; w^2)$$
$$= (1-9w^2)^{-1} F\left(\tfrac{9}{8}, -\tfrac{3}{4}; 1,1,1,1; \frac{w^2}{w^2 - \frac{1}{9}}\right) . \quad (21)$$

Joyce [6] has shown that this Heun function is related to the simple-cubic lattice Green function

$$P(z) = \frac{1}{\pi^3} \int\!\!\int\!\!\int_0^{\pi} \frac{dx_1 dx_2 dx_3}{1 - \frac{z}{3}(\cos x_1 + \cos x_2 + \cos x_3)} \quad (22)$$

through

$$F(\tfrac{9}{8}, -\tfrac{3}{4}; 1,1,1,1; x_3)$$
$$= [P(t)]^{\frac{1}{2}} (1 - \tfrac{3}{4}x_1)^{-\frac{1}{4}} (1-x_1)^{\frac{1}{2}} (1 - \tfrac{8}{9}x_3)^{-\frac{1}{2}}, \quad (23)$$

where

$$x_3 = \frac{9w^2}{9w^2-1} = \frac{1}{2} + \frac{x_2}{4} - \frac{1}{2}\sqrt{(1-x_2)\left(1-\frac{x_2}{4}\right)}, \tag{24a}$$

$$x_2 = \frac{x_1}{x_1-1}, \tag{24b}$$

$$x_1 = \frac{1}{2} + \frac{x}{6} - \frac{1}{2}\sqrt{(1-x)\left(1-\frac{x}{9}\right)}, \tag{24c}$$

and $x = t^2$. Also

$$P(t) = \left(1-\frac{3}{4}x_1\right)^{\frac{1}{2}} (1-x_1)^{-1} \left(\frac{2}{\pi}\right)^2 K(k_+)K(k_-) , \tag{25}$$

where

$$k_\pm^2 = \frac{1}{2} \pm \frac{x_2}{4}(4-x_2)^{\frac{1}{2}} - \frac{1}{4}(2-x_2)(1-x_2)^{\frac{1}{2}} , \tag{26}$$

and $K(k)$ is the complete elliptic integral of the first kind. Hence we conclude that

$$Z_3^2(w^2) = \left(\frac{2}{\pi}\right)^2 (1-9w^2)^{-1}(1-w^2)^{-1}K(k_+)K(k_-), \tag{27}$$

where the argument of the complete elliptic integral is given implicitly as a function of w through Eqs. (22) and (24), and so $G_3(x^2)$ follows immediately from (27) and (5).

Similarly, for $d = 4$, the Heun function can also be transformed (Snow, VII.13) to give

$$\begin{aligned} Z_4(x^2) &= [F(\tfrac{1}{4},-\tfrac{1}{8};\tfrac{1}{2},\tfrac{1}{2},1,\tfrac{1}{2};4x^2)]^2 \\ &= [F(4,-\tfrac{1}{2};\tfrac{1}{2},\tfrac{1}{2},1,\tfrac{1}{2};16x^2)]^2 \\ &= \frac{4}{\pi^2}K(k_+)K(k_-), \end{aligned} \tag{28}$$

where $k_\pm^2 = \frac{1}{2} \pm 8x^2(1-4x^2)^{\frac{1}{2}} - \frac{1}{2}(1-8x^2)(1-16x^2)^{\frac{1}{2}}$. Note that $Z_4(x^2)$ is simply related to the lattice Green function for the face-centered-cubic and diamond lattices, as [6]

$$P(z)_{\rm fcc} = \frac{3}{3+z}\left[F\left(4,-\tfrac{1}{2};\tfrac{1}{2},\tfrac{1}{2},1,\tfrac{1}{2};\frac{4z}{3+z}\right)\right]^2 \tag{29}$$

and

$$P(z)_{\rm diam} = [F(4,-\tfrac{1}{2};\tfrac{1}{2},\tfrac{1}{2},1,\tfrac{1}{2};z^2)]^2 . \tag{30}$$

Finally, $G_4(x^2)$ follows immediately from (28) and (5).

For $d > 4$ the theory of generalized hypergeometric functions with five or more regular singular points is not known to us, though the full singularity structure of the differential equations is clear from (12d) and (12e).

Thus we have explicitly solved the problem of staircase polygons in dimensionality $d \le 4$. For $d > 4$ a Fuchsian differential equation with transparent singularity structure is given for $d = 5$ and $d = 6$, and is readily constructable for other values of d. We have found an unexpected connection between the generating function for multinomial coefficients in $d = 3$ and $d = 4$ and Heun functions, and hence between multinomial coefficients and lattice Green functions and complete elliptic integrals of the first kind. Since the complete elliptic integral can be expressed as an ordinary hypergeometric function, an additional connection between these Heun functions and the hypergeometric function can also be deduced. Additional connections with the generating function for random returns to the origin — a closely related problem — with lattice Green functions and with lattice dynamics can be deduced from the work of Joyce [6].

This connection becomes clearer if one considers the fact that the projection of a d-dimensional directed walk along the directed axis leads to a restricted random walk on a hypertriangular lattice in $d-1$ dimensions. Thus d-dimensional staircase polygons can be interpreted as (restricted) random returns on such a lattice [12].

We note that the critical exponents of the staircase polygon model are clearly rational for all dimensionality. Whether this is true for more realistic systems for $d > 2$, or whether it is due to the simplicity of the model remains a tantalizing open question.

A.J.G. would like to thank Dr. G. S. Joyce for introducing him to Heun functions many years ago, and for recent helpful discussions. We would also like to thank Professor J. W. Essam and Professor L. Glasser for helpful comments on the manuscript, and to acknowledge the ARC for financial support.

* Permanent address: Department of Mathematics, The University of Melbourne, Parkville, Victoria 3052, Australia.

[1] A.J. Guttmann, in *Proceedings of the Conference on Computer-aided Statistical Physics*, edited by Chin-Kun Hu, AIP Conf. Proc. No. 248 (AIP, New York, 1992), p. 34.

[2] M. Delest, J. Math. Chem. **8**, 3 (1991).

[3] X.G. Viennot, in *Séries Formelles et Combinatoire Algébrique*, edited by P. Leroux and C. Reutenauer, LACIM Conf. Proc. No. 11 (LACIM, Montreal, 1992).

[4] I.G. Enting, A.J. Guttmann, L.B. Richmond, and N.C. Wormald, Random Struct. Algorithms (to be published).

[5] A.J. Guttmann and I.G. Enting (unpublished).

[6] G.S. Joyce, Philos. Trans. R. Soc. London **273**, 583 (1973).

[7] A.J. Guttmann, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz (Academic, London, 1989), Vol. 13.

[8] A. Erdèlyi *et al., Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 3, p. 57.

[9] C. Snow, in *Hypergeometric and Legendre Functions with Applications,* Natl. Bur. Stand. (U.S.) Wash. Appl. Math. Ser. No. 19 (U.S. GPO, Washington, DC, 1952).

[10] *Proceedings of the Centennial Workshop on Heun's Equation—Theory and Applications, Schloss Ringberg*, edited by A. Seeger and W. Lay (Max-Planck-Institut für Metallforschung, Stuttgart, 1990).

[11] M. Appell, C.R. Acad. Sci. **91**, 211 (1880).

[12] J.W. Essam (unpublished).