Staircase polygons, elliptic integrals and Heun functions

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Abstract

We discuss the perimeter generating function of d-dimensional staircase polygons and relate these to the generating function of the square of the d-dimensional multinomial coefficients. These are found to satisfy differential equations of order $d-1$. The equations are solved for $d < 5$, and the singularity structure deduced for all values of d. The connection with complete elliptic integrals, Heun functions and lattice Green functions is also found. The original article by A. J. Guttmann and T. Prellberg can be found in [4].

1. Staircase polygons

Any d-dimensional staircase polygon [3, 6] 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 neighbouring points on the lattice $\mathbb{Z}^d$. 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. The number of paths of length n having k_i steps in direction i $(1 \leq i \leq d)$ is $\binom{k_1+\cdots+k_d}{k_1,\ldots,k_d}$ with $k_1 + \cdots + k_d = n$. Then the number of pairs of such paths is $\binom{n}{k_1,\ldots,k_d}^2$. The generating function $Z_d(x_1,\ldots,x_d)$ for these pairs of paths, including a walk of zero length for later convenience, is

$$Z_d(x_1,\ldots,x_d) = \sum_{k_1,\ldots,k_d=0}^{\infty} \binom{k_1+\cdots+k_d}{k_1,\ldots,k_d}^2 x_1^{2k_1}\cdots x_d^{2k_d}.$$

This generating function produces a chain of staircase polygons, each links of which comprises either a staircase polygon or a double bond. The generating function for double bonds is $\sum_{i=1}^{d} x_i^2$ and we denote the generating function of staircase polygons in d dimensions by $G_d(x_1,\ldots,x_d)$. Let $H(x_1,\ldots,x_d)$ be the generating function for a link

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

Due to the orientability of walks, each staircase polygon is produced twice in the definition of $H(x_1,\ldots,x_d)$. We set $x_1 = \cdots = x_d = x$. The construction "chain of" corresponds to the functional relation

$$Z(x) = \frac{1}{1-H(x)}.$$

Hence, by inspection

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

with

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

For $d = 1$ we get $S_n^{(1)} = 1$ and $G_1(x^2) = 0$. For $d = 2$ from the identity $\sum_{k=0}^{n} \binom{n}{k}^2 = \binom{2n}{n}$ we find

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

For $d > 2$ we observe the recursion

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

By expansion and inspection (aided by computer algebra), we get

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

These recurrences can be reexpressed as differential equations

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

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

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

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

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

where B_d is a constant whose amplitude can be calculated.

2. Heun functions and lattice Green Functions

For $d = 3$ the differential equation can be rewritten as Heun's equation [7], a generalization of the ${}_2F_1$ hypergeometric equation to the case of four, rather than three, regular points. We denote the solution as

$$Z_3(x^2) = F\left(\frac{1}{9}, -\frac{1}{3}; 1, 1, 1, 1; x^2\right) = \frac{1}{1-9x^2} F\left(\frac{9}{8}, -\frac{3}{4}; 1, 1, 1, 1; \frac{x^2}{x^2 - 1/9}\right).$$

Joyce [5] (and Watson for $P_3(1)$) has shown that this Heun function is related to the simple-cubic lattice Green function

$$P_3(z) = \frac{1}{\pi^3}\iiint_0^\pi \frac{dx_1 dx_2 dx_3}{1 - \frac{z}{3}(\cos x_1 + \cos x_2 + \cos x_3)} \tag{2}$$

through

$$F\left(\frac{9}{8}, -\frac{3}{4}; 1,1,1,1; x_3\right) = (P_3(t))^{\frac{1}{2}}\left(1 - \frac{3}{4}x_1\right)^{-\frac{1}{4}}(1-x_1)^{\frac{1}{2}}\left(1 - \frac{8}{9}x_3\right)^{-\frac{1}{2}},$$

$$x_3 = \frac{1}{2} + \frac{x_2}{4} - \frac{1}{2}\sqrt{(1-x_2)(1-x_2/4)} = \frac{9\omega^2}{9\omega^2-1}, \qquad x_2 = \frac{x_1}{x_1 - 1}, \tag{3}$$

$$x_1 = \frac{1}{2} + \frac{x}{6} - \frac{1}{2}\sqrt{(1-x)(1-x/9)}, \qquad x = t^2. \tag{4}$$

Further

$$P_3(t) = \left(1 - \frac{3}{4}x_1\right)^{\frac{1}{2}}(1-x_1)^{-1}\left(\frac{2}{\pi}\right)^2 K(k_+)K(k_-)$$

where

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

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

$$Z_3^2(\omega^2) = \left(\frac{2}{\pi}\right)^2 (1-9\omega^2)^{-1}(1-\omega^2)^{-1}K(k_+)K(k_-) \tag{5}$$

where the argument of the complete elliptic integral is given implicitly as a function of ω through equations (2), (3) and (4), and so $G_3(x^2)$ follows immediately from (5) and (1).

Similarly, for $d = 4$, the Heun function can also be transformed [1, 7] to give

$$\begin{aligned} Z_4(x^2) &= \left(F\left(\frac{1}{4}, -\frac{1}{8}; \frac{1}{2}, \frac{1}{2}, 1, \frac{1}{2}; 4x^2\right)\right)^2 = \left(F\left(4, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}, 1, \frac{1}{2}; 16x^2\right)\right)^2 \\ &= \frac{4}{\pi^2}K(k_+)K(k_-). \end{aligned} \tag{6}$$

where

$$k_\pm^2 = \frac{1}{2} \pm 8x^2\left(1-4x^2\right)^{\frac{1}{2}} - \frac{1}{2}(1-8x^2)(1-16x_2)^{\frac{1}{2}}.$$

Note that $Z_4(x^2)$ is simply related to the lattice Green function [5] for the face-centered-cubic lattice as

$$P_{f.c.c.}(z) = \frac{3}{3+z}\left(F\left(4, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}, 1, \frac{1}{2}; \frac{4z}{3+z}\right)\right)^2$$

and for the diamond lattice as

$$P_{diam}(z) = \left(F\left(4, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}, 1, \frac{1}{2}; z^2\right)\right)^2.$$

Finally, $G_4(x^2)$ follows from (1) and (6).

For $d > 4$ the theory of generalized hypergeometric functions with five or more regular singular point is not known to us, though the full singularity structure of the differential equations is given for $d = 5$ and $d = 6$, and is readily constructible for other values of d.

3. Bessel functions

Bessel functions [8] are the solutions of the differential equations

$$z^2 f''(z) + z f'(z) + (z^2 - \nu^2) f(z) = 0. \tag{7}$$

Let $J_\nu(z)$ be a solution of (7) which is analytic near the origin. Then we have

$$J_\nu(z) = \sum_{m=0}^{\infty} \frac{(-1)^m \left(\frac{1}{2}z\right)^{\nu+2m}}{m!\Gamma(\nu+m+1)}$$

when 2ν is not an integer. $J_{-\nu}(z)$ is also such a solution. The first of the two series defines a function called a Bessel function of order ν and argument z, of the first kind. When ν is an integer, the function

$$Y_n(z) = \lim_{\nu\to n} \frac{J_\nu(z) - (-1)^n J_{-\nu}(z)}{\nu - n}$$

is called a Bessel function of the second kind of order n. Note that

$$Y_n(z) = \left[\frac{\partial J_\nu(z)}{\partial \nu} - (-1)^n \frac{\partial J_{-\nu}(z)}{\partial \nu}\right]_{\nu=n}.$$

It has seemed desirable to Nielsen to regard the pair of the functions $J_\nu(z) \pm iY_\nu(z)$ as standard solutions of Bessel's equation (7). In honour of Hankel, Nielsen denotes them by the symbol H

$$H_\nu^{(1)} = J_\nu(z) + iY_\nu(z), \qquad H_\nu^{(2)} = J_\nu(z) - iY_\nu(z).$$

Physicists consider the equation

$$z^2 f''(z) + z f'(z) - (z^2 + \nu^2) f(z) = 0. \tag{8}$$

The solutions of this equation are called modified Bessel functions. It is usually desirable to present the solution of (8) in a real form, and the fundamental systems $J_\nu(iz)$ and $J_{-\nu}(iz)$ or $J_\nu(iz)$ and $Y_\nu(iz)$ are unsuited for this purpose. The function $e^{-\frac{1}{2}\nu i\pi} J_\nu(iz)$ is real in z and is a solution of (8). It is customary to denote the modified Bessel function of the first kind by $I_\nu(z)$ so that

$$I_\nu(z) = \sum_{m=0}^{\infty} \frac{\left(\frac{1}{2}z\right)^{\nu+2m}}{m!\Gamma(\nu+m+1)}.$$

The modified Bessel function of the second kind is

$$K_n(z) = \lim_{\nu\to n} \frac{(-1)^n}{2}\left(\frac{I_\nu(z) - I_{-\nu}(z)}{\nu - n}\right).$$

Note that

$$K_\nu(z) = \frac{\pi}{2}\left(\frac{I_{-\nu}(z) - I_\nu(z)}{\sin(\nu\pi)}\right).$$

The following formulæ are valid:

$$\begin{aligned} (m!)^2 &= \int_0^\infty t(t/2)^{2m} K_0(t)\, dt, & e^{-s} &= \frac{2s}{\pi}\int_0^1 \frac{K_0(s/u)}{u^2\sqrt{1-u^2}}\, du, \\ I_0(z) &= \sum_{n=0}^{\infty} \frac{z/2)^{2n}}{(n!)^2} = \frac{1}{\pi}\int_0^\infty e^{z\cos\theta}\, d\theta, & \frac{1}{z} &= \int_0^\infty e^{-sz}\, ds. \end{aligned} \tag{9}$$

Philippe Flajolet remarks that a natural tool to attack the calculation of $G_d(z)$ are Bessel generating functions [2]. The Bessel generating function of a sequence s_n of numbers is defined as the sum

$$\sum_{n=0}^{\infty} \frac{s_n z^n}{(n!)^2}.$$

For instance, the Bessel generating function of the constant sequence $s_n = 1$ is given by the modified Bessel function

$$j(z) := I_0\left(2\sqrt{z}\right) = \sum_{n=0}^{\infty} \frac{z^n}{(n!)^2}.$$

The Bessel generating function of the number of pairs of paths with same origin and end and positive steps in a d-dimensional lattice is given by the product

$$\prod_{i=1}^{d} j(x_i),$$

where x_i marks the steps in dimension i. It follows that the Bessel generating function of the numbers $S_n^{(d)}$ with respect to the length n of the paths is $j(x)^d$. In dimension 2, the generating function $Z_2(x)$ is algebraic. In higher dimension, $Z_d(x)$ belongs to the larger class of holonomic functions. This class is closed under sum, product, Borel and inverse Borel transforms. The Borel transform is related to the inverse Laplace transform and is defined by

$$\text{Borel}\left(\sum_{n=0}^{\infty} s_n x^n\right) = \sum_{n=0}^{\infty} \frac{s_n x^n}{n!}.$$

We proceed to get $Z_d(x)$ by the formula

$$Z_d(x) = \left(\text{Borel}^{(-2)}\right)\left(j(x)^d\right).$$

4. The 4D simple-cubic lattice Green function

This section is due to the help of L. Glasser. The 4D simple-cubic lattice Green function is

$$\begin{aligned} P_4(z) &= \frac{1}{\pi^4} \iiiint_0^{\pi} \frac{dx_1 dx_2 dx_3 dx_4}{1 - \frac{z}{4}(\cos x_1 + \cos x_2 + \cos x_3 + \cos x_4)} \\ &= \frac{1}{\pi^4} \int_0^{\infty} e^{-s} \left(\int_0^{\pi} e^{zs \cos k}\, dk\right)^4 ds = \int_0^{\infty} e^{-s} I_0^4(sz)\, ds. \end{aligned}$$

From (9)

$$\begin{aligned} P_4(z) &= \sum_{n_1,n_2,n_3,n_4=0}^{\infty} \frac{(z/2)^{2(n_1+n_2+n_3+n_4)}}{(n_1!n_2!n_3!n_4)^2} \int_0^{\infty} e^{-s} s^{2(n_1+n_2+n_3+n_4)}\, ds \\ &= \sum \{n_i\} \frac{2\left(\sum n_i\right)!}{(n_1!n_2!n_3!n_4)^2} (z/2)^{2\sum n_i} = \sum_{n=0}^{\infty} A_n (z/2)^{2n}, \end{aligned}$$

where $A_n = \sum_{n_1+n_2+n_3+n_4=n} \frac{(2n)!}{(n_1!n_2!n_3!n_4)^2}$. But if we remark that

$$\sum_{n_1+n_2+n_3+n_4=n} (n_1!n_2!n_3!n_4)^{-2} = 2^{2n} \sum_{n_1+n_2=n} \frac{(1/2)_{n_1}(1/2)_{n_2}}{(n_1!n_2!)^3} = 2^{2n} S_n$$

where $(1/2)_{n_1} = \Gamma(n_1 + 1/2)/\Gamma(1/2)$, then we have

$$P_4(z) = \int_0^\infty e^{-s} I_0^4(sz)\, ds = \sum_{n=0}^{\infty} z^{2n}(2n)! \sum_{n_1+n_2=n} \frac{(1/2)_{n_1}(1/2)_{n_2}}{(n_1! n_2!)^3}.$$

Using the following identities

$$(1/2)_{n-k} = \Gamma(n-k+1/2)/\Gamma(1/2) = \frac{(-1)^{n-k}\pi}{\Gamma(1/2)\Gamma(1/2-n)(1/2-n)_k} \text{ and } (n-k)! = \frac{(-1)^k n!}{(-n)_k}$$

we obtain

$$S_n = \frac{(-1)^n \pi^{1/2}}{\Gamma(1/2-n)(n!)^3} \sum \frac{(1/2)_k(-n)_k(-n)_k(-n)_k}{(1)_k(1)_k(1/2-n)_k k!} = \frac{(-1)^n \pi^{1/2}}{\Gamma(1/2-n)(n!)^3}\, {}_4F_3\left[\begin{matrix} 1/2, -n, -n, -n; \\ 1, 1, 1/2-n; \end{matrix}\; 1\right]$$

and

$$A_n = \frac{4^n (2n)!(1/2)_n}{(n!)^3}\, {}_4F_3\left[\begin{matrix} 1/2, -n, -n, -n; \\ 1, 1, 1/2-n; \end{matrix}\; 1\right].$$

We can also solve the fourth order differential equation with 4 regular singular points (0, 1/16, 1/4, ∞). An indirect method leads to an integral representation whereas a direct method leads to Kampé de Fériet functions.

For $d > 4$, we have

$$P_d(z) = \frac{1}{\pi^d} \int \cdots \int_0^\pi \frac{dx_1 \cdots dx_d}{1 - \frac{z}{d}(\cos x_1 + \cdots + \cos x_d)} = \int_0^\infty e^{-s} I_0(sz/d)\, ds = \frac{2}{\pi} \int_0^1 \frac{Z_d(u^2 z^2/d^2)}{\sqrt{1-u^2}}\, du$$

$$\text{with } Z_d(x) = \int_0^\infty t K_0(t) I_0^d(xt)\, dt.$$

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