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FAST TRACK COMMUNICATION

Lattice Green functions and Calabi–Yau differential equations

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Abstract
By making the connection between four-dimensional lattice Green functions (LGFs) and Picard–Fuchs ordinary differential equations of Calabi–Yau manifolds, we have given explicit forms for the coefficients of the four-dimensional LGFs on the simple-cubic and body-centred cubic lattices, in terms of finite sums of products of binomial coefficients, and have shown that the corresponding four-dimensional face-centred cubic LGF satisfies a fourth-order ODE of degree 7, which we have found but not solved. The fact that the Picard–Fuchs equations that appear here are similar to those that appear in string theory perhaps makes the first connection between these two apparently unrelated topics.

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1. Introduction

Lattice Green functions (LGFs) are remarkable integrals that arise in many problems of solid-state physics, including ferromagnetism, phonon spectra and lattice vibrations. The study of random walks, which is a central problem in probability theory, also gives rise to lattice Green functions which, along with certain integrals of Ramanujan, Onsager and Selberg, are amongst the most remarkable that appear in mathematical physics. Higher dimensional LGFs, for lattices of dimensionality greater than 3, have been sought since the 1930s [4]. We show here that LGFs satisfy the Picard–Fuchs ordinary differential equations (ODEs) of Calabi–Yau manifolds, which are ubiquitous in string theory [5, 6]. This allows us to compute LGFs in $D \geqslant 4$ dimensions and to make possible connections between two subjects that were hitherto unrelated.

The Picard–Fuchs equations of Calabi–Yau manifolds that appear here also appear in string theory [5, 6]. This connection appears to be new but is analogous to that between plane partitions and topological strings [6, 7]. The latter connection continues to be mathematically fruitful, and we hope that the connection made in this communication will be similarly fruitful.

1.1. Lattice walk structure functions

Consider a random walk on a D-dimensional lattice with i.i.d steps [4]. Let $\mathbf{x}$ be the position vector of a point on the lattice[1] and $p[\mathbf{x}' - \mathbf{x}]$ be the probability of a single-step transition from $\mathbf{x}$ to $\mathbf{x}'$. The discrete Fourier transform of $p[\mathbf{x}]$ is the lattice walk structure function $\lambda[\mathbf{k}] = \sum_{\mathbf{x}} \mathrm{e}^{\mathrm{i}\mathbf{x}\cdot\mathbf{k}} p[\mathbf{x}]$. For the three-dimensional body-centred cubic (BCC), face-centred cubic (FCC) and simple cubic (SC) lattices, the structure functions are

$$\lambda[\mathbf{k}] = \begin{cases} \cos k_1 \cos k_2 \cos k_3 & \text{BCC} \\ \frac{1}{3}(\cos k_1 \cos k_2 + \cos k_1 \cos k_3 + \cos k_2 \cos k_3) & \text{FCC} \\ \frac{1}{3}(\cos k_1 + \cos k_2 + \cos k_3) & \text{SC.} \end{cases} \tag{1}$$

Let $a_n[\mathbf{x}]$ be the probability that a random walk starts at $\mathbf{0}$ and ends at $\mathbf{x}$ after n steps. The lattice Green function is the generating function

$$P(\mathbf{x}; z) = \sum_{n=0}^{\infty} a_n[\mathbf{x}] z^n = \frac{1}{(2\pi)^D} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \frac{\mathrm{e}^{\mathrm{i}\mathbf{x}\cdot\mathbf{k}}}{1 - z\lambda[\mathbf{k}]} \, \mathrm{d}^D\mathbf{k}. \tag{2}$$

Evaluating $P(\mathbf{x}; z)$ in one dimension is straightforward, while in two dimensions, it requires basic knowledge of complete elliptic integrals [4]. In three dimensions, the problem suddenly becomes difficult, and in the following we restrict our attention to $P(\mathbf{0}; z)$ which we write as $P(z)$. For the three-dimensional BCC lattice, $P(1)$ was computed by W F van Peype, a student of H A Kramers, in 1938 [8]. For the three-dimensional FCC and SC lattices, $P(1)$ was computed by G N Watson in 1939 [9], and together these three integrals are known as *the Watson integrals.*

For the general three-dimensional case $P(z)$, almost all advances since 1971 were made by G S Joyce and S Katsura and their co-workers. For surveys, see [4, 10]. Remarkably, for the three-dimensional BCC, FCC, SC lattices, and also for the three-dimensional diamond lattice, all results can be written in the form

$$P(z) = f_1(z)(K(f_2(z)))^2, \tag{3}$$

where $f_1(z)$ and $f_2(z)$ are simple, lattice-dependent algebraic functions of z and $K(q)$ is the complete elliptic integral of the first kind with modulus q.

2. $P(z)$ in $D \geqslant 4$ dimensions

Few exact results are available for $D \geqslant 4$ LGFs. We will outline the known results. For the four-dimensional BCC lattice the problem is completely straightforward, since $\lambda[\mathbf{k}]$ is factorized, as we can see from equation (1), so that

$$\begin{aligned} P(z) &= \frac{1}{(\pi)^4} \int_0^{\pi} \cdots \int_0^{\pi} \frac{\mathrm{d}k_1\, \mathrm{d}k_2\, \mathrm{d}k_3\, \mathrm{d}k_4}{1 - z \cos k_1 \cos k_2 \cos k_3 \cos k_4} \\ &= \frac{1}{\pi^4} \sum_{n=0}^{\infty} z^n \left(\int_0^{\pi} \cos^n k \, \mathrm{d}k \right)^4 = \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n \left(\frac{1}{2}\right)_n \left(\frac{1}{2}\right)_n \left(\frac{1}{2}\right)_n}{(1)_n (1)_n (1)_n n!} z^{2n} \\ &= {}_4F_3\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}; 1, 1, 1; z^2\right) = \sum_{n=0}^{\infty} \binom{2n}{n}^4 \left(\frac{z}{16}\right)^{2n}, \end{aligned} \tag{4}$$

[1] We use boldface letters to denote vector quantities.

which clearly readily generalizes to all D. Using the notation $\theta = z\frac{\mathrm{d}}{\mathrm{d}z}$ allows the underlying ODE to be written in a surprisingly compact form, and we find that $P(z)$ in equation (4) satisfies the fourth-order ODE of degree 1:[2]

$$\left(\theta^4 - 256z\left(\theta + \tfrac{1}{2}\right)^4\right)P(16z) = 0. \tag{5}$$

In 1994, Glasser and Guttmann found that the four-dimensional SC LGF $P(z) = \sum_{n\geqslant 0} a_n z^n$ satisfies the fourth-order ODE of degree 2:

$$(\theta^4 - 4z(2\theta+1)^2(5\theta^2+5\theta+2) + 2^8 z^2(\theta+1)^2(2\theta+1)(2\theta+3))P(z) = 0, \tag{6}$$

and expressed its solution as a double hypergeometric function [11] and also in terms of Kampé de Fériet functions. Whilst this was technically a solution, it was not a particularly transparent or simple solution. In the following section, we give a simpler solution in terms of finite sums of products of binomial coefficients.

For the hyper-cubic lattice, Bender *et al* [1] obtained asymptotics for random walks in arbitrary (nonintegral) dimensionality. In 2001, Joyce and Zucker [2] gave a rapidly convergent numerical procedure to calculate the Watson integral $P(1)$ for the hypercubic lattice in any dimension.

3. Calabi–Yau ODEs

The central new idea in this paper that now allows us to compute $D \geqslant 4$ LGFs is the connection to Calabi–Yau manifolds, which are ubiquitous in modern string theory, via the Picard–Fuchs equations [5, 6]. Once we know that an ODE has *maximal unipotent monodromy (MUM)*, then the Frobenius method gives us a constructive way to write a basis of the solutions. If in addition, the ODE satisfies the *Calabi–Yau condition*, then we have enough constraints on the solutions that it is frequently solvable.

3.1. Calabi–Yau manifolds

The Picard–Fuchs equations are a set of linear ODEs in the moduli parameter of the complex structure on a particular complex manifold $\mathcal{M}_n$ of complex dimension n, satisfying certain additional properties that need not concern us here.

An ODE is the Picard–Fuchs ODE of a Calabi–Yau manifold when it satisfies a certain *Calabi–Yau condition*. In the following, we refer to Picard–Fuchs ODEs of Calabi–Yau manifolds as *Calabi–Yau ODEs*.

In the presence of branch cuts, the solutions to an ODE acquire phase factors when transported around a branch cut. These phases are coded in a monodromy matrix M. An order-n ODE has maximal unipotent monodromy if $M^p = 1$ only when p is an integral multiple of n. In the presence of maximal unipotent monodromy, one can use the Frobenius method to obtain a basis for the solutions. The Calabi–Yau ODEs we consider here have MUM at the origin, a consequence of which is that all the exponents at the origin are zero.

Consider the fourth-order ODE

$$y^{(4)} + a_3(z)y^{(3)} + a_2(z)y'' + a_1(z)y' + a_0(z)y = 0 \tag{7}$$

with four solutions around the origin, y_0, y_1, y_2, y_3. Using the Frobenius method, maximal unipotent monodromy at the origin implies that

$$y_0 = 1 + \sum_{n\geqslant 1} \alpha_n z^n \tag{8}$$

[2] The degree is the maximum power of z that occurs in the differential operator.

$$y_1 = y_0 \log z + \sum_{n\geqslant 1} \beta_n z^n \tag{9}$$

$$\begin{aligned} y_2 &= \frac{y_0}{2}\log^2 z + \left(\sum_{n\geqslant 1}\beta_n z^n\right)\log z + \sum_{n\geqslant 1}\gamma_n z^n \\ y_3 &= \frac{y_0}{6}\log^3 z + \frac{1}{2}\left(\sum_{n\geqslant 1}\beta_n z^n\right)\log^2 z + \left(\sum_{n\geqslant 1}\gamma_n z^n\right)\log z + \sum_{n\geqslant 1}\delta_n z^n. \end{aligned} \tag{10}$$

The condition for equation (7) to be a Picard–Fuchs equation of a Calabi–Yau manifold is

$$a_1 = \tfrac{1}{2}a_2 a_3 - \tfrac{1}{8}a_3^3 + a_2' - \tfrac{3}{4}a_3 a_3' - \tfrac{1}{2}a_3'', \tag{11}$$

which puts stringent conditions on the solutions that frequently allow us to determine them [12].

A list of Calabi–Yau ODEs has been tabulated by Almkvist *et al* [13]. It contains more than 300 Calabi–Yau ODEs, many of which were found to have solutions in terms of sums of products of binomial coefficients.

Anticipating results given below, we remark on the unexpected, and so far unexplained, observation that almost all known higher dimensional LGF ODEs also appear in the list of [13]. For example, equation (5) is Calabi–Yau ODE number **3** in [13], while equation (6) of Glasser and Guttmann is Calabi–Yau ODE number **16**, which is given along with its solution. So, for the LGF generating function coefficient a_n, we have

$$a_n = \binom{2n}{n}\sum_{j+k+l+m=n}\left(\frac{n!}{j!k!l!m!}\right)^2 = \binom{2n}{n}\sum_{k=0}^{n}\binom{n}{k}^2\binom{2k}{k}\binom{2n-2k}{n-k}.$$

The first equality follows from a result of Glasser and Montaldi [14], who related the hypercubic LGF to the generating function of the squares of multinomial coefficients, which had been given earlier by Guttmann and Prellberg [15], but the second equality is new, and gives the coefficient as a finite sum of products of binomial coefficients.

3.2. Four-dimensional FCC LGF

The four-dimensional FCC LGF has not previously been found. It is defined as

$$P(z) = \frac{1}{(\pi)^4}\int_0^{\pi}\cdots\int_0^{\pi}\frac{\mathrm{d}k_1\,\mathrm{d}k_2\,\mathrm{d}k_3\,\mathrm{d}k_4}{1-\frac{z}{6}\lambda[\mathbf{k}]},$$

where $\lambda[\mathbf{k}] = (c_1c_2 + c_1c_3 + c_1c_4 + c_2c_3 + c_2c_4 + c_3c_4)$, with $c_i = \cos k_i$. We set $u = 1 - \frac{z}{6}(c_2c_3 + c_2c_4 + c_3c_4)$ and $v = \frac{z}{6}(c_2 + c_3 + c_4)$. Then the integrand is $[u - v\cos k_1]^{-1}$. We use

$$\frac{1}{\pi}\int_0^{\pi}\frac{\mathrm{d}\theta}{u - v\cos\theta} = \frac{1}{\sqrt{u^2-v^2}} = \frac{1}{\sqrt{(u+v)(u-v)}}$$

to eliminate k_1.

Next we write $(u+v)(u-v) = e(c-\cos k_2)(d-\cos k_2)$, where c, d, e are independent of k_2, and use

$$\int_0^{\pi}\frac{\mathrm{d}\theta}{\sqrt{(c-\cos\theta)(d-\cos\theta)}} = \frac{2K(k)}{\sqrt{(c-1)(d+1)}}$$

to eliminate k_2, where $k^2 = \frac{2(c-d)}{(c-1)(d+1)}$, and $K(k)$ is the complete elliptic integral of the first kind. We are left with a two-dimensional integral, which was expanded as a power series in z

and integrated term by term in Maple. We obtained 40 terms in a few hours and then searched for, and found, the ODE generating the coefficients. It is

$$\begin{aligned}(\theta^4 - z(39\theta^4 - 30\theta^3 - 19\theta^2 - 4\theta) + 2z^2(16\theta^4 - 1070\theta^3 - 1057\theta^2 - 676\theta - 192)\\ - 36z^3(171\theta^3 + 566\theta^2 + 600\theta + 316)(3\theta + 2)\\ - 2^5 3^3 z^4(384\theta^4 + 1542\theta^3 + 2635\theta^2 + 2173\theta + 702)\\ - 2^6 3^3 z^5(1393\theta^3 + 5571\theta^2 + 8378\theta + 4584)(1 + \theta)\\ - 2^{10} 3^5 z^6(31\theta^2 + 105\theta + 98)(1 + \theta)(\theta + 2)\\ - 2^{12} 3^7 z^7(\theta + 1)(\theta + 2)^2(\theta + 3))P(z) = 0.\end{aligned} \tag{12}$$

This is a fourth-order, degree 7 Calabi–Yau ODE with regular singular points at 0, $1/24$, $-1/4$, $-1/8$, $-1/12$, $-1/18$ and ∞. It is not (yet) on the list [13], but turns out to be one of only three known fourth-order, degree 7 Calabi–Yau ODEs [16].

It is straightforward to obtain the five-dimensional BCC and SC LGF ODEs. The five-dimensional BCC LGF follows by a straightforward generalization of equation (4), and satisfies a fifth-order ODE, which can be *pulled back*[3] to a fourth-order ODE. Similarly, the five-dimensional SC LGF satisfies a fifth-order ODE of degree 3, which can be *pulled back* to a fourth-order degree 12 ODE. It is number **188** in [13]. Remarkably, all the above ODEs also turn out to be Calabi–Yau ODEs! We are yet to obtain the five-dimensional FCC LGF.

3.3. Mirror symmetry

A deep result from modern string theory is that Calabi–Yau manifolds come in pairs $\{X_n, Y_n\}$ that are *mirror symmetric* [5–7]. Consider the solutions of equation (7) given by equations (8)–(10) and define $q(z) = \exp(y_1/y_0) = \sum_{n\geqslant 0} t_n z^n$. If z is the moduli parameter of the complex structure on X_n, then q is the moduli parameter of the Kähler structure on Y_n, and the inverse function $z(q) = \sum_{n\geqslant 0} u_n q^n$ is the *mirror map*. Given a mirror pair $\{X_n, Y_n\}$, one can compute the Yukawa coupling $K(q)$ of certain fields in the effective field theory limit of a string theory compactified on Y_n. The result is

$$K(q) = \left(q\frac{\mathrm{d}}{\mathrm{d}q}\right)^2\left(\frac{y_2}{y_0}\right) = 1 + \sum_{k=1}^{\infty}\frac{k^3q^k}{1-q^k}N_k, \tag{13}$$

where N_k is the degree-k instanton number, that is, the number of degree k holomorphic maps from the projective line to Y_n. The sum on the right-hand side of equation (13) is the full string theoretic contribution to the Yukawa coupling. Equation (13) is a major achievement of modern string theory. It led to great advances in enumerative geometry [6, 7].

From this definition, we can calculate the instanton numbers N_k from the LGF ODEs. In all cases we find that, up to a small integer multiple, they comprise an integer sequence. Presumably they count something of combinatorial or probabilistic significance. At this stage, what this something is remains a completely open, but potentially very interesting, question.

4. Conclusion

We have given explicit forms for the coefficients of the four-dimensional LGFs on the SC and BCC lattices, in terms of finite sums of products of binomial coefficients, and have shown that the corresponding FCC LGF satisfies a fourth-order ODE of degree 7, which we have found but not solved. We have also given the solution, in terms of hypergeometric functions, of the LGF for the five-dimensional BCC lattice and identified the relevant ODE for the five-dimensional

[3] By this, we mean that the solutions can be expressed in terms of the solutions of an ODE of a lower degree.

SC lattice. Neither calculation is particularly difficult. However what is remarkable is that, in both cases, a pull-back to a fourth-order ODE can be achieved and that all these LGFs are solvable in terms of Calabi–Yau ODEs.

It took more than 20 years to find a unifying viewpoint for all three-dimensional LGFs as products of two elliptic integrals of the first kind. Glasser and Guttmann [11] showed that the four-dimensional BCC LGF can be expressed as a 1D integral of a product of two elliptic integrals of the first kind. Glasser [3] has suggested that this result may hold for all four-dimensional lattices. If so, that would then provide a unifying viewpoint of four-dimensional LGFs.

The physical meaning of the connection between LGFs and Calabi–Yau ODEs remains to be explained. The answer will potentially provide insights into both LGFs and Calabi–Yau ODEs. A related aspect is to use the mirror symmetry of Calabi–Yau manifolds to obtain deeper information about LGFs and explain the combinatorial significance of the instanton numbers. The fact that the Picard–Fuchs equations of Calabi–Yau manifolds that appear in this paper are the same as those that appear in string theory [5, 6] hopefully marks the beginning of a cross-fertilization between these different topics. On a more general level, we can draw a parallel with some integrals that arise in the study of the two-dimensional Ising model susceptibility [17]. There it is argued that the algebraic nature of the integrand give rise to globally nilpotent Fuchsian ODEs with rational exponents. Similar conclusions should apply to the LGFs we consider here, from which follows that the solutions are highly specialized and selected. It remains to link this somewhat vague observation with something more precise to explain the occurrence of the CY condition for these ODEs.

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