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Vassiliev invariants and a strange identity related to the Dedekind eta-function

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Abstract

In this paper the "function" $F(q) = \sum_{n=0}^{\infty}(1-q)(1-q^2)\cdots(1-q^n)$ is studied. The series does not converge in any open set, but has well-defined values and derivatives of all orders when q is a root of unity. It is shown that the coefficients of its Taylor expansion at $q=1$ are equal to the numbers ξ_D of "regular linearized chord diagrams" as defined by Stoimenow and hence give an upper bound (the best currently known) for the number of linearly independent Vassiliev invariants of degree D. There are similar expansions at other roots of unity. The same values and derivatives of all orders at all roots of unity are obtained as the limiting value of the function $-\frac{1}{2}\sum_{n\in\mathbb{Z}}(-1)^n|6n+1|q^{(3n^2+n)/2}$, the "derivative of order one-half" of the Dedekind eta-function, and also exhibit a kind of modular behavior which can be seen as an example of a generalization of the classical theory of periods of modular forms to the case of half-integral weight. Functions of a similar type also occurred in recent joint work with Lawrence in connection with the Witten–Reshetikhin–Turaev invariants of knots.

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Introduction

An important open problem of knot theory is the determination of the number $V(D)$ of linearly independent Vassiliev invariants of degree D, or equivalently of chord diagrams of degree D modulo the 4-term relation. In a recent paper, Stoimenow [6] introduced the notion of "regular linearized chord diagrams" (the definition is recalled in Section 1) and proved that $V(D)$ is bounded by the number ξ_D of such diagrams of degree D. He gave an explicit, but somewhat complicated,

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algorithm (Eqs. (8)–(11) below) to compute the numbers ξ_D and used it to show that $\xi_D \leqslant C(M)D^{-M}D!$ for any $M > 0$, improving the previously known upper bound $(D-2)!/2$ for the number of Vassiliev invariants, but observed that the numerical computations (up to $D = 30$) actually suggested a better estimate "something like $D!/1.5^D$". In this paper we will give another and simpler description of Stoimenow's numbers ξ_D and use it to deduce that $\xi_D/D!$ tends to 0 exponentially fast (like $1.644\ldots^{-D}$). The analysis involves a series of surprising identities related to the Dedekind eta-function. These identities also provide the first indication of the existence of a period theory (or theory of Eichler integrals) for modular forms of half-integral weight.

Specifically, we will show (Theorem 1) that Stoimenow's numbers ξ_D are given by the simple generating function identity

$$\sum_{n=0}^{\infty} (1-q)(1-q^2)\cdots(1-q^n) = \sum_{D=0}^{\infty} \xi_D (1-q)^D \tag{1}$$

in $\mathbb{Z}[[1-q]]$. This identity, apart from its elegance, makes the numerical evaluation of the ξ_D very easy. Calculating the values up to $D = 200$ and interpolating numerically suggested an asymptotic formula of the form

$$\xi_D \sim \frac{D!\sqrt{D}}{(\pi^2/6)^D}\left(C_0 + \frac{C_1}{D} + \frac{C_2}{D^2} + \cdots\right) \tag{2}$$

with $C_0 \approx 2.704332490062429595$, $C_1 \approx -1.52707$ and $C_2 \approx -0.269009$. Our second main result (Theorem 4 in Section 3) is a proof of this formula with explicitly computable constants C_i. In particular,

$$C_0 = \frac{12\sqrt{3}}{\pi^{5/2}} e^{\pi^2/12}, \tag{3}$$

which agrees to the accuracy given above with the empirically obtained value. The proof of (2) is based on the following surprising identity of formal power series (Theorem 3 in Section 2):

$$e^{-t/24} \sum_{n=0}^{\infty} (1-e^{-t})\cdots(1-e^{-nt}) = \sum_{n=0}^{\infty} \frac{T_n}{n!}\left(\frac{t}{24}\right)^n. \tag{4}$$

Here the numbers $T_0 = 1, T_1 = 23, T_2 = 1681, \ldots$ (which occur in the literature under the name "Glaisher's T-numbers"; cf. [5], sequence #5138), are integers given by the generating function

$$\sum_{n=0}^{\infty} \frac{T_n}{(2n+1)!} x^{2n+1} = \frac{\sin 2x}{2\cos 3x} \quad \left(= \frac{\sin x}{1 - 4\sin^2 x}\right) \tag{5}$$

or in closed form by the formulas

$$T_n = 6\frac{(-144)^n}{n+1}\left[B_{2n+2}\left(\frac{1}{12}\right) - B_{2n+2}\left(\frac{5}{12}\right)\right] = \frac{(2n+1)!}{2\sqrt{3}} \frac{L(2n+2,\chi)}{(\pi/6)^{2n+2}}, \tag{6}$$

where $B_n(x)$ denotes the nth Bernoulli polynomial and $L(s,\chi)$ is the Dirichlet L-series associated to the quadratic character $\chi = (12/\cdot)$ of conductor 12.

Identity (4) is surprising, but not strange: it is a normal identity between two formal power series. The "strange identity" of the title is the "formula"

$$\sum_{n=0}^{\infty} (1-q)(1-q^2)\cdots(1-q^n) = -\frac{1}{2}\sum_{n=1}^{\infty} n\chi(n) q^{(n^2-1)/24}. \tag{7}$$

What is strange about it, apart from the factor $-\frac{1}{2}$ on the right-hand side, is that the two sides never make sense simultaneously: the left-hand side is divergent both as a power series in q and as a complex-valued function in the region $|q| < 1$ (or of course $|q| > 1$), but has a well-defined value when q is a root of unity, while the right-hand side converges as a formal power series and in the disk $|q| < 1$, but nowhere on the unit circle. The meaning of the equality is that the function on the left agrees at roots of unity with the radial limit of the function on the right, and similarly for the derivatives of all orders. Eq. (7), of which (4) is a consequence, is related to the Dedekind η-function and the theory of periods of modular forms. This will be discussed briefly in Section 6, and at more length in a later paper.

I end this introduction with a few words on the origin of the formulas above. The expression occurring on the left-hand side of (1) occurred in a lecture on analytic continuation of Feynman integrals given by Maxim Kontsevich in the Max-Planck-Institut für Mathematik in October 1997. He had studied the values of this expression when q is a root of unity (in which case the sum terminates) and discovered a very surprising asymptotic formula (Eq. (34) below) for these values when $q = \mathrm{e}^{2\pi \mathrm{i}/k}$ with $k \to \infty$. I gave an interpretation of his formula as a statement about a certain "period function" associated to the Dedekind eta-function and showed that it would follow from identity (7). As part of the attempt to prove (7) and its special case (4) I calculated the first few Taylor coefficients at $q = 1$ of the left-hand side of (1) and discovered by using the on-line version of [5] that the same numbers had occurred in [6] in the context of counting chord diagrams. Studying the recursions in [6] led to a proof of identity (1) and to a derivation of the asymptotic Eq. (2) modulo identity (4), for which I finally found an elementary direct proof.

1. The number of regular linearized chord diagrams

We define a *linearized chord diagram* (LCD) of degree D as a fixed-point free involution τ on the set $\{1,2,\dots,2D\}$. (Think of the chords as the semi-circles in the upper half-plane with end-points i and $\tau(i)$ for $1 \leqslant i \leqslant 2D$.) The diagram is called *regular* if $[i, i+1] \subseteq [\tau(i+1), \tau(i)]$ whenever $\tau(i+1) < \tau(i)$. For instance, in degree 2 there are two regular LCDs (12)(34) and (13)(24) and one irregular one (14)(23), while in degree 3 there are five regular LCDs (12)(34)(56), (12)(35)(46), (13)(25)(46), (13)(24)(56) and (14)(25)(36) and ten irregular ones. It is well known that the dimension of the space of Vassiliev invariants of degree D is equal to the dimension of the space of LCDs of degree D modulo a certain relation (the four-term relation). The total number of LCDs of degree D is equal to

$$\frac{(2D)!}{2^D D!} \sim \frac{2^D D!}{\sqrt{\pi D}},$$

so this is a trivial upper bound on the dimension in question. This bound was improved to $(D-1)!$ by Chmutov and Duzhin [2] and to $(D-2)!/2$ by Ng and Stanford [4]. In a recent paper [6], Stoimenow showed that any linearized chord diagram is equivalent modulo the four-term relation to a linear combination of regular ones, so that the dimension $V(D)$ of the space of Vassiliev invariants is also bounded by the number ξ_D of regular LCDs. In this section we will prove the generating function identity (1) for these numbers.

In fact, we will prove a slightly more precise generating function identity. Following Stoimenow, we define $\xi_{D,k}$ for all $k \geqslant 1$ as the number of regular LCSs of degree D whose leftmost chord has length k (i.e. $\tau(1) = k+1$). The numbers $\xi_{D,k}$ vanish for $k > D$ and are related to the numbers ξ_D by

$$\xi_D = \sum_{k=1}^{D} \xi_{D,k} = \xi_{D+1,1}. \tag{8}$$

Stoimenow gave the following recursive formula to compute the numbers $\xi_{D,k}$:

$$\xi_{1,1} = 1 \quad \text{and} \quad \xi_{D,k} = \sum_{l=k-1}^{D-1} \sum_{p=1}^{l} \hat{\xi}_{D-1,l,p} \eta_{l,k-1,p} \quad \text{for } D \geqslant 2, \tag{9}$$

where $\hat{\xi}_{D,l,p}$ is defined by the formula

$$\hat{\xi}_{D,l,p} = \sum_{j=1}^{p} (-1)^{p-j} \binom{p-1}{j-1} \xi_{D+j-l,j} \tag{10}$$

and the coefficients $\eta_{l,k,p}$ by the generating function

$$\sum_{k,l,p \geqslant 0} \eta_{l,k,p} x^k y^l z^p = \frac{1-x}{1-x-z(y/(1-y)-x^2y/(1-xy))}. \tag{11}$$

From these one can compute numerical values. Here is a table for $D \leqslant 7$:

D	$k=1$	2	3	4	5	6	7	ξ_D
1	1							1
2	1	1						2
3	2	2	1					5
4	5	6	3	1				15
5	15	21	12	4	1			53
6	53	84	54	20	5	1		217
7	217	380	270	110	30	6	1	1014

We extend the definition to all $D, k \geqslant 0$ by setting $\xi_{D,k} = 0$ whenever $Dk = 0$ except for $\xi_{0,0} = 1$.

Theorem 1. *The numbers $\xi_{D,k}$ are given by the generating function*

$$\sum_{D,k \geqslant 0} \xi_{D,k} X^D Y^k = \sum_{n=0}^{\infty} (1-a)(1-qa)\cdots(1-q^{n-1}a) \in \mathbb{Z}[Y][[X]], \tag{12}$$

where q and a are related to X and Y by

$$q = 1 - X, \qquad a = 1 - XY. \tag{13}$$

Specializing to $Y = 1$, $a = q$ and using (8), we obtain the generating function identity (1).

Proof. We can rewrite (9) (with $D+1, k+1$ in place of D, k) as

$$\begin{aligned} \xi_{D+1,k+1} &= \sum_{l=k}^{D} \sum_{p=1}^{l} \left(\sum_{j=1}^{p} (-1)^{p-j} \binom{p-1}{j-1} \xi_{D+j-l,j} \right) \eta_{l,k,p} \\ &= \sum_{l=k}^{D} \sum_{j=1}^{l} \xi_{D+j-l,j}\, \eta^*_{l,k,j} \end{aligned}$$

with

$$\eta^*_{l,k,j} = \sum_{p=j}^{l} (-1)^{p-j} \binom{p-1}{j-1} \eta_{l,k,p} \quad (l \geqslant j \geqslant 1).$$

Using the generating function (11) we compute

$$\begin{aligned}\sum_{l \geqslant j \geqslant 1,\, k \geqslant 0} \eta^*_{l,k,j} x^k y^l z^j &= \sum_{l \geqslant p \geqslant j \geqslant 1,\, k \geqslant 0} (-1)^{p-j} \binom{p-1}{j-1} \eta_{l,k,p} x^k y^l z^j \\ &= \sum_{l \geqslant p \geqslant 1,\, k \geqslant 0} \eta_{l,k,p} x^k y^l z (z-1)^{p-1} \\ &= \frac{z}{z-1} \left(\frac{(1-y)(1-xy)}{(1-y)(1-xy) - y(z-1)(1+x-xy)} - 1 \right) \\ &= \frac{yz(1+x-xy)}{1-yz(1+x-xy)},\end{aligned}$$

which gives the explicit formula

$$\begin{aligned}\eta^*_{l,k,j} &= \text{coefficient of } x^k y^{l-j} \text{ in } (1 + x(1-y))^j \\ &= (-1)^{l-j} \binom{j}{k} \binom{k}{l-j}.\end{aligned}$$

(In particular $\eta^*_{l,k,j} = 0$ unless $l \geqslant j \geqslant k \geqslant l - j \geqslant 0$.) In other words, we have replaced (9)–(11) by the simpler recursion relation

$$\xi_{D+1,k+1} = \sum_{r=0}^{k} \sum_{j=k}^{D-r} (-1)^r \binom{k}{r} \binom{j}{k} \xi_{D-r,j} \quad (D \geqslant 1) \tag{14}$$

and this recursion remains true for $D = 0$ with the conventions above.

Now let $F(X, Y)$ be the generating function defined by the left-hand side of Eq. (12). Then the recursion relation (14) translates into the identity

$$\begin{aligned}F(X,Y) &= 1 + \sum_{D,k \geqslant 0} \xi_{D+1,k+1} X^{D+1} Y^{k+1} \\ &= 1 + XY \sum_{D \geqslant j \geqslant k \geqslant r \geqslant 0} (-1)^r \binom{k}{r} \binom{j}{k} \xi_{D,j} X^{D+r} Y^k \\ &= 1 + XY \sum_{D \geqslant j \geqslant k \geqslant 0} \binom{j}{k} \xi_{D,j} X^D Y^k (1-X)^k \\ &= 1 + XY \sum_{D \geqslant j \geqslant 0} \xi_{D,j} X^D (1 + Y - XY)^j \\ &= 1 + XYF(X, 1 + Y - XY).\end{aligned}$$

Now make the change of variables (13). Then $F(X, Y)$ becomes a power series $f(q, a)$ in $1 - q$ and $1 - a$ (because $\xi_{D,k} = 0$ for $k > D$) and the functional equation just proved translates into the simpler functional equation

$$f(q, a) = 1 + (1 - a) f(q, qa).$$

Iterating this, we find that $f(q, a)$ is equal to the expression on the right-hand side of (12). □

2. Some beautiful power series identities

Set

$$F(q) = \sum_{n=0}^{\infty} (1 - q) \cdots (1 - q^n), \tag{15}$$

where the empty product as usual is taken to be 1. This expression does not make any sense either as a formal power series in q (since the terms tend to a non-zero limit in $\mathbb{Z}[[q]]$) or as a function of a complex variable (since the series diverges both for $|q| < 1$ and for $|q| > 1$), but does make sense when q is a root of unity (since the series then terminates) and also as a formal power series in $1 - q$ or in $\zeta - q$ for any root of unity ζ. The values and power series expansions of q at general roots of unity will be discussed in Section 5; for now, we consider only the expansion of F around $q = 1$, our immediate goal being to prove identity (4) describing expansion of $F(\mathrm{e}^{-t})$ as a power series in t. We use the standard notation $(a)_n$ for the product $(1 - a)(1 - qa) \cdots (1 - q^{n-1}a)$ (to be taken as 1 if $n = 0$), so that $F(q)$ can be written simply as $\sum_{n \geqslant 0} (q)_n$.

Our first step is to replace F by another function which makes sense both as a function of the complex variable q and as a power series in q. By partial summation or induction on N we have

$$\sum_{n=0}^{N-1} [(q)_n - (q)_N] = \sum_{n=1}^{N} n (q)_{n-1} q^n \tag{16}$$

for any integer $N \geqslant 1$, and letting $N \to \infty$ we see that the series

$$F_1(q) = \sum_{n=1}^{\infty} n\, (q)_{n-1}\, q^n, \tag{17}$$

which makes sense both as a function of q (for $|q| < 1$) and as a power series in either q or $1 - q$, equals $F(q)$ as a power series in $(1 - q)$ (or in $\zeta - q$ for any root of unity ζ), while the series

$$F_2(q) = \sum_{n=0}^{\infty} [(q)_n - (q)_\infty] \tag{18}$$

agrees with $F_1(q)$ both as a power series in q and as a function in the disk of radius 1. We will prove an identity for the function $F_1 = F_2 \in \mathbb{Z}[[q]]$. To state it, we introduce two more power series.

Let $\chi(\cdot) = (12/\cdot)$ be the unique primitive character of conductor 12, already mentioned in the introduction. Euler's famous "pentagonal number theorem" $(q)_\infty = \sum_{k \in \mathbb{Z}} (-1)^k q^{k(3k+1)/2}$ can be written in the form

$$(q)_\infty := \prod_{n=1}^{\infty} (1-q^n) = \sum_{n=1}^{\infty} \chi(n)\, q^{(n^2-1)/24} = 1 - q + q^2 + q^5 + q^7 + \cdots; \tag{19}$$

this has a natural interpretation (which we will return to in Section 6) as saying that the Dedeind eta-function $q^{1/24}(q)_\infty$ is a theta series. We define a new power series $H(q) \in \mathbb{Z}[[q]]$ by

$$H(q) = \sum_{n=1}^{\infty} n\chi(n)\, q^{(n^2-1)/24} = 1 - 5q - 7q^2 + 11q^5 + 13q^7 - \cdots, \tag{20}$$

i.e., formally by "differentiating the Dedekind eta-function half a time" (this, too, will be discussed in more detail in Section 6). Finally, we define a power series $E(q) = q + 2q^2 + 2q^3 + 3q^4 + \cdots$ by

$$E(q) = -\frac{\mathrm{d}}{\mathrm{d}x}[\log(qx)_\infty]|_{x=1} = \sum_{n=1}^{\infty} \frac{q^n}{1-q^n} = \sum_{n=1}^{\infty} d(n)\, q^n, \tag{21}$$

where $d(n)$ denotes the number of divisors of an integer n.

Theorem 2. *The power series F_1, H and E are related by*

$$F_1(q) = -\tfrac{1}{2}H(q) + (\tfrac{1}{2} - E(q))(q)_\infty. \tag{22}$$

Proof. Define a power series in q, a and x by the formula

$$S(a,x) = \sum_{n=0}^{\infty} (1-a)(1-qa)\cdots(1-q^{n-1}a)\, x^n = \sum_{n=0}^{\infty} (a)_n\, x^n.$$

(Here q is considered as fixed and is suppressed in the notation.) The two recursions

$$(1-x)\, S(a,x) = 1 - ax\, S(a,qx), \quad S(a,x) = 1 + (1-a)\, x\, S(qa,x)$$

are immediately verified, and from them we deduce that the series

$$S(x) := (1-x)\, S(qx,x) = \sum_{n=0}^{\infty} (x)_{n+1} x^n \in Z[[q,x]]$$

satisfies the recursion $S(x) = 1 - qx^2 - q^2x^3\, S(qx)$, whence

$$S(x) = \sum_{n=1}^{\infty} \chi(n) x^{(n-1)/2} q^{(n^2-1)/24}. \tag{23}$$

(This is Exercise 10, p. 29, of [1].) In particular, for ε small we have

$$S(1-\varepsilon) = \sum_{n=1}^{\infty} \chi(n)\, q^{(n^2-1)/24} - \varepsilon \sum_{n=1}^{\infty} \frac{n-1}{2} \chi(n)\, q^{(n^2-1)/24} + O(\varepsilon^2).$$

On the other hand, directly from the definition we have

$$S(x) = (qx)_\infty + (1-x) \sum_{n=0}^{\infty} [(qx)_n - (qx)_\infty] x^n$$

which gives (cf. Eq. (21))

$$S(1-\varepsilon)=(q)_\infty+[E(q)(q)_\infty+F_2(q)]\varepsilon+O(\varepsilon^2).$$

The theorem now follows by comparing the coefficients of ε and recalling that $F_1=F_2$. $\square$

Remark. An amusing consequence of (22) is the formula

$$\frac{\sum_{n\geqslant 1} n\,\chi(n)\,q^{n^2/24}}{\sum_{n\geqslant 1}\chi(n)\,q^{n^2/24}}=1-2\sum_{n=1}^{\infty}\frac{q^n}{1-q^n}\left(1+\frac{1}{(1-q)\cdots(1-q^n)}\right)$$

for what one could call the "$\frac{1}{2}$-logarithmic derivative of the Dedekind eta-function".

Theorem 2 concerned power series expansions near $q=0$. We now consider the expansion of $F(q)$ at $q=1$, or rather, three different expansions, defining coefficients $\{a_n\}$, $\{b_n\}$, $\{c_n\}$ in $\mathbb{Z}$ by

$$F(1-x)=\sum_{n=0}^{\infty}a_n\,x^n,\quad F(\mathrm{e}^{-t})=\sum_{n=0}^{\infty}\frac{b_n}{n!}\,t^n,\quad \mathrm{e}^{-t/24}F(\mathrm{e}^{-t})=\sum_{n=0}^{\infty}\frac{c_n}{24^n n!}t^n, \tag{24}$$

so Theorem 1 asserts the equality $\xi_D=a_D$ and Eq. (4) the identity $c_n=T_n$. (An interpretation of the intermediate coefficients b_n will be given in Section 6.) We give a small table of these coefficients to illustrate their size; the precise asymptotics will be discussed in the next section.

n	0	1	2	3	4	5	6	7
a_n	1	1	2	5	15	53	217	1014
b_n	1	1	3	19	207	3451	81663	2602699
c_n	1	23	1681	257543	67637281	27138236663	15442193173681	11828536957233383

Theorem 3. *The coefficients c_n defined by the generating function* (24) *agree for all n with the Glaisher T-numbers T_n defined by the generating function* (5) *or by the closed formula* (6).

Proof. We have already seen that $F(q)$ and $F_1(q)$ agree to all orders as q approaches 1 (or any other root of unity) radially from within the unit disk. From Theorem 2 it follows that $F(q)$ also agrees with $-\frac{1}{2}H(q)$ to all orders, since $(q)_\infty$ vanishes to infinite order as we approach any root of unity and $E(q)$ blows up at worst like $(1-|q|)^{-2}$ (because the coefficients $d(n)$ in (21) are trivially bounded by n). It follows that the function $H(q)$ has an asymptotic expansion in powers of $1-q$ as q tends to 1 and that, if we define coefficients $\{\gamma_n\}$ by the asymptotic expansion

$$\mathrm{e}^{-t/24}H(\mathrm{e}^{-t})=\sum_{m=1}^{\infty}m\chi(m)\mathrm{e}^{-m^2t/24}\sim\sum_{n=0}^{\infty}\gamma_n\,t^n\quad\text{as } t\searrow 0,$$

then $c_n/24^n n!=-\gamma_n/2$ for all n. But a standard argument shows that

$$\gamma_n=\frac{(-1)^n}{24^n n!}\,L(-2n-1,\chi) \tag{25}$$

for all $n \geqslant 0$, where $L(-2n-1,\chi)$ is the value defined by analytic continuation of the L-series $L(s,\chi) = \sum \chi(m) m^{-s}$. Indeed,

$$\int_0^\infty \mathrm{e}^{-t/24} H(\mathrm{e}^{-t}) t^{s-1}\,\mathrm{d}t = \sum_{m=1}^\infty m\,\chi(m) \int_0^\infty \mathrm{e}^{-m^2 t/24} t^{s-1}\,\mathrm{d}t = 24^s\,\Gamma(s)\,L(2s-1,\chi),$$

while on the other hand we have

$$\int_0^C \mathrm{e}^{-t/24} H(\mathrm{e}^{-t}) t^{s-1}\,\mathrm{d}t = \int_0^C \left(\sum_{n=0}^{N-1} \gamma_n\, t^n + \mathrm{O}(t^N)\right) t^{s-1}\,\mathrm{d}t = \sum_{n=0}^{N-1} \frac{\gamma_n}{s+n} + R_N(s)$$

with $R_N(s)$ holomorphic in $\Re(s) > -N$ (N any positive integer), and comparing the residues at $s = -n$ gives Eq. (24). But by the functional equation of $L(s,\chi)$ we find that the number T_n defined by (6) is equal to $(-1)^{n-1} L(-2n-1,\chi)/2$, and combining this with formula (25) and the equality $c_n/24^n n! = -\gamma_n/2$ we obtain the main assertion of the theorem. To relate the generating function (5) and the formula for T_n in terms of Bernoulli polynomials in (6), one applies the same method to the function $\sum_m \chi(m)\,\mathrm{e}^{-mt} = (\mathrm{e}^{-t} - \mathrm{e}^{-5t})/1 + \mathrm{e}^{-6t}) = \sinh 2t/\cosh 3t$ instead of $\sum_m m\,\chi(m)\,\mathrm{e}^{-m^2 t/24}$. □

Remark. The same method applied to the full identity (23) gives the two-variable identity

$$\mathrm{e}^{-t/24} \sum_{n=0}^\infty (1-\mathrm{e}^{-u})(1-\mathrm{e}^{-t-u}) \cdots (1-\mathrm{e}^{-nt-u})\mathrm{e}^{-(n+1/2)u} = \sum_{n,r \geqslant 0} T_{n+r} \frac{t^n}{24^n n!} \frac{(-1)^r u^{2r+1}}{2^{2r}(2r+1)!}.$$

3. Asymptotic formula for ξ_D

In [6], Stoimenow used his recursive formulas (8)–(11) to compute a table up to $D = 30$ and to prove that $\xi_D/D!$ goes to 0 faster than any power of $1/D$, but observed that the numerical results in fact suggested a faster exponential decrease roughly like 1.5^{-D}. Using (1) we can compute the numbers ξ_D much more easily, e.g. the first k values can be computed by the one-line PARI program

```
s = 1 + o(x^k); p = s; q = s; for (n = 1,k,q = q − q*x; p = p − p*q; s = s+p); vec(s)
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which takes about 0.5 s on a SUN workstation for $k = 100$ and about 11 s for $k = 200$, the corresponding final values being

$$\xi_{100} = 6.0918680481\ldots \times 10^{137}, \qquad \xi_{200} = 1.7722937748\ldots \times 10^{333}.$$

To make Stoimenow's guess about the asymptotics of ξ_D precise, we make the Ansatz

$$\frac{\xi_D}{D!} \sim D^\alpha A^{-d}(C_0 + C_1 D^{-1} + C_2 D^{-2} + \cdots) \tag{26}$$

with some unknown constants $\alpha, A, C_0, C_1, \ldots$ and then try to fit these to the numerical data. The easiest way to do this is to note that (26) implies that $\xi_{D+1}/D\xi_D$ has an asymptotic expansion

$b_0 + b_1 D^{-1} + \cdots$ with some coefficients $b_0 = 1/A$, $b_1 = (\alpha + 1)/A, \ldots$. Given a function $D \mapsto f(D)$ for which such an asymptotic expansion is expected, one can determine the b_i's numerically by multiplying the function $f(D)$ by D^r for some moderately small value of r (say, $r = 10$) and taking the rth difference of the resulting function $D^r f(D) = b_0 D^r + b_1 D^{r-1} + \cdots + b_r + b_{r+1} D^{-1} + \cdots$. This difference equals $r! b_0 + O(D^{-r-1})$ and hence tends very rapidly to $r! b_0$ as D gets large, and once one has computed b_0 one can compute b_1 by applying the same process to $D(f(D) - b_0)$ and then continue the process iteratively. Applying this procedure in our case we found (to 20-digit accuracy) that the numbers α and A in (26) were given by $\frac{1}{2}$ and $\pi^2/6$, respectively, and that the first few coefficients C_i had the numerical values given in the introduction.

Theorem 4. *The numbers ξ_D defined by* (1) *have an asymptotic expansion of the form* (2) *with computable coefficients C_i and with C_0 as given in Eq.* (3). *In particular, the number of Vassiliev invariants of degree D is $O(D!\sqrt{D}/(\pi^2/6)^D)$.*

Proof. We know from Theorem 1 that $\xi_D = a_D$, with a_D defined by Eq. (24). We use that formula to express the a_n in terms of the b_n and the c_n. First, we have

$$b_n = \frac{1}{24^n} \sum_{k=0}^{n} \binom{n}{k} c_k.$$

Substituting into this the formula $c_n = T_n$ and the asymptotic formula

$$T_n = \frac{1}{2\sqrt{3}} \frac{(2n+1)!}{(\pi/6)^{2n+2}} (1 + O(5^{-2n})),$$

which follows immediately from (6), we find

$$b_n \sim 4\sqrt{3} \frac{(2n+1)!}{(2\pi^2/3)^{n+1}} \left(1 + \frac{\pi^2/72}{2n+1} + \frac{(\pi^2/72)^2/2!}{(2n+1)(2n-1)} + \cdots \right)$$

and hence by Stirling's formula

$$b_n \sim \frac{12\sqrt{3n}}{\pi^{5/2}} \frac{n!^2}{(\pi^2/6)^n} \left(1 + \frac{\beta_1}{n} + \frac{\beta_2}{n^2} + \cdots \right) \tag{27}$$

with computable coefficients $\beta_1 = \frac{\pi^2}{144} + \frac{3}{8}$, $\beta_2, \ldots$. Now we use the generating function

$$\frac{t^m}{m!} = \sum_{n=m}^{\infty} S_{n,m} \frac{(1 - e^{-t})^n}{n!},$$

where $S_{n,m}$ denotes the Stirling number of the first kind (defined as the number of elements of $\mathfrak{S}_n$ with exactly m cycles, or as the coefficient of x^m in $x(x+1) \cdots (x+n-1)$) to deduce from (24) the relation

$$a_n = \frac{1}{n!} \sum_{k=0}^{n-1} S_{n,n-k} b_{n-k} \tag{28}$$

between a_n and b_n. From $S_{n,n}=1$ and the recursion $S_{n+1,m}=S_{n,m-1}+nS_{n,m}$ we have

$$S_{n,n-k}=\frac{n^{2k}}{2^k k!}\left(1-\frac{c_1(k)}{n}+\frac{c_2(k)}{n^2}+\cdots\right)$$

with computable coefficients $c_1(k)=(2k^2+k)/3$, $c_2(k),\ldots$. Together with (27) and (28) this gives

$$a_n\sim\frac{b_n}{n!}\sum_{k\geqslant 0}\frac{(\pi^2/12)^k}{k!}\left(1+\frac{2k^2-11k}{6n}+\cdots\right)\sim\frac{n!\sqrt{n}}{(\pi^2/6)^n}\left(C_0+\frac{C_1}{n}+\cdots\right)$$

with C_0 given by (3), $C_1=C_0(\frac{3}{8}-\frac{17\pi^2}{144}+\frac{\pi^4}{432})$, and all C_i effectively computable. □

4. Enumeration of connected regular chord diagrams

In Section 4 of [6], Stoimenow also gave an algorithm, similar to but more complicated than (8)–(11), to compute the number λ_D^c of *connected* regular LCDs of degree D, which is an upper bound for the number of primitive Vassiliev invariants of this degree. Here again we can partly solve the recursions to give a fairly simple formula for the generating function

$$\Lambda(X)=\sum_{D=1}^{\infty}\lambda_D^c X^D=X+X^2+2X^3+5X^4+16X^5+63X^6+293X^7+1561X^8+\cdots.$$

To do this, we define a power series $\Phi_X(\varepsilon)=1+X-\varepsilon+2X^2-2X\varepsilon+\varepsilon^2+\cdots\in\mathbb{Z}[[X,\varepsilon]]$ by

$$\Phi_X(\varepsilon)=\sum_{n=0}^{\infty}\frac{(1-q)\cdots(1-q^n)}{(1+\varepsilon)(1+q\varepsilon)\cdots(1+q^n\varepsilon)}\quad(q=1-X).\tag{29}$$

Using the identity $\Phi_X(q\varepsilon)=(1+\varepsilon)\Phi_X(\varepsilon)-\varepsilon/(1+\varepsilon)$ we get the alternative expression

$$\Phi_X(\varepsilon)=\sum_{n=0}^{\infty}[1+(1-q^{n+1})+(1-q^{n+1})(1-q^{n+2})+\cdots](-\varepsilon)^n.\tag{30}$$

Theorem 5. *The generating function $\Lambda(X)$ equals $\Phi_X^{-1}(1)$.*

Proof. We give a sketch only, since the details are similar to, but more tedious than, those of the proof of Theorem 1. We use the notations and formulas of [6], Section 4, without restating them. The recursions for the numbers $\xi_{D,k,n}^2$ translate to the functional equation

$$(1-XY+XYZ)F(X,Y,Z)=Z+XYZF(X,1+Y-XY,Z)$$

for the generating function $F(X,Y,Z)=\sum\xi_{D,k,n}^2X^DY^kZ^n$. Iterating this, we obtain

$$F(X,Y,Z)=\frac{1}{1+\varepsilon}+\frac{1-a}{(1+\varepsilon)(1+q\varepsilon)}+\frac{(1-a)(1-qa)}{(1+\varepsilon)(1+q\varepsilon)(1+q^2\varepsilon)}+\cdots,$$

where q and a are defined by (13) and $\varepsilon=a(1-Z)/Z$. In particular,

$$F(X,1,Z)=\Phi_X\left(q\frac{1-Z}{Z}\right)=\frac{1}{Z}\Phi_X\left(\frac{1-Z}{Z}\right)-1+Z.$$

On the other hand, Eq. (2) of [6] is equivalent to the relation

$$P_\lambda(X,Y,Z) = 1 + \Lambda(X, Z\,P_\lambda(X,Y,Z))$$

between the two generating functions

$$P_\lambda(X,Y,Z) = 1 + \sum_{D,n,l\geqslant 0} \lambda_{D,n,l} X^D Y^l Z^n, \quad \Lambda(X,Z) = \sum_{D,n\geqslant 1} \lambda^{\mathrm{c}}_{D,n} X^D Z^n.$$

Finally, from $\sum_{k\geqslant 1} \xi^2_{D,k,n} = \xi^2_{D,n} = \sum_{l\geqslant 1} \lambda_{D,n,l}$ we get $P_\lambda(X,1,Z) = 1 - Z + F(X,1,Z)$. Combining these equations leads to the "closed" formula

$$\Lambda(X,Z) = Z\Phi_X^{-1}(Z) - 1 + Z.$$

The theorem is obtained by specializing to $Z = 1$. □

Theorem 5 lets us compute the λ^{c}_D very quickly. For instance, the evaluation of

$$\lambda^{\mathrm{c}}_{30} = 44390236643156201288 6101206$$

took just 1 s of CPU time on a Sun workstation as compared to the 30 h cited in [6]. Computing further to $D = 100$ (time: 3 min) and interpolating numerically in the way explained in the previous section, we find empirically that λ^{c}_D satisfies an asymptotic formula like (2) but with the coefficients C_j replaced by other coefficients C_j^*, with $C_0/C_0^* = 2.7182818285$ to 11 decimals, confirming Stoimenow's guess that $\lambda^{\mathrm{c}}_D \sim \xi_D/e$ as $D \to \infty$. In particular, considering λ^{c}_D rather than ξ_D can give at most a very modest improvement of the bound on $V(D)$ in Theorem 4.

5. Expansions of $F(q)$ near roots of unity

As already remarked, the series $F(q)$ in (15) makes sense not only for q equal or near to 1, but also for q equal or near to any root of unity $\xi = \mathrm{e}^{2\pi i\alpha}$, $\alpha \in \mathbb{Q}$. We can write its Taylor expansion near such a root of unity in three different sets of coordinates, setting

$$F(\xi(1-X)) = \sum_{n=0}^{\infty} a_n(\xi) X^n, \quad F(\xi \mathrm{e}^{-t}) = \sum_{n=0}^{\infty} \frac{b_n(\xi)}{n!} t^n, \quad \mathrm{e}^{-t/24} F(\xi \mathrm{e}^{-t}) = \sum_{n=0}^{\infty} \frac{c_n(\xi)}{24^n n!} t^n, \tag{31}$$

where $a_n(\xi)$, $b_n(\xi)$, and $c_n(\xi)$ belong to $\mathbb{Z}[\xi]$. The following result generalizes Theorem 3.

Theorem 6. *Let $\xi = \mathrm{e}^{2\pi i\alpha}$ be a root of unity. Then the coefficients $c_n(\xi)$ defined by* (31) *are given by the generating function*

$$\frac{1}{1-\mathrm{e}^{-Nt}} \sum_{m=1}^{N} \chi(m) \xi^{(m^2-1)/24} \mathrm{e}^{-mt} \sim 2 \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} c_n(\xi) t^{2n+1} \quad (t \to 0), \tag{32}$$

where N is any positive multiple of 12 *such that $\xi^{N/12} = 1$.*

Proof. The proof is similar to that of Theorem 3. Using Mellin transforms, we see that the function H defined by (20) has the asymptotic expansion

$$e^{-t/24}H(\xi e^{-t}) = \sum_{m=1}^{\infty} m\chi(m)\xi^{(m^2-1)/24}e^{-m^2t/24} \sim \sum_{n=0}^{\infty} \frac{L_\xi(-2n-1,\chi)}{n!}\left(-\frac{t}{24}\right)^n$$

around the point ξ, where $L_\xi(s,\chi)$ is the twisted L-series defined by

$$L_\xi(s,\chi) = \sum_{m=1}^{\infty} \chi(m)\xi^{(m^2-1)/24}m^{-s}$$

if $\Re(s) > 1$ and by analytic continuation otherwise. From Theorem 2 and (32) it follows that

$$c_n(\xi) = (-1)^{n-1}L_\xi(-2n-1,\chi)/2. \tag{33}$$

On the other hand, the same Mellin transform argument shows that $(-1)^n L_\xi(-n,\chi)$ for any $n \geqslant 0$ is the coefficient of $t^n/n!$ in the Taylor expansion of $\sum_{m=1}^{\infty}\chi(m)\xi^{(m^2-1)/24}e^{-mt}$ at $t=0$, and since the function $m \mapsto \chi(m)\,\xi^{(m^2-1)/24}$ is periodic of period N, this latter function is equal to the left-hand side of (32). (One must also check that this sum, which obviously has an expansion in $t^{-1}\mathbb{C}[[t]]$, is finite at $t=0$ and is an odd function of t, but this is easy.) Combining these statements gives the desired result. □

We can write (32) more explicitly in the form

$$c_n(\xi) = \frac{(-1)^n N^{2n+1}}{2n+2}\sum_{m=1}^{N/2} \chi(m)\xi^{(m^2-1)/24}B_{2n+2}\left(\frac{m}{N}\right),$$

where $B_n(x)$ denotes the nth Bernoulli polynomial. (Cf. (6), where $\xi = 1$, $N = 12$.) For the special case $n = 0$ this becomes

$$F(\xi) = \frac{1}{4N}\sum_{m=1}^{N} m^2\chi(m)\xi^{(m^2-1)/24}.$$

Here is a small table of $c_n(\xi)$ for the first four roots of unity $\xi = 1, -1, \omega = e^{2\pi i/3}$ and i:

n	$c_n(1)$	$c_n(-1)$	$c_n(\omega)$	$c_n(i)$
0	1	3	$5-\omega$	$8-3i$
1	23	261	$955-215\omega$	$2728-1125i$
2	1681	76083	$625925-141841\omega$	$3180983-1317369i$
3	257543	46620501	$862948795-195611975\omega$	$7796806408-3229519605i$

As in the special case $\xi = 1$, the coefficients $b_n(\xi)$ and $a_n(\xi)$ defined by (31) grow more slowly than the $c_n(\xi)$, e.g. the sequence $\{b_n(-1)\}_{n\geqslant 0}$ begins 3, 11, 133, 3389, … and the sequence $\{a_n(-1)\}_{n\geqslant 0}$ begins 3, 11, 72, 635, … . The asymptotics of these sequences could be determined, if so desired, by the method of Section 3.

6. Modular properties

As mentioned at the end of the introduction, Kontsevich originally introduced the function $F(q)$ defined by (15), noted that it makes sense whenever q is a root of unity, and performed numerical computations which led to the conjectural asymptotic formula

$$F(\mathrm{e}^{2\pi\mathrm{i}/k}) \sim \exp\left(-\frac{\pi\mathrm{i}}{12}\left(k-3+\frac{1}{k}\right)\right)k^{3/2} + \sum_{n\geqslant 0}\frac{b_n}{n!}\left(-\frac{2\pi\mathrm{i}}{k}\right)^n \quad (k\to\infty) \tag{34}$$

with the first few coefficients b_n given empirically by

$$b_0 = 1, \quad b_1 = 1, \quad b_2 = 3, \quad b_3 = 19, \quad b_4 = 207, \ldots \ . \tag{35}$$

Comparing (35) with the table given in Section 2 suggests that the coefficients b_n are indeed the same as the coefficients b_n defined there using the generating function expansion (24). The attempt to understand the reason for the asymptotic development (34) and to identify the coefficients (35) led to the results of the present paper. In this section we will establish the asymptotic expansion (34), with b_n as given in (24), and find the corresponding statement for the expansion of F near other roots of unity. We give only brief indications of the proofs, since this is part of a more general theory of "period functions for modular forms of half-integral weight" which will be developed in more detail in [7].

The first remark is that (34) becomes simpler if we multiply both sides by $\mathrm{e}^{\pi\mathrm{i}/12k}$, namely

$$\zeta_{24k}\,F(\zeta_k) \sim \zeta_{24}^{-k+3}\,k^{3/2} + \sum_{n\geqslant 0}\frac{c_n}{n!}\left(-\frac{\pi\mathrm{i}}{12k}\right)^n \quad (k\to\infty), \tag{36}$$

where ζ_m for any $m\in\mathbb{N}$ denotes $\mathrm{e}^{2\pi\mathrm{i}/m}$ and the c_n are related to the b_n as in (24). We can write this in a more enlightening way by defining a function $\varphi:\mathbb{Q}\to\mathbb{C}$ by

$$\varphi(\alpha) = \mathrm{e}^{\pi\mathrm{i}\alpha/12}\,F(\mathrm{e}^{2\pi\mathrm{i}\alpha}) \quad (\alpha\in\mathbb{Q}). \tag{37}$$

(The factor $\mathrm{e}^{\pi\mathrm{i}\alpha/12}$ is suggested by Theorem 2, since both the functions $H(q)$ and $(q)_\infty$ become more natural when multiplied by $q^{1/24}$.) Then φ obviously satisfies

$$\varphi(\alpha+1) = \zeta_{24}\,\varphi(\alpha) \quad (\alpha\in\mathbb{Q}), \tag{38}$$

so $\varphi(k) = \zeta_{24}^k\varphi(0) = \zeta_{24}^k$ and Eq. (36) and its complex conjugate can be rewritten as

$$\varphi(\pm 1/k) \sim \zeta_8^{\pm 3}k^{3/2}\varphi(\mp k) + \sum_{n\geqslant 0}\frac{c_n}{n!}\left(\mp\frac{\pi\mathrm{i}}{12k}\right)^n \quad (k\to\infty).$$

Together with (38), this formula suggests some kind of modular transformation behavior of the function φ under the generators $\alpha\to\alpha+1$, $\alpha\to -1/\alpha$ of $PSL(2,\mathbb{Z})$, and indeed this is the case.

Theorem. *The function $\varphi:\mathbb{Q}\to\mathbb{C}$ defined by* (37) *satisfies the modular transformation equations* (38) *and*

$$\varphi(\alpha) + (\mathrm{i}\alpha)^{-3/2}\varphi(-1/\alpha) = g(\alpha) \quad (\alpha\in\mathbb{Q},\ \alpha\neq 0), \tag{39}$$

where $(\mathrm{i}\alpha)^{-3/2}$ is the principal branch $(=\zeta_8^{\pm 3}|\alpha|^{-3/2}$ for $\pm\alpha>0)$ and $g:\mathbb{R}\to\mathbb{C}$ is a C^∞ function which is real-analytic everywhere except at $x=0$ and whose derivatives at $x=0$ are given by

$g^{(n)}(0) = (-\pi i/12)^n c_n$ ($n = 0, 1, \ldots$). *More generally,* φ *satisfies*

$$\varphi(\alpha) - v(\gamma)(c\alpha + d)^{-3/2}\varphi(\gamma(\alpha)) = g_\gamma(\alpha) \quad (\alpha \in \mathbb{Q},\ \gamma(\alpha) \neq \infty)$$

for all matrices $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SL(2,\mathbb{Z})$, *where* $v(\gamma)$ *is a* 24*th root of unity related to the multiplier of the Dedekind eta-function and* g_γ *is a* C^∞ *function on* $\mathbb{R}$ *which is real-analytic except at* $\gamma^{-1}(\infty)$.

We do not give the complete proof, since this theorem is a special case of results to be proved in more detail in [7], but only give an indication of the reason for the theorem and the definition of the function g. In the classical theory of periods of modular forms, we assign to a cusp form $f(z) = \sum_{n=1}^{\infty} a(n)e^{2\pi i n z}$ of integral weight $k \geqslant 2$ on $SL(2,\mathbb{Z})$ its *Eichler integral* $\tilde{f}(z) = \sum_{n=1}^{\infty} n^{1-k} a(n) e^{2\pi i n z}$. Then the modularity of f and the fact that $(d/dz)^{k-1}\tilde{f}$ is a multiple of f imply that $\tilde{f}$ is "nearly modular" of weight $2-k$: we have $\tilde{f}(z+1) = \tilde{f}(z)$ and $z^{k-2}\tilde{f}(-1/z) = \tilde{f}(z) + g(z)$ for a certain polynomial g of degree $\geqslant k-2$, the *period polynomial* of f, given explicitly by the formula $g(x) = c_k \int_0^\infty f(z)(z-x)^{k-2}\,dz$ where c_k is a constant depending only on k. More generally, for an arbitrary element $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ in the modular group we have $(cz+d)^{k-2}\tilde{f}(\gamma(z)) = \tilde{f}(z) + g_\gamma(z)$ where g_γ is a polymomial given by the same integral formula, but with the integral taken from $\gamma^{-1}(\infty) = -d/c$ to ∞.

In our case we replace f with the Dedekind eta-function

$$\eta(z) = e^{\pi z/12} \prod_{n=1}^{\infty} (1 - e^{2\pi i n z}) = \sum_{n=1}^{\infty} \chi(n)\, e^{\pi i n^2 z/12},$$

which is a modular form of weight $\frac{1}{2}$ on $SL(2, \mathbb{Z})$:

$$\eta(z+1) = \zeta_{24}\eta(z), \qquad \eta(-1/z) = (z/i)^{1/2}\eta(z), \qquad \eta(\gamma(z)) = v_\eta(\gamma)(cz+d)^{1/2}\eta(z),$$

where $v_\eta(\gamma)$ is a certain 24th root of unity, depending on γ and on the determination of the square root of $cz + d$, whose value was determined by Dedekind. If we formally define the Eichler integral $\tilde{\eta}(z)$ by the same formula as before, then it is (up to a constant) the power series $\sum n\chi(n)e^{\pi i n^2 z/12}$ with integer coefficients (because $k - 1 = \frac{1}{2}$ in this case and the exponents occurring in the Fourier expansion of η are proportional to perfect squares). The integral which we previously used to define the period polynomial g would be $g(x) = c\int_0^\infty (z-x)^{-3/2}\eta(z)\,dz$. This does not make sense for x in the upper half-plane, because of the two-valuedness and singularity at $z = x$ of the factor $(z-x)^{-3/2}$, and indeed there is no direct analogue for $\tilde{\eta}$ of the "nearly modular" property of $\tilde{f}$ valid in the upper half-plane. But the integral *does* make sense for x real, and it turns out that the limiting values of $\tilde{\eta}$ at rational points (and, indeed, its full asymptotic expansions at all rational points) do satisfy modular transformation properties analogous to those of the Eichler integral $\tilde{f}$ of a modular form f of integral weight. Together with Theorem 2, which shows that the limiting value of $\tilde{\eta}$ at any rational point α is $-2\varphi(\alpha)$, this gives the results stated in the theorem, with $g(x)$ given by the above integral formula and $g_\gamma(x)$ by the same integral but with the lower limit replaced by $\gamma^{-1}(\infty) = -d/c$.

As a final remark, we mention that formulas of the type discussed in this paper have a second connection with knot theory, quite separate from the generating function (1): it turns out that the

Witten–Reshitikhin–Turaev invariants of certain 3-manifolds lead to a formalism and to generating functions which are very similar to those occurring here, but this time related to the period functions of modular forms of weight $\frac{3}{2}$ (rather than $\frac{1}{2}$) and to the "mock theta functions" of Ramanujan. This connection is discussed in [3].

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