JOURNAL OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 26, Number 4, October 2013, Pages 1191–1207
S 0894-0347(2013)00765-1
Article electronically published on March 4, 2013

JUHL'S FORMULAE FOR GJMS OPERATORS AND Q-CURVATURES

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1. Introduction

GJMS operators and Q-curvatures are important objects in conformal geometry which have been studied intensely during the past decade. The GJMS operators are conformally invariant scalar differential operators whose principal part is a power of the Laplacian. They generalize the Yamabe operator $P_2 = \Delta - \frac{n-2}{4(n-1)}R$ (also called the conformal Laplacian). They arise naturally in a number of situations, for instance, in the sharp Moser-Trudinger inequality. The Q-curvatures are the zeroth order terms of the GJMS operators. Their importance was emphasized by Branson. They too arise in many circumstances, for instance, in the consideration of anomalies for functional determinants.

In [J2], [J3], building on previous work beginning with [J1], Juhl has derived remarkable formulae for GJMS operators and Q-curvatures, which reveal unexpected algebraic structure. In this paper we give direct proofs of Juhl's formulae starting from the original construction of [GJMS].

Juhl's formulae are expressed in terms of quantities arising in the expansion of a Poincaré metric, or equivalently an ambient metric, associated to a given pseudo-Riemannian metric. Let g be a pseudo-Riemannian metric of signature (p, q), $p + q = n \geq 3$, on an n-dimensional manifold M. A Poincaré metric in normal form relative to g is a metric g_+ on $M \times (0, \epsilon)$ of the form

$$g_+ = r^{-2}\left(dr^2 + h_r\right),$$

where h_r is a smooth 1-parameter family of metrics on M satisfying $h_0 = g$, for which $\mathrm{Ric}(g_+) + ng_+ = 0$ in the following asymptotic sense. If n is odd, then $\mathrm{Ric}(g_+) + ng_+ = O(r^\infty)$, while if n is even, then $\mathrm{Ric}(g_+) + ng_+ = O(r^{n-2})$ and the tangential trace of $r^{2-n}\left(\mathrm{Ric}(g_+) + ng_+\right)$ vanishes at $r = 0$. Set

$$V(r) = \sqrt{\frac{\det h_r}{\det h_0}}$$

and $W(r) = \sqrt{V(r)}$. Let δ denote the divergence operator on vector fields with respect to g, given by $\delta\varphi = \nabla_i\varphi^i$. Define a 1-parameter family $\mathcal{M}(r)$ of second order differential operators on M by

$$\mathcal{M}(r) = \delta(h_r^{-1}d) - U(r), \tag{1.1}$$

Received by the editors March 26, 2012 and, in revised form, December 5, 2012.
2010 *Mathematics Subject Classification.* Primary 53A30, 53A55.
This work was partially supported by NSF grants DMS 0901040 and DMS 0906035.

where

$$U(r) = \frac{\left[\partial_r^2 - (n-1)r^{-1}\partial_r + \delta(h_r^{-1}d)\right] W(r)}{W(r)}$$

acts as a zeroth order term. (We write $U(r)$ in the form given in v1 of [J3]. v2 of [J3] expresses it in a different form; see Lemma 8.1 of v2.) Use $\mathcal{M}(r)$ as a generating function for second order differential operators $\mathcal{M}_{2N}$ on M defined for $N \geq 1$ (and $N \leq n/2$ if n is even) by

$$\mathcal{M}(r) = \sum_{N\geq 1} \mathcal{M}_{2N} \frac{1}{(N-1)!^2} \left(\frac{r^2}{4}\right)^{N-1}. \tag{1.2}$$

The $\mathcal{M}_{2N}$ are natural scalar differential operators. Natural scalar invariants W_{2N} are defined by

$$W(r) = 1 + \sum_{N\geq 1} W_{2N} r^{2N} \tag{1.3}$$

for $N \geq 1$ (and $N \leq n/2$ if n is even).

Juhl's formulae involve constants n_I, m_I which are parametrized by ordered lists $I = (I_1, \ldots, I_r)$ of positive integers. I is referred to as a composition of the sum $|I| = I_1 + I_2 + \cdots + I_r$. Sometimes compositions are written in the form (I, a) singling out the last entry. In this case the convention is that I is allowed to be empty but $a > 0$. The constants appearing in Juhl's formulae are

$$\begin{aligned} n_I &= (|I|-1)!^2 \prod_{j=1}^{r} \frac{1}{(I_j-1)!^2} \prod_{j=1}^{r-1} \frac{1}{\left(\sum_{k=1}^{j} I_k\right)\left(\sum_{k=j+1}^{r} I_k\right)}, \\ m_I &= (-1)^{r+1}|I|!(|I|-1)! \prod_{j=1}^{r} \frac{1}{I_j!(I_j-1)!} \prod_{j=1}^{r-1} \frac{1}{I_j + I_{j+1}}. \end{aligned} \tag{1.4}$$

Empty products are always interpreted as 1. Observe when $r = 1$ that $n_{(N)} = m_{(N)} = 1$. Although it will not be important for us, we remark that all n_I and m_I are integers. For the n_I, this follows from the fact that each n_I can be rewritten as a product of binomial coefficients; see (2.2), (2.3) of [J3]. For the m_I, it follows from the fact that each m_I can be written as a polynomial in the n_J with integer coefficients. This is a consequence of the characterization of the m_I as the coefficients in polynomial relations which are inverse to lower-triangular polynomial relations with coefficients the n_J. (See the first paragraph of §4.)

Let P_{2N} denote the GJMS operators, with sign convention determined by $P_{2N} = \Delta^N + \ldots$ with $\Delta = \delta(g^{-1}d)$. These are defined for all $N \geq 1$ for n odd and for $1 \leq N \leq n/2$ for n even. Iterated compositions of the P_{2N} and the $\mathcal{M}_{2N}$ are denoted by $P_{2I} = P_{2I_1} \circ \cdots \circ P_{2I_r}$ and $\mathcal{M}_{2I} = \mathcal{M}_{2I_1} \circ \cdots \circ \mathcal{M}_{2I_r}$.

Juhl proves four formulae: an explicit formula and a recursive formula each for GJMS operators and for Q-curvatures. All four formulae are universal in the dimension.

Theorem 1.1 (Explicit formula for GJMS operators). *For $N \geq 1$ (and $N \leq n/2$ if n is even),*

$$P_{2N} = \sum_{|I|=N} n_I \mathcal{M}_{2I}. \tag{1.5}$$

Theorem 1.2 (Recursive formula for GJMS operators)**.** *For $N \geq 1$ (and $N \leq n/2$ if n is even),*

$$P_{2N} = -\sum_{\substack{|I|=N \\ I\neq(N)}} m_I P_{2I} + \mathcal{M}_{2N}. \tag{1.6}$$

Clearly the explicit formula expresses P_{2N} in terms of the second order building blocks $\mathcal{M}_{2M}$, $M \leq N$. The recursive formula expresses each P_{2N} as a sum of compositions of lower order GJMS operators, modulo the second order term $\mathcal{M}_{2N}$. For $N = 1$ both formulae state that $\mathcal{M}_2 = P_2$, the Yamabe operator. For $N = 2$ the formulae express the Paneitz operator as $P_4 = \mathcal{M}_2^2 + \mathcal{M}_4 = P_2^2 + \mathcal{M}_4$. The principal part of $\mathcal{M}_{2N}$ for $N > 1$ involves curvature, and $\mathcal{M}_{2N} = 0$ for $N > 1$ if g is flat. Further discussion and specializations of the formulae may be found in [J3].

The Q-curvatures are defined in terms of the zeroth order terms of the GJMS operators:

$$P_{2N}(1) = (-1)^N \Big(\frac{n}{2} - N\Big) Q_{2N}. \tag{1.7}$$

Q_{2N} is defined for all $N \geq 1$ if n is odd and for $1 \leq N \leq n/2$ if n is even. For n even, both sides vanish in the critical case $N = n/2$ and Q_n is defined by an analytic continuation.

Theorem 1.3 (Explicit formula for Q-curvatures)**.** *For $N \geq 1$ (and $N \leq n/2$ if n is even),*

$$(-1)^N Q_{2N} = \sum_{|(I,a)|=N} n_{(I,a)} a!(a-1)! 2^{2a} \mathcal{M}_{2I}(W_{2a}). \tag{1.8}$$

Theorem 1.4 (Recursive formula for Q-curvatures)**.** *For $N \geq 1$ (and $N \leq n/2$ if n is even),*

$$(-1)^N Q_{2N} = -\sum_{\substack{|(I,a)|=N \\ a<N}} m_{(I,a)} (-1)^a P_{2I}(Q_{2a}) + N!(N-1)! 2^{2N} W_{2N}. \tag{1.9}$$

The explicit formula expresses Q_{2N} in terms of the operators $\mathcal{M}_{2M}$ and the coefficients W_{2a}. The recursive formula expresses Q_{2N} in terms of GJMS operators applied to Q_{2a} with $a < N$, modulo the multiple of W_{2N}. Observe that the factor $n/2 - N$ in the definition which vanished in the critical case no longer appears. So the Q-curvature formulae do not follow immediately from the GJMS operator formulae just by taking constant terms.

If g is Einstein or locally conformally flat, then there is an invariantly defined Poincaré metric to infinite order also if n is even. It can be written explicitly; see [FG]. In these cases, P_{2N} and Q_{2N} are invariantly defined for all $N \geq 1$ also for n even. For such g, Juhl's formulae and our proofs are valid for all N.

The GJMS operators are known to be self-adjoint. This is exhibited by the formulae (1.5) and (1.6), since $\mathcal{M}(r)$ is evidently self-adjoint with respect to g for each r so that the $\mathcal{M}_{2N}$ are all self-adjoint and since $n_I = n_{I^{-1}}$ and $m_I = m_{I^{-1}}$ where $I^{-1} = (I_r, \ldots, I_1)$. However, the self-adjointness is not obvious from the original GJMS construction. If one desires to understand Juhl's formulae in terms of the original construction, it is reasonable to start by asking the modest question of how to see the self-adjointness from that derivation. It turns out that understanding this is the key to unlocking the mysteries of Juhl's formulae.

The operators P_{2N} were derived in [GJMS] via the Laplacian of the ambient metric associated to g. In normal form, this is the metric

$$\widetilde{g} = 2\rho dt^2 + 2tdtd\rho + t^2 g_\rho \tag{1.10}$$

on $\mathbb{R}_+ \times M \times (-\epsilon, \epsilon)$, where $t \in \mathbb{R}_+$, $\rho \in (-\epsilon, \epsilon)$, and $g_\rho = h_r$ with $\rho = -r^2/2$. The asymptotic vanishing of $\mathrm{Ric}(g_+) + ng_+$ at $r = 0$ translates into asymptotic vanishing of $\mathrm{Ric}(\widetilde{g})$ at $\rho = 0$. See [FG] for details. If $f \in C^\infty(M)$ and $\widetilde{f} \in C^\infty(M \times (-\epsilon, \epsilon))$ satisfies $\widetilde{f}(x, 0) = f$, then the GJMS definition is

$$P_{2N} f = \widetilde{\Delta}^N (t^{N-n/2} \widetilde{f})|_{\rho=0, t=1} \tag{1.11}$$

where $\widetilde{\Delta}$ denotes the Laplacian in the metric $\widetilde{g}$. The right-hand side is shown to be independent of the choice of $\widetilde{f}$ extending f.

It is straightforward to calculate the Laplacian $\widetilde{\Delta}$ of a metric of the form (1.10). Evidently there is a term involving the Laplacian Δ_{g_ρ} in the metric g_ρ for fixed ρ acting in the M factor (see (2.1) below). This term is not self-adjoint with respect to $g = g_0$, so P_{2N} obtained by iterating $\widetilde{\Delta}$ and restricting to $\rho = 0$ does not appear to be self-adjoint either. This is the reason that self-adjointness of the P_{2N} is not apparent from this construction. However, if we set

$$v(\rho) = \sqrt{\frac{\det g_\rho}{\det g_0}} \tag{1.12}$$

(so that $v(\rho) = V(r)$ with $\rho = -r^2/2$), then multiplying the volume form for g by $v(\rho)$ gives the volume form for g_ρ. It follows that for each ρ the operator $v(\rho)\Delta_{g_\rho}$ is self-adjoint with respect to g. Pre- and post-composing a self-adjoint operator with multiplication by a smooth real function gives another self-adjoint operator. Therefore the operator $v^{1/2} \circ \Delta_{g_\rho} \circ v^{-1/2}$ is also self-adjoint with respect to g. This motivates consideration of

$$\widetilde{\Delta}_v := v^{1/2} \circ \widetilde{\Delta} \circ v^{-1/2},$$

as we are guaranteed that the operator acting along M when $\widetilde{\Delta}_v$ is written out will be self-adjoint with respect to g. Moreover, $\widetilde{\Delta}_v^N = v^{1/2} \circ \widetilde{\Delta}^N \circ v^{-1/2}$ since the middle factors of $v^{\pm 1/2}$ cancel. The pre- and post-multiplications by $v^{\pm 1/2}$ affect neither the extension property nor the restriction back to $\rho = 0$ since $v = 1$ at $\rho = 0$. Hence (1.11) can be rewritten as

$$P_{2N} f = \widetilde{\Delta}_v^N (t^{N-n/2} \widetilde{f})|_{\rho=0, t=1}. \tag{1.13}$$

Now a direct calculation which we carry out in §2 shows that

$$\widetilde{\Delta}_v (t^\gamma \widetilde{f}) = t^{\gamma-2} \left[-2\rho \partial_\rho^2 + (2\gamma + n - 2)\partial_\rho + \widetilde{\mathcal{M}}(\rho) \right] \widetilde{f}, \tag{1.14}$$

where $\widetilde{\mathcal{M}}(\rho) = \mathcal{M}(r)$, $\rho = -r^2/2$. This is the key identity. It explains the previously mysterious appearance of both $W = \sqrt{V}$ and the generating function $\mathcal{M}(r)$ in Juhl's theory. Since $\left[-2\rho\partial_\rho^2 + (2\gamma + n - 2)\partial_\rho \right] \rho^k = c_{k,\gamma,n} \rho^{k-1}$ for constants $c_{k,\gamma,n}$, upon choosing $\widetilde{f}$ to be independent of ρ we see that iterating (1.14) and restricting to $\rho = 0$, $t = 1$ gives a formula for P_{2N} as a linear combination of compositions of the Taylor coefficients of $\widetilde{\mathcal{M}}(\rho)$, i.e. of the $\mathcal{M}_{2I}$. Showing that the coefficients in the linear combination are the n_I reduces to a (rather nontrivial) combinatorial identity which we derive in §3. This proves Theorem 1.1. Theorem 1.3 reduces to an equivalent combinatorial identity upon calculating $P_{2N} 1$ using (1.13), (1.14) and taking the extension $\widetilde{f}$ to be $v^{1/2}$ rather than 1. This reduction is included in §2 and the proof of the relevant combinatorial identity in §3.

Theorem 1.2 can be derived from Theorem 1.1 by inverting (1.5), viewed as a formal transformation law from the $\mathcal{M}_{2N}$ to the P_{2N}. A proof in the opposite direction due to Krattenthaler was presented in §2 of [J3] and immediately implies the direction we need here. Likewise, Theorem 1.4 follows from Theorem 1.3 upon inverting (1.8), viewed as a formal transformation from the W_{2N} to the Q_{2N}. In §4 we review Krattenthaler's proof of the inversion for the operators following the presentation in [J3] and then present the similar but more complicated proof for the Q-curvatures.

It is also possible to prove both the explicit and recursive formulae for Q-curvatures by taking the constant term in the corresponding formula for the GJMS operators and then rewriting by deriving and substituting expressions for the $\mathcal{M}_{2N}(1)$. This approach is closely related to arguments in [J3], where the scalar invariants $\mathcal{M}_{2N}(1)$ play a prominent role.

We still find these formulae to be quite astonishing. Juhl deserves great credit for their discovery as subtle consequences of the recursive structure of his residue families. Even though we now see that this theory of residue families and their factorization identities is not required for their proofs, this theory, linking ideas from conformal geometry, representation theory and spectral theory, appears deep and fascinating and deserves further exploration.

2. Explicit formulae

In this section we give the details of the argument outlined in the introduction which reduces Theorem 1.1 to a combinatorial identity and then we show how similar reasoning reduces Theorem 1.3 to an equivalent combinatorial identity.

The first task is to establish (1.14) by direct calculation. The inverse of the metric (1.10) is

$$\widetilde{g}^{IJ} = \begin{pmatrix} 0 & 0 & t^{-1} \\ 0 & t^{-2}g_\rho^{ij} & 0 \\ t^{-1} & 0 & -2\rho t^{-2} \end{pmatrix},$$

where the blocks correspond to $(t, x^i, \rho) \in \mathbb{R}_+ \times M \times (-\epsilon, \epsilon)$. Thus $\sqrt{|\det \widetilde{g}|} = t^{n+1}\sqrt{|\det g_\rho|}$. Using this in

$$\widetilde{\Delta} = \frac{1}{\sqrt{|\det \widetilde{g}|}} \partial_I \left(\widetilde{g}^{IJ} \sqrt{|\det \widetilde{g}|} \partial_J \right)$$

gives

$$\widetilde{\Delta}(t^\gamma \varphi) = t^{\gamma-2} \left[-2\rho\varphi'' + (2\gamma + n - 2 - 2\rho v'/v)\,\varphi' + (\Delta_{g_\rho} + \gamma v'/v)\varphi \right] \tag{2.1}$$

(cf. (3.5) of [GJMS]). Here v is given by (1.12), $'$ denotes ∂_ρ, and φ is independent of t. Set $w = v^{1/2}$ and $\varphi = w^{-1}\psi$. Then $v'/v = 2w'/w$ and

$$\begin{aligned} \varphi' &= w^{-1}\psi' - w^{-2}w'\psi, \\ \varphi'' &= w^{-1}\psi'' - 2w^{-2}w'\psi' + (2w^{-3}w'^2 - w^{-2}w'')\psi. \end{aligned}$$

Substituting and simplifying gives

$$\begin{aligned} w\big[-2\rho\varphi'' &+ (2\gamma + n - 2 - 2\rho v'/v)\varphi' + \gamma(v'/v)\varphi \big] \\ &= -2\rho\psi'' + (2\gamma + n - 2)\psi' + w^{-1}\big[2\rho w'' - (n-2)w'\big]\psi. \end{aligned} \tag{2.2}$$

For the remaining term in (2.1) we have

Lemma 2.1.

$$w \circ \Delta_{g_\rho} \circ w^{-1} = \delta(g_\rho^{-1} d) - w^{-1}\delta(g_\rho^{-1} dw). \tag{2.3}$$

(Recall that δ denotes the divergence operator with respect to $g = g_0$.) The second term on the right-hand side acts as a zeroth order operator.

Proof. For fixed ρ it is clear that $w \circ \Delta_{g_\rho} \circ w^{-1}$ and $\delta(g_\rho^{-1} d)$ are second order differential operators whose principal parts agree. We observed in the introduction that the first is self-adjoint with respect to g, and clearly this is the case for the second. So their difference is zeroth order. Evaluating on w identifies the zeroth order term. □

Multiplying (2.1) by w and then substituting (2.2) and (2.3) yields

$$w\widetilde{\Delta}(t^\gamma w^{-1}\psi) = t^{\gamma-2}\left[-2\rho\psi'' + (2\gamma+n-2)\psi' + \left(\delta(g_\rho^{-1}d) - \widetilde{U}(\rho)\right)\psi\right] \tag{2.4}$$

where

$$\widetilde{U}(\rho) = \frac{\left[-2\rho\partial_\rho^2 + (n-2)\partial_\rho + \delta(g_\rho^{-1}d)\right] w(\rho)}{w(\rho)}.$$

The chain rule with $\rho = -r^2/2$ shows that $\widetilde{U}(\rho) = U(r)$ so that $\delta(g_\rho^{-1}d) - \widetilde{U}(\rho) = \widetilde{\mathcal{M}}(\rho)$. Hence (2.4) becomes (1.14). This completes the derivation of (1.14).

Set

$$\mathcal{R}_k = -2\rho\partial_\rho^2 + 2k\partial_\rho + \widetilde{\mathcal{M}}(\rho)$$

and note that (1.2) becomes

$$\widetilde{\mathcal{M}}(\rho) = \sum_{N\ge 1} \mathcal{M}_{2N}\frac{1}{(N-1)!^2}\left(-\frac{\rho}{2}\right)^{N-1}.$$

Iterating (1.14) gives

$$\widetilde{\Delta}_v^N(t^{N-n/2}\widetilde{f}) = t^{-N-n/2}\mathcal{R}_{1-N}\mathcal{R}_{3-N}\cdots\mathcal{R}_{N-3}\mathcal{R}_{N-1}\widetilde{f},$$

so we deduce that $\mathcal{R}_{1-N}\mathcal{R}_{3-N}\cdots\mathcal{R}_{N-3}\mathcal{R}_{N-1}\widetilde{f}|_{\rho=0}$ depends only on $\widetilde{f}|_{\rho=0}$. Taking $\widetilde{f}$ to be independent of ρ, it follows upon expanding the right-hand side that $\mathcal{R}_{1-N}\mathcal{R}_{3-N}\cdots\mathcal{R}_{N-3}\mathcal{R}_{N-1}|_{\rho=0}$ is a linear combination of the compositions $\mathcal{M}_{2I}$. In the next section we will prove the combinatorial identity

$$\mathcal{R}_{1-N}\mathcal{R}_{3-N}\cdots\mathcal{R}_{N-3}\mathcal{R}_{N-1}|_{\rho=0} = \sum_{|I|=N} n_I\mathcal{M}_{2I}, \tag{2.5}$$

which identifies the constants in the linear combination. Theorem 1.1 then follows via (1.13).

We next show that Theorem 1.3, the explicit formula for Q-curvatures, reduces to a similar combinatorial identity, which we will see in the next section is equivalent to (2.5). By definition we have $(-1)^N(n/2-N)Q_{2N} = P_{2N}1$. Use (1.13) to calculate $P_{2N}1$, taking $\widetilde{f} = v^{1/2}$ to be the extension of $f=1$. Thus

$$(-1)^N(n/2-N)Q_{2N} = \widetilde{\Delta}_v^{N-1}\left(v^{1/2}\widetilde{\Delta}(t^{N-n/2})\right)|_{\rho=0,t=1}.$$

Equation (2.1) gives

$$\widetilde{\Delta}(t^{N-n/2}) = t^{N-n/2-2}(N-n/2)v'/v = 2t^{N-n/2-2}(N-n/2)w'/w.$$

The factors of $(N - n/2)$ cancel, and it follows that

$$(-1)^N Q_{2N} = -2\widetilde{\Delta}_v^{N-1}(t^{N-n/2-2}w')|_{\rho=0,t=1}. \tag{2.6}$$

Iterating (1.14) gives

$$(-1)^N Q_{2N} = -2\mathcal{R}_{1-N}\mathcal{R}_{3-N}\cdots\mathcal{R}_{N-3}(w')|_{\rho=0}. \tag{2.7}$$

Now $w = 1 + \sum_{a\geq 1} W_{2a}(-2\rho)^a$, so

$$w' = \sum_{a\geq 1} a(-2)^a W_{2a}\rho^{a-1}. \tag{2.8}$$

As will be shown in the next section, the following is equivalent to (2.5).

Proposition 2.2. *Let $1 \leq a \leq N$ and let f be a function on M (i.e. independent of ρ). Then*

$$\mathcal{R}_{1-N}\mathcal{R}_{3-N}\cdots\mathcal{R}_{N-3}(f\rho^{a-1})|_{\rho=0} = \sum_{|I|=N-a} n_{(I,a)}(a-1)!^2(-2)^{a-1}\mathcal{M}_{2I}(f). \tag{2.9}$$

Substituting (2.8) into (2.7) and then applying (2.9) termwise gives

$$(-1)^N Q_{2N} = \sum_{(I,a)=N} n_{(I,a)}a!(a-1)!2^{2a}\mathcal{M}_{2I}(W_{2a}),$$

which is the explicit formula for Q_{2N}.

For n even, the above argument applies also for the critical case $N = n/2$ since Q_n is defined by removing the factor of $n/2 - N$. The critical case may also be deduced without this argument of analytic continuation in the dimension by using the realization

$$(-1)^{n/2}Q_n = -\widetilde{\Delta}^{n/2}(\log t)|_{\rho=0,t=1}$$

derived in [FH]. First write

$$\widetilde{\Delta}^{n/2}(\log t)|_{\rho=0,t=1} = \widetilde{\Delta}_v^{n/2-1}\big(w\widetilde{\Delta}(\log t)\big)|_{\rho=0,t=1}.$$

Direct calculation gives $w\widetilde{\Delta}(\log t) = 2t^{-2}w'$. So we recover (2.6), and the argument proceeds as above.

3. Combinatorial identities

In this section we derive the combinatorial identities (2.5) and (2.9) to which Theorems 1.1 and 1.3 were reduced above. Begin with (2.5). First change variables by setting

$$s = -\frac{\rho}{2}, \qquad x_N = \frac{\mathcal{M}_{2N}}{(N-1)!^2}, \qquad X(s) = \widetilde{\mathcal{M}}(\rho) = \sum_{N=0}^{\infty} x_{N+1}s^N. \tag{3.1}$$

As far as this identity is concerned, $x_1, x_2, \ldots$ can simply be regarded as noncommuting variables, all of which commute with s. In the new variables, the $\mathcal{R}_k$ become the differential operators

$$\mathcal{L}_k = s\frac{d^2}{ds^2} - k\frac{d}{ds} + X(s),$$

where $X(s)$ acts as a zeroth order multiplication operator. We only have to verify the constant term in ∂_ρ of (2.5), which becomes

Theorem 3.1. *Let $N \geq 1$. Then*

$$\mathcal{L}_{1-N}\mathcal{L}_{3-N}\cdots\mathcal{L}_{N-3}\mathcal{L}_{N-1}1|_{s=0} = \sum_{|I|=N} \bar{n}_I\; x_{I_1}x_{I_2}\cdots x_{I_r}, \tag{3.2}$$

where

$$\bar{n}_I = \frac{(N-1)!^2}{\prod_{k=1}^{r-1}\Big(\sum_{j=1}^{k} I_j\Big)\Big(\sum_{j=k+1}^{r} I_j\Big)}.$$

Set $\bar{\mathcal{L}}_j = \mathcal{L}_{N+1-2j}$ so that $\mathcal{L}_{1-N}\mathcal{L}_{3-N}\cdots\mathcal{L}_{N-3}\mathcal{L}_{N-1} = \bar{\mathcal{L}}_N\bar{\mathcal{L}}_{N-1}\cdots\bar{\mathcal{L}}_2\bar{\mathcal{L}}_1$. Since $\bar{n}_I = \bar{n}_{I^{-1}}$, (3.2) can be rewritten as

$$\bar{\mathcal{L}}_N\bar{\mathcal{L}}_{N-1}\cdots\bar{\mathcal{L}}_2\bar{\mathcal{L}}_1 1|_{s=0} = \sum_{|I|=N} \bar{n}_I\; x_{I_r}x_{I_{r-1}}\cdots x_{I_1}. \tag{3.3}$$

Fix positive integers $I_1,\dots,I_r$, where $r \geq 1$. We will prove (3.3) by verifying the coefficient of $x_{I_r}x_{I_{r-1}}\cdots x_{I_1}$ in $\bar{\mathcal{L}}_N\bar{\mathcal{L}}_{N-1}\cdots\bar{\mathcal{L}}_2\bar{\mathcal{L}}_1 1|_{s=0}$ for each choice of $I_1,\dots,I_r$.

For $1 \leq l \leq r$, set

$$\mu_l = I_1 + I_2 + \cdots + I_l$$

so that $1 \leq \mu_1 < \mu_2 < \cdots < \mu_{r-1} < \mu_r$. Consider the calculation of $\bar{\mathcal{L}}_N\bar{\mathcal{L}}_{N-1}\cdots\bar{\mathcal{L}}_2\bar{\mathcal{L}}_1 1$ by successive multiplication from the left. For $1 \leq j \leq N$, $\bar{\mathcal{L}}_j\bar{\mathcal{L}}_{j-1}\cdots\bar{\mathcal{L}}_1 1$ is a formal power series in s whose coefficients are polynomials in the x's. The only monomials in the x's appearing in $\bar{\mathcal{L}}_j\bar{\mathcal{L}}_{j-1}\cdots\bar{\mathcal{L}}_1 1$ which can ultimately contribute to the coefficient of $x_{I_r}x_{I_{r-1}}\cdots x_{I_1}$ in $\bar{\mathcal{L}}_N\bar{\mathcal{L}}_{N-1}\cdots\bar{\mathcal{L}}_2\bar{\mathcal{L}}_1 1$ are of the form $x_{I_l}x_{I_{l-1}}\cdots x_{I_1}$ for some l, $1 \leq l \leq r$. The term $sd^2/ds^2 - (N+1-2k)d/ds$ in one of the factors $\bar{\mathcal{L}}_k$ reduces the power of s by 1 and multiplies by a constant. The term $X(s)$ is linear in the x's. So in order for a monomial $x_{I_l}x_{I_{l-1}}\cdots x_{I_1}$ to appear in the expansion of $\bar{\mathcal{L}}_j\bar{\mathcal{L}}_{j-1}\cdots\bar{\mathcal{L}}_1 1$, it must be that the zeroth order term $X(s)$ has contributed in exactly l of these $\bar{\mathcal{L}}_k$. Thus the differentiation in s terms have contributed in exactly $j-l$ of the $\bar{\mathcal{L}}_k$. It follows that the power of s multiplying $x_{I_l}x_{I_{l-1}}\cdots x_{I_1}$ is $s^{\mu_l - l-(j-l)} = s^{\mu_l - j}$. Hence we have

$$\bar{\mathcal{L}}_j\bar{\mathcal{L}}_{j-1}\cdots\bar{\mathcal{L}}_1 1 = \sum_{l=1}^{\min(j,r)} c_{j,l}\; x_{I_l}x_{I_{l-1}}\cdots x_{I_1} s^{\mu_l - j} + \dots \tag{3.4}$$

for some constants $c_{j,l}$, where $\dots$ indicates terms involving monomials in the x's which cannot contribute in the end. The $c_{j,l}$ are defined for $1 \leq j \leq N$, $1 \leq l \leq \min(j,r)$, and we have $c_{1,1} = 1$ and $c_{j,l} = 0$ if $\mu_l < j \leq N$.

From (3.4) it follows first that the coefficient of $x_{I_r}\cdots x_{I_1}$ in $\bar{\mathcal{L}}_N\bar{\mathcal{L}}_{N-1}\cdots\bar{\mathcal{L}}_2\bar{\mathcal{L}}_1 1|_{s=0}$ is zero unless $|I| = N$. In fact, taking $j = N$, the term $x_{I_r}\cdots x_{I_1}$ on the right-hand side is multiplied by $s^{\mu_r - N}$. This vanishes at $s = 0$ unless $\mu_r = N$, i.e. $|I| = N$. Theorem 3.1 therefore reduces to the statement that $c_{N,r} = \bar{n}_I$ if $|I| = N$. We assume henceforth that $|I| = N$, i.e. $\mu_r = N$.

Extend the definition of the $c_{j,l}$ to $0 \leq j \leq N$, $0 \leq l \leq r$ by defining $c_{0,0} = 1$ and $c_{j,l} = 0$ if $0 \leq j < l \leq r$ or if $l = 0$ and $1 \leq j \leq N$. We claim that these constants satisfy the recursion relation

$$c_{j+1,l} = -(\mu_l - j)(N - \mu_l - j)c_{j,l} + c_{j,l-1} \tag{3.5}$$

for $0 \le j \le N-1$, $1 \le l \le r$. For $1 \le j \le N-1$ and $1 \le l \le \min(j+1, r)$, this follows by applying $\bar{\mathcal{L}}_{j+1}$ to (3.4). For $j = 0$, $l = 1$, both sides are 1, and for all the other values both sides vanish. Now extend the definition of the $c_{j,l}$ to $j > N$, $0 \le l \le r$ by setting $c_{j,0} = 0$ for $j > N$ and by requiring that (3.5) hold for $j \ge N$, $1 \le l \le r$. The resulting $c_{j,l}$ are defined for $j \ge 0$, $0 \le l \le r$, and (3.5) holds for $j \ge 0$, $1 \le l \le r$.

Define generating functions

$$F_l(y) = \sum_{j=0}^{\infty} \frac{c_{j,l}}{(j!)^2} y^j, \qquad 0 \le l \le r.$$

The definitions of the $c_{j,0}$ and $c_{0,l}$ show that

$$F_0 = 1 \qquad \text{and} \qquad F_l(0) = 0, \quad 1 \le l \le r. \tag{3.6}$$

The recursion (3.5) turns into a differential equation relating F_l and F_{l-1}. For a fixed positive integer N as above, define ordinary differential operators

$$\mathcal{D}_\mu = y(1+y)\frac{d^2}{dy^2} + [1 - (N-1)y]\frac{d}{dy} + \mu(N-\mu).$$

Lemma 3.2. *Let*

$$u = \sum_{j=0}^{\infty} \frac{u_j}{(j!)^2} y^j, \qquad f = \sum_{j=0}^{\infty} \frac{f_j}{(j!)^2} y^j \tag{3.7}$$

be formal power series. Then $\mathcal{D}_\mu u = f$ if and only if

$$u_{j+1} = -(\mu - j)(N - \mu - j)u_j + f_j, \qquad j \ge 0. \tag{3.8}$$

The proof is to substitute the expansions into the equation and to compare coefficients of like powers of y. Comparing (3.5) and (3.8) then gives immediately that

$$\mathcal{D}_{\mu_l} F_l = F_{l-1}, \qquad 1 \le l \le r. \tag{3.9}$$

Now $\mathcal{D}_\mu$ has a regular singularity at $y = 0$ with indicial root 0 of multiplicity 2. By general Frobenius theory or just by staring at (3.8), there exists a unique formal power series solution of $\mathcal{D}_\mu u = 0$ with $u(0) = 1$. Also, for any formal power series f there exists a unique formal power series solution u to $\mathcal{D}_\mu u = f$ with $u(0) = 0$. In particular, (3.6) and (3.9) together characterize the functions F_l. Combining the solutions of the homogeneous and inhomogeneous problems shows that for any f there is a unique solution u to $\mathcal{D}_\mu u = f$ with $u(0)$ any prescribed value.

Since the y^N coefficient of $F_r(y)$ is $c_{N,r}/(N!)^2$, the above considerations show that the statement $c_{N,r} = \bar{n}_I$ to which Theorem 3.1 reduced is a consequence of the following.

Proposition 3.3. *Let $r \ge 1$ and $1 \le \mu_1 < \mu_2 < \cdots < \mu_r = N$, $\mu_l \in \mathbb{N}$. Define formal power series $F_l(y)$ for $0 \le l \le r$ by* (3.6) *and* (3.9)*. Then F_r is a polynomial of degree N and its y^N coefficient is*

$$\left[N^2 \prod_{l=1}^{r-1} \mu_l (N - \mu_l) \right]^{-1}.$$

Remarks. It follows easily from the discussion below (or from the definition of the $c_{j,l}$) that F_l is a polynomial with $\deg F_l \leq \mu_l$. For $l < r$ it often happens that $\deg F_l < \mu_l$. It is easily seen from the definition of the $c_{j,l}$ (or from (3.5)) that the lowest power of y occurring in F_l with nonzero coefficient is y^l, and its coefficient is 1.

We prove Proposition 3.3 by expressing the $F_l(y)$ in terms of special solutions of the differential equations. Let P_μ denote the formal power series defined by

$$\mathcal{D}_\mu P_\mu = 0, \qquad P_\mu(0) = 1.$$

Then $P_\mu = P_{N-\mu}$ since $\mathcal{D}_\mu = \mathcal{D}_{N-\mu}$. Clearly $P_0(y) = 1$. We claim that if μ is an integer satisfying $0 \leq \mu \leq N$, then P_μ is a polynomial with $\deg P_\mu = \min(\mu, N-\mu)$. This is clear from (3.8) with $f = 0$ since the multiplicative factor first vanishes when $j = \min(\mu, N-\mu)$. Up to a simple linear change of independent variable and overall multiplicative factor, the P_μ are particular instances of Jacobi polynomials.

Next observe that the same reasoning applies if f is a polynomial with $\deg f < \min(\mu, N-\mu)$: the unique solution u with $u(0)$ any prescribed value is a polynomial with $\deg u \leq \min(\mu, N-\mu)$. The multiplicative factor $(\mu-j)(N-\mu-j)$ also vanishes for $j = \max(\mu, N-\mu)$. Again the same reasoning shows that if f is a polynomial with $\deg f < \max(\mu, N-\mu)$, then u is a polynomial with $\deg u \leq \max(\mu, N-\mu)$. In particular, if $\mu \neq N/2$, the conditions

$$\mathcal{D}_\mu Q_\mu = P_\mu, \qquad Q_\mu(0) = 0$$

uniquely determine a polynomial Q_μ with $\deg Q_\mu \leq \max(\mu, N-\mu)$. Again $Q_\mu = Q_{N-\mu}$. In the special case $\mu = 0$, we have

Lemma 3.4. *The y^N coefficient of Q_0 is N^{-2}.*

Proof. We have $P_0 = 1$. So (3.8) with $j = 0$ and $u_0 = 0$ gives $u_1 = 1$. Setting $\mu = 0$ and iterating (3.8) for higher j gives

$$u_j = (j-1)!(N-j+1)(N-j+2)\cdots(N-1).$$

Hence $u_N = (N-1)!^2$. The result now follows from (3.7). □

Proof of Proposition 3.3. Begin by observing that the definition of the F_l and the conclusion both remain unchanged if any μ_l is replaced by $N - \mu_l$. We use this observation to redefine some of the μ_l. Namely, if $1 \leq l \leq r-1$ and μ_l satisfies the two conditions that $\mu_l > N/2$ and for no k is it the case that $\mu_k = N - \mu_l$, then we replace μ_l by $N - \mu_l$. The new sequence of μ_l need no longer be increasing, but that will be irrelevant; it suffices to prove the statement of the theorem with the F_l defined using these μ_l. It is still the case that all μ_l are distinct, and we now have the property that if for some l one has $\mu_l > N/2$, then necessarily there is $k < l$ for which $N - \mu_l = \mu_k$.

For convenience, let us set $\mu_0 = 0$ and enlarge the set of μ's to include μ_0. Then $\mu_0 = 0$ and $\mu_r = N$ are both in our enlarged set of μ's, and now the property stated above that if $\mu_l > N/2$, then there is $k < l$ for which $N - \mu_l = \mu_k$ holds also for $l = r$.

Define polynomials p_l, $0 \leq l \leq r$, as follows:

$$\begin{aligned} p_l &= P_{\mu_l} \qquad \text{if} \quad \mu_l \leq N/2, \\ p_l &= Q_{\mu_l} \qquad \text{if} \quad \mu_l > N/2. \end{aligned}$$

Clearly $\deg p_l \leq \mu_l$.

Claim. There are constants $a_{j,l}$ for $0 \le l \le r$, $0 \le j \le l$, satisfying

$$F_l = \sum_{j=0}^{l} a_{j,l} p_j, \qquad 0 \le l \le r, \tag{3.10}$$

$$a_{0,l} = \left[\prod_{j=1}^{l} \mu_j (N - \mu_j)\right]^{-1}, \qquad 0 \le l \le r-1, \tag{3.11}$$

$$a_{r,r} = \left[\prod_{l=1}^{r-1} \mu_l (N - \mu_l)\right]^{-1}. \tag{3.12}$$

In (3.11) and (3.12) an empty product is interpreted as 1.

Proposition 3.3 follows immediately from the Claim. In fact, $\deg p_j < N$ for $0 \le j \le r-1$ and $\deg p_r = \deg Q_0 = N$ by Lemma 3.4. Thus (3.10) for $l = r$, together with (3.12), shows that $\deg F_r = N$. Only $p_r = Q_0$ contributes to its y^N coefficient, which by Lemma 3.4 is $N^{-2} a_{r,r}$.

The Claim is proved by induction on l. It is clear for $l = 0$ since $F_0 = p_0 = 1$. Suppose that the Claim is established for $l-1$ and assume first that $l < r$. The argument is slightly different for the last induction step passing from $l = r-1$ to $l = r$.

Now F_l is defined by

$$\mathcal{D}_{\mu_l} F_l = F_{l-1} = \sum_{j=0}^{l-1} a_{j,l-1} p_j, \qquad F_l(0) = 0.$$

For each j, $0 \le j \le l-1$, we will solve $\mathcal{D}_{\mu_l} u_j = p_j$, $u_j(0) = 0$, with u_j a linear combination of the p_k, $0 \le k \le l$. Then $F_l = \sum_{j=0}^{l-1} a_{j,l-1} u_j$ is of the desired form.

The construction of the u_j's is based on the observation that

$$\mathcal{D}_{\mu_l} = \mathcal{D}_{\mu_j} + [\mu_l(N-\mu_l) - \mu_j(N-\mu_j)]. \tag{3.13}$$

Consider different cases for j. If $\mu_j \le N/2$ and $\mu_j(N-\mu_j) \ne \mu_l(N-\mu_l)$, then $p_j = P_{\mu_j}$ solves $\mathcal{D}_{\mu_j} p_j = 0$. Hence (3.13) gives

$$\mathcal{D}_{\mu_l}\left([\mu_l(N-\mu_l) - \mu_j(N-\mu_j)]^{-1} p_j\right) = p_j.$$

Correct the value at $y = 0$ by subtracting a multiple of the solution of the homogeneous equation. Set

$$u_j = [\mu_l(N-\mu_l) - \mu_j(N-\mu_j)]^{-1}(p_j - P_{\mu_l}).$$

Clearly u_j solves the equation and the initial condition. Now P_{μ_l} is of the form p_k for some k with $1 \le k \le l$: if $\mu_l \le N/2$, then $P_{\mu_l} = p_l$, while if $\mu_l > N/2$, then $P_{\mu_l} = p_k$, where $k < l$ is the index such that $N - \mu_l = \mu_k$. Thus we have constructed u_j of the desired form in this case. Note that if $j = 0$, then $\mu_j = 0$ and our solution is $u_0 = [\mu_l(N-\mu_l)]^{-1}(p_0 - P_{\mu_l})$. The coefficient of p_0 is $[\mu_l(N-\mu_l)]^{-1}$, and p_0 has coefficient zero when any of the u_j with $j > 0$ is expressed as a linear combination of the p's.

Next consider the construction of u_j in case $\mu_j \le N/2$ but $\mu_j(N-\mu_j) = \mu_l(N-\mu_l)$. This case might not occur at all, and if it does it can occur for only one j. Since $j < l$ we have $\mu_j \ne \mu_l$, so it must be that $\mu_l > N/2$ and $\mu_j = N - \mu_l$. Therefore $p_j = P_{\mu_j}$ and $p_l = Q_{\mu_l}$. Since $\mathcal{D}_{\mu_l} Q_{\mu_l} = P_{\mu_l} = P_{\mu_j}$ and $Q_{\mu_l}(0) = 0$, we just take $u_j = Q_{\mu_l} = p_l$. p_0 does not occur in the expression of this u_j as a linear combination of the p's.

The remaining possibility is $\mu_j > N/2$. Now we need to solve $\mathcal{D}_{\mu_l} u_j = p_j = Q_{\mu_j}$. Once again we apply (3.13) to conclude that

$$\begin{aligned}\mathcal{D}_{\mu_l} Q_{\mu_j} &= \mathcal{D}_{\mu_j} Q_{\mu_j} + [\mu_l(N-\mu_l) - \mu_j(N-\mu_j)]Q_{\mu_j} \\ &= P_{\mu_j} + [\mu_l(N-\mu_l) - \mu_j(N-\mu_j)]Q_{\mu_j}.\end{aligned}$$

Since $j < l$ it is impossible that $\mu_l = N - \mu_j$. Therefore $\mu_l(N-\mu_l) - \mu_j(N-\mu_j) \neq 0$. Arguing exactly as in the first case above we conclude that we can solve $\mathcal{D}_{\mu_l} v_j = P_{\mu_j}$, $v_j(0) = 0$, with v_j a linear combination of the p_k for $1 \le k \le l$. Then we take

$$\begin{aligned}u_j = &\ [\mu_l(N-\mu_l) - \mu_j(N-\mu_j)]^{-1}(Q_{\mu_j} - v_j) \\ = &\ [\mu_l(N-\mu_l) - \mu_j(N-\mu_j)]^{-1}(p_j - v_j).\end{aligned}$$

Once again, p_0 has coefficient zero when u_j is expressed as a linear combination of the p's.

This concludes the induction step for $l < r$: $F_l = \sum_{j=0}^{l-1} a_{j,l-1} u_j$ is of the desired form. Since p_0 entered only in the construction of u_0 and its coefficient in u_0 was $[\mu_l(N-\mu_l)]^{-1}$, we have

$$a_{0,l} = [\mu_l(N-\mu_l)]^{-1} a_{0,l-1}.$$

Thus (3.11) follows by induction as well.

Finally consider the last inductive step, passing from $r-1$ to r. Now $\mu_l = N$ so $N - \mu_l = \mu_0 = 0$. We again divide $\{j : 0 \le j \le r-1\}$ into the same three cases as above and solve for the u_j using the same methods. The difference now is that $j = 0$ occurs in the second case instead of the first, since $\mu_0(N-\mu_0) = \mu_r(N-\mu_r)$. So $u_0 = Q_0 = p_r$. In no other u_j does p_r occur with nonzero coefficient. From $F_r = \sum_{j=0}^{r-1} a_{j,r-1} u_j$ we therefore deduce $a_{r,r} = a_{0,r-1}$, which gives (3.12). □

This completes the proof of Theorem 3.1 and thus of (2.5). It remains to prove Proposition 2.2. It is evident upon expanding the $\mathcal{R}_k$'s that the left-hand side of (2.9) is a linear combination of $\mathcal{M}_{2I}(f)$. Again make the change of variables (3.1). Then (2.9) becomes

$$\begin{aligned}\mathcal{L}_{1-N}\mathcal{L}_{3-N}\cdots\mathcal{L}_{N-3}(s^{a-1})|_{s=0} &= \sum_{|I|=N-a} n_{(I,a)}(a-1)!^2(I_1-1)!^2\cdots(I_r-1)!^2\ x_I \\ &= \sum_{|I|=N-a} \bar{n}_{(I,a)}\ x_I.\end{aligned}$$

But this is equivalent to (3.2), which stated that

$$\mathcal{L}_{1-N}\mathcal{L}_{3-N}\cdots\mathcal{L}_{N-3}\mathcal{L}_{N-1}1|_{s=0} = \sum_{|J|=N} \bar{n}_J\, x_J = \sum_{|(I,a)|=N} \bar{n}_{(I,a)}\ x_I x_a,$$

as one sees upon evaluating $\mathcal{L}_{N-1}1 = X(s) = \sum_{a\ge 1} x_a s^{a-1}$.

4. Recursive formulae

In this section we present the proofs of Theorems 1.2 and 1.4. First consider Theorem 1.2. Since $n_{(N)} = 1$, (1.5) can be written as $P_{2N} = \mathcal{M}_{2N} + \sum_{|I|=N, I\neq(N)} n_I \mathcal{M}_{2I}$. The second term on the right-hand side only involves $\mathcal{M}_{2M}$ with $M < N$. Thus this is a polynomial lower-triangular system, and it follows that there are constants a_I determined inductively by inverting this relation so that $\mathcal{M}_{2N} = P_{2N} + \sum_{|I|=N, I\neq(N)} a_I P_{2I}$. Observe that (1.6) is another relation of this same form. §2 of [J3] presents a proof due to Krattenthaler that (1.5) and (1.6) are inverse relations in the other direction. Specifically, Krattenthaler showed that if $\overline{\mathcal{M}}_{2N}$ are defined by

$$\overline{\mathcal{M}}_{2N} = \sum_{|I|=N} m_I P_{2I}, \tag{4.1}$$

then

$$P_{2N} = \sum_{|I|=N} n_I \overline{\mathcal{M}}_{2I}. \tag{4.2}$$

Our desired identity (1.6) follows from the uniqueness of the inverse. Concretely, from (4.2) one deduces $\overline{\mathcal{M}}_{2N} = P_{2N} + \sum_{|I|=N, I\neq(N)} a_I P_{2I}$ by precisely the same inductive inversion as for the $\mathcal{M}_{2N}$. Hence $\overline{\mathcal{M}}_{2N} = \mathcal{M}_{2N}$, and (1.6) follows.

We review Krattenthaler's proof of (4.2) as presented in §2 of [J3] as a warm-up for the proof of Theorem 1.4. Substitution of (4.1) into (4.2) shows that (4.2) is equivalent to

$$P_{2N} = \sum_{|I|=N} \sum_{|J_1|=I_1,\dots,|J_r|=I_r} n_I m_{J_1}\cdots m_{J_r} P_{2J_1}\cdots P_{2J_r}. \tag{4.3}$$

The coefficient of P_{2N} on the right-hand side is 1, so one is reduced to showing that for $K = (K_1, \dots, K_s)$ with $s > 1$, the coefficient of P_{2K} in (4.3) vanishes. Given K, the choice of J's corresponds to a choice of subset $A = \{a_1, \dots, a_{r-1}\}$ of $[s-1] = \{1, \dots, s-1\}$ (including the empty set) of cardinality $r-1$, which we order by $1 \le a_1 < a_2 < \cdots < a_{r-1} \le s-1$. The parameterization is

$$\begin{aligned} J_1 = (K_1, \dots, K_{a_1}), \quad J_2 = (K_{a_1+1}, \dots, K_{a_2}), \ \dots, \\ J_{r-1} = (K_{a_{r-2}+1}, \dots, K_{a_{r-1}}), \quad J_r = (K_{a_{r-1}+1}, \dots, K_s). \end{aligned} \tag{4.4}$$

The J's determine I by $I = (|J_1|, \dots, |J_r|)$. The coefficient of $P_{2K_1}\cdots P_{2K_s}$ is then

$$\sum_{A\subset[s-1]} n_I m_{J_1}\cdots m_{J_r}, \tag{4.5}$$

so (4.2) reduces to showing that this vanishes for all $(K_1, \dots, K_s)$ with $s > 1$.

Sums such as (4.5) can be evaluated using the following ingenious lemma of Krattenthaler.

Lemma 4.1. *Let $s > 1$ and let $K_1, \dots, K_s \in \mathbb{N}$. Set $|K| = \sum_{j=1}^s K_j$. For $A = \{a_1, \dots, a_{r-1}\} \subset [s-1]$, define $J_1, \dots, J_r$ and I as above. Then*

$$\begin{aligned} \sum_{A\subset[s-1]} (-1)^r I_1\cdots I_{r-1}(I_r + X)\cdot \frac{\prod_{a\in A}(K_a + K_{a+1} + Y\chi(a = s-1))}{\prod_{i=1}^{r-1}(\sum_{k=1}^i I_k)(\sum_{k=i+1}^r I_k)} \\ = \frac{X(|K| - K_s) + Y(K_s + X)}{|K| - K_1}. \end{aligned} \tag{4.6}$$

Here $\chi(\mathcal{S}) = 1$ if $\mathcal{S}$ is true and $\chi(\mathcal{S}) = 0$ otherwise. X and Y are formal variables; the identity holds as polynomials in X and Y.

This is Lemma 2.1 in [J3]. The proof is by induction on s, decomposing the family of subsets $A \subset [s]$ according to their last element. The proof is not at all obvious, but the real ingenuity was to introduce the variables X and Y and to find the identity (4.6) amenable to a proof by induction. For the purposes of this paper it suffices to know (4.6) in the case $X = Y$. An examination shows that the proof by induction actually applies to this case directly; it is not necessary for our purposes to introduce both independent variables X and Y. We rewrite the identity for the case $X = Y$ in the form we will need in the proof of Theorem 1.4. Setting $X = Y = -b$ and then replacing K_s by $K_s + b$ in (4.6) gives

$$\sum_{A\subset[s-1]} (-1)^r I_1 \cdots I_r \frac{\prod_{a\in A}(K_a + K_{a+1})}{\prod_{i=1}^{r-1}(\sum_{k=1}^{i} I_k)(\sum_{k=i+1}^{r} I_k + b)} = -\frac{b|K|}{|K| - K_1 + b}. \tag{4.7}$$

This holds also for $s = 1$, since in that case both sides are $-K_1$. As usual, empty products are interpreted as 1. The form (4.7) seems natural: the induction hypothesis arises naturally in its proof by induction and the function $\chi(a = s-1)$ does not appear.

We use Lemma 4.1 to finish the proof of (4.2). Substitution of the definitions (1.4) of n_I and the m_{J_i} into (4.5) shows that

$$\sum_{A\subset[s-1]} n_I m_{J_1} \cdots m_{J_r} = (-1)^s(|K|-1)!^2 \prod_{j=1}^{s} \frac{1}{K_j!(K_j-1)!} \prod_{j=1}^{s-1} \frac{1}{K_j + K_{j+1}} \cdot \Sigma,$$

where Σ is the expression occurring on the left-hand side of (4.6) with $X = Y = 0$. Lemma 4.1 (or (4.7) with $b = 0$) shows that this vanishes. Thus (4.2) follows, and hence also Theorem 1.2.

We turn now to the proof of Theorem 1.4. Recall that the scalar invariants W_{2N} are defined by (1.3). It will be convenient to introduce

$$\overline{W}_{2N} = 2^{2N} N!(N-1)!\, W_{2N}, \qquad N \geq 1,$$

so that (1.8) takes the form

$$(-1)^N Q_{2N} = \sum_{|(I,b)|=N} n_{(I,b)} \mathcal{M}_{2I}(\overline{W}_{2b}) \tag{4.8}$$

and (1.9) becomes

$$\overline{W}_{2N} = \sum_{|(L,d)|=N} m_{(L,d)} (-1)^d P_{2L}(Q_{2d}).$$

Substitution of (4.8) for each $(-1)^d Q_{2d}$ shows that (1.9) is equivalent to

$$\overline{W}_{2N} = \sum_{|(L,d)|=N} \sum_{|(I,b)|=d} m_{(L,d)} n_{(I,b)} P_{2L} \mathcal{M}_{2I}(\overline{W}_{2b}).$$

The term on the right-hand side with $L = I = \emptyset$ is $\overline{W}_{2N}$, so it suffices to prove

$$\sum_{|(L,d)|=N} \sum_{|(I,b)|=d} m_{(L,d)} n_{(I,b)} P_{2L} \mathcal{M}_{2I} = 0$$

for each fixed b such that $1 \le b < N$. Substitution of (1.6) for each $\mathcal{M}_{2I_j}$ rewrites this as

(4.9)
$$\sum_{|(L,d)|=N} \sum_{|(I,b)|=d} \sum_{|J_1|=I_1,\dots,|J_r|=I_r} m_{(L,d)} n_{(I,b)} m_{J_1} \cdots m_{J_r} P_{2L} P_{2J_1} \cdots P_{2J_r} = 0.$$

Fix $K_1, \dots, K_s$ with $s \ge 1$ and each $K_j \ge 1$ and consider the coefficient of $P_{2K_1} \cdots P_{2K_s}$ in (4.9). We must have $L = (K_1, \dots, K_p)$ for some p, $0 \le p \le s$. Each J_i satisfies $|J_i| \ge 1$, although $r = 0$ is allowed corresponding to $p = s$. For $p < s$, the choice of J's corresponds to a choice of subset $A = \{a_1, \dots, a_{r-1}\}$ of $[s-p-1] = \{1, \dots, s-p-1\}$ (including the empty set) of cardinality $r-1$, which we order by $1 \le a_1 < a_2 < \cdots < a_{r-1} \le s-p-1$. Here

$$\begin{aligned} J_1 = (K_{p+1}, \dots, K_{p+a_1}), \quad J_2 = (K_{p+a_1+1}, \dots, K_{p+a_2}), \ \dots, \\ J_{r-1} = (K_{p+a_{r-2}+1}, \dots, K_{p+a_{r-1}}), \quad J_r = (K_{p+a_{r-1}+1}, \dots, K_s). \end{aligned} \tag{4.10}$$

For $p = s-1$, the only possibility for A is the empty set, in which case $J_1 = (K_s)$. The J's determine I by $I = (|J_1|, \dots, |J_r|)$ as above. The coefficient of $P_{2K_1} \cdots P_{2K_s}$ is then

$$m_{(K,b)} + \sum_{p=0}^{s-1} m_{(L,|K|-|L|+b)} \sum_{A \subset [s-p-1]} n_{(I,b)} m_{J_1} \cdots m_{J_r}. \tag{4.11}$$

So Theorem 1.4 reduces to showing that this vanishes for all $b \ge 1$ and all $(K_1, \dots, K_s)$ with $s \ge 1$.

We use Lemma 4.1 in the form (4.7) to evaluate the inner sum. Set $K'_j = K_{p+j}$ for $1 \le j \le s-p$. Substitution of (1.4) for $n_{(I,b)}$ and the m_{J_i} shows that

(4.12)
$$\begin{aligned} &\sum_{A \subset [s-p-1]} n_{(I,b)} m_{J_1} \cdots m_{J_r} \\ &\qquad = (-1)^{s-p} \frac{(|K'|+b-1)!^2}{|K'|\, b!\, (b-1)!} \prod_{j=1}^{s-p} \frac{1}{K'_j!(K'_j-1)!} \prod_{j=1}^{s-p-1} \frac{1}{K'_j + K'_{j+1}} \cdot \Sigma \end{aligned}$$

where

$$\Sigma = \sum_{A \subset [s-p-1]} (-1)^r I_1 \cdots I_r \frac{\prod_{a \in A} (K'_a + K'_{a+1})}{\prod_{i=1}^{r-1} (\sum_{k=1}^{i} I_k)(\sum_{k=i+1}^{r} I_k + b)}.$$

Replacement of s by $s-p$ and K_j by K'_j in (4.7) shows that

$$\Sigma = -\frac{b|K'|}{|K'| - K_{p+1} + b}. \tag{4.13}$$

Substitute (4.13) into (4.12) and multiply by $m_{(L,|K|-|L|+b)}$. One obtains

(4.14)
$$\begin{aligned} &m_{(L,|K|-|L|+b)} \sum_{A \subset [s-p-1]} n_{(I,b)} m_{J_1} \cdots m_{J_r} \\ &\qquad = (-1)^{s+1} \frac{(|K|+b)!(|K|+b-1)!}{(b-1)!^2} \prod_{j=1}^{s} \frac{1}{K_j!(K_j-1)!} \prod_{j=1}^{s-1} \frac{1}{K_j + K_{j+1}} \cdot R_p \end{aligned}$$

where

$$R_p = \frac{K_p + K_{p+1}}{(\sum_{i=p}^{s} K_i + b)(\sum_{i=p+1}^{s} K_i + b)(\sum_{i=p+2}^{s} K_i + b)}, \qquad 1 \leq p \leq s-1,$$

and

$$R_0 = \frac{1}{(\sum_{i=1}^{s} K_i + b)(\sum_{i=2}^{s} K_i + b)}.$$

Empty sums are interpreted as 0.

Set $b = K_{s+1}$ and substitute (4.14) into (4.11). After cancellation of factors in common with $m_{(K,b)}$, one finds that the vanishing of (4.11) is equivalent to

$$\sum_{p=1}^{s-1} \frac{K_p + K_{p+1}}{(\sum_{i=p}^{s+1} K_i)(\sum_{i=p+1}^{s+1} K_i)(\sum_{i=p+2}^{s+1} K_i)} = \frac{1}{K_{s+1}(K_s + K_{s+1})} - \frac{1}{(\sum_{i=1}^{s+1} K_i)(\sum_{i=2}^{s+1} K_i)}.$$

This is proved by induction on s. For $s = 1$ the sum on the left-hand side is empty and the right-hand side vanishes. Suppose the identity holds for s. Write

$$\begin{aligned}\sum_{p=1}^{s} \frac{K_p + K_{p+1}}{(\sum_{i=p}^{s+2} K_i)(\sum_{i=p+1}^{s+2} K_i)(\sum_{i=p+2}^{s+2} K_i)} =& \frac{K_1 + K_2}{(\sum_{i=1}^{s+2} K_i)(\sum_{i=2}^{s+2} K_i)(\sum_{i=3}^{s+2} K_i)} \\ &+ \sum_{p=2}^{s} \frac{K_p + K_{p+1}}{(\sum_{i=p}^{s+2} K_i)(\sum_{i=p+1}^{s+2} K_i)(\sum_{i=p+2}^{s+2} K_i)}\end{aligned}$$

and use the induction hypothesis on the second term on the right-hand side to obtain that the above equals

$$\begin{aligned}&\frac{K_1 + K_2}{(\sum_{i=1}^{s+2} K_i)(\sum_{i=2}^{s+2} K_i)(\sum_{i=3}^{s+2} K_i)} + \frac{1}{K_{s+2}(K_{s+1} + K_{s+2})} - \frac{1}{(\sum_{i=2}^{s+2} K_i)(\sum_{i=3}^{s+2} K_i)} \\ &= \frac{1}{K_{s+2}(K_{s+1} + K_{s+2})} + \frac{1}{(\sum_{i=2}^{s+2} K_i)(\sum_{i=3}^{s+2} K_i)} \left(\frac{K_1 + K_2}{\sum_{i=1}^{s+2} K_i} - 1 \right) \\ &= \frac{1}{K_{s+2}(K_{s+1} + K_{s+2})} - \frac{1}{(\sum_{i=1}^{s+2} K_i)(\sum_{i=2}^{s+2} K_i)}.\end{aligned}$$

This completes the proof of the vanishing of (4.11) and thus also of Theorem 1.4.

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