# THE COMBINATORICS OF TRACES OF HECKE OPERATORS

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#### In celebration of Dick Askey's 70th birthday.

ABSTRACT. We investigate the combinatorial properties of the traces of the *n*-th Hecke operators on the spaces of weight 2k cusp forms of level *N*. We establish examples in which these traces are expressed in terms of classical objects in enumerative combinatorics (e.g. tilings and Motzkin paths). We establish in general that Hecke traces are explicit rational linear combinations of values of Gegenbauer (a.k.a. ultraspherical) polynomials. These results arise from "packaging" the Hecke traces into power series in weight aspect. These generating functions are easily computed using the Eichler-Selberg trace formula.

#### 1. INTRODUCTION AND STATEMENT OF RESULTS

Throughout, let k be a positive integer, and let  $S_{2k}(\Gamma_0(N))$ (resp.  $S_{2k}^{\text{new}}(\Gamma_0(N))$ ) denote the space generated by the weight 2k cusp forms (resp. newforms) on the congruence subgroup  $\Gamma_0(N)$  (see [9], [10] for background on modular forms). For positive integers n and N which are coprime, define the integers  $\text{Tr}_{2k}(\Gamma_0(N), n)$  and  $\text{Tr}_{2k}^{\text{new}}(\Gamma_0(N), n)$  by

(1.1) 
$$\operatorname{Tr}_{2k}^{\operatorname{new}}(\Gamma_0(N), n) := \operatorname{trace} \text{ of the } n \text{-th Hecke op-erator on } S_{2k}^{\operatorname{new}}(\Gamma_0(N)),$$

(1.2) 
$$\operatorname{Tr}_{2k}(\Gamma_0(N), n) := \text{trace of the } n\text{-th Hecke operator on } S_{2k}(\Gamma_0(N)).$$

Recent works (for example, see [1], [5], [11], [12]) have proven congruences between such traces and combinatorial numbers such as the Apéry numbers

$$A(n) := \sum_{j=0}^{n} \binom{n+j}{j}^2 \binom{n}{j}^2.$$

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For example, Ahlgren and the second author [1] confirmed a conjecture of Beukers that

$$\operatorname{Tr}_4^{\operatorname{new}}(\Gamma_0(8), p) \equiv A\left(\frac{p-1}{2}\right) \pmod{p^2}$$

for every odd prime p. Many more such congruences for traces are obtained by the authors in [5].

In view of these congruences, it is natural to investigate the instrinsic combinatorial properties of these traces. In the *n*-aspect (i.e. where 2k and N are fixed), one does not expect to find a simple combinatorial description of these traces. However, in the weight aspect these traces are indeed combinatorial numbers. We begin by presenting four examples of this phenomenon.

There are many instances where these traces are combinatorial numbers analogous to the Apéry numbers. For example, we establish the following fact.

**Theorem 1.1.** If  $k \geq 2$ , then

$$\operatorname{Tr}_{2k}(\Gamma_0(7), 2) = -2 - \sum_{r=0}^{k-1} \binom{k+r-1}{2r} \cdot (-2)^{k-r-1}.$$

Theorem 1.1 provides a combinatorial formula for the trace of  $T_2$  on the space of cusp forms for the congruence subgroup  $\Gamma_0(7)$ . Such formulas are often closely connected to hypergeometric functions. First we recall the traditional notation for these functions. If n is a positive integer, then define  $(a)_n$  by

(1.3) 
$$(a)_n := a(a+1)(a+2)\cdots(a+n-1).$$

If n = 0, then let  $(a)_n := 1$ . Gauss'  $_2F_1$  hypergeometric functions are defined by

(1.4) 
$$_2F_1\left(\begin{array}{c}a, b\\c\end{array}\middle| x\right) := \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{(c)_n n!} \cdot x^n.$$

We establish the following formula involving  $_2F_1$  functions (which are Gegenbauer polynomials).

**Theorem 1.2.** If  $k \geq 3$ , then

$$\operatorname{Tr}_{2k}(\Gamma_0(17),3) = -2 + 3(-2)^{k-1} \cdot {}_2F_1\left( \begin{array}{c} (2-k)/2, & (3-k)/2 \\ 2-k \end{array} \middle| 9 \right) \\ + (-2)^k \cdot {}_2F_1\left( \begin{array}{c} (1-k)/2, & (2-k)/2 \\ 1-k \end{array} \middle| 9 \right).$$

In general we shall see that, apart from certain simple summands, Hecke traces are almost always sums of such  $_2F_1$  evaluations.

In view of the combinatorial formulas in Theorems 1.1 and 1.2, it is natural to wonder whether these traces are connected to classical topics in enumerative combinatorics. The next two examples confirm this speculation.

If n is a non-negative integer, then let

(1.5) 
$$T(n) := \#\{\text{tilings of a } 3 \times n \text{ rectangle using} \\ 1 \times 1 \text{ and } 2 \times 2 \text{ tiles}\}.$$

For example, here are the five tilings when n = 3.



FIGURE 1. Square tilings of  $3 \times 3$  rectangles

It turns out that  $\operatorname{Tr}_{12}(\Gamma_0(3), 2) = 6 \cdot T(3) = 30$ , an example of the following more general result.

**Theorem 1.3.** If  $k \geq 3$ , then

$$\operatorname{Tr}_{2k}(\Gamma_0(3), 2) = 6(-1)^k \cdot T(k-3).$$

As another example, we consider Motzkin paths. An *elevated Motzkin path* of length n is a lattice path which lies strictly above the *x*-axis, apart from its endpoints (0,0) and (n,0), with steps of the form (1,1), (1,-1) and (1,0). If  $n \geq 2$ , then let

(1.6)  $M_a(n) := \text{sum of areas bounded by length } n$ elevated Motzkin paths and the xaxis.

For example, here are the four elevated Motzkin paths of length 5:



FIGURE 2. Motzkin paths of length 5

Therefore,  $M_a(5) = 20$ . It turns out that  $\text{Tr}_{12}(\Gamma_0(4), 3) = 12 \cdot M_a(5) = 240$ . This formula also generalizes to other weights, as given in the following result.

**Theorem 1.4.** If  $k \geq 3$ , then

$$\operatorname{Tr}_{2k}(\Gamma_0(4),3) = 12(-1)^k \cdot M_a(k-1).$$

The four theorems above are special cases of a general theorem concerning the combinatorial properties of the traces of Hecke operators in weight aspect. To illustrate this general phenomenon, consider the cusp forms in  $S_{2k}(\Gamma_0(N^3))$  given by

(1.7) 
$$F_{2k}^{\text{new}}(N;z) := \sum_{\substack{n=1\\ \gcd(N,n)=1}}^{\infty} \operatorname{Tr}_{2k}^{\text{new}}(\Gamma_0(N),n)q^n$$

(note that  $q := e^{2\pi i z}$  throughout). By Atkin-Lehner theory, such a cusp form is essentially (and often exactly) the sum of the newforms in the space  $S_{2k}^{\text{new}}(\Gamma_0(N))$ .

To study the coefficients of these cusp forms, it is convenient to employ the Eichler-Selberg trace formula (for example, see [3], [4], [8], [13]). Although these formulas are quite formidable at first glance, we make some elementary observations which reveal some surprisingly simple properties leading to results such as the theorems above.

For the group  $\Gamma_0(8)$ , consider the forms  $F_{2k}^{\text{new}}(8;z)$ :

$$F_{4}^{\text{new}}(8;z) = q -4q^{3} -2q^{5} +24q^{7} + \cdots$$

$$F_{6}^{\text{new}}(8;z) = q +20q^{3} -74q^{5} -24q^{7} + \cdots$$

$$F_{8}^{\text{new}}(8;z) = 2q -40q^{3} +348q^{5} -1680q^{7} + \cdots$$

$$\vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots$$

For general N, we use these coefficients, grouped by column, to define the power series

(1.9) 
$$R^{\text{new}}(\Gamma_0(N), n; x) := \sum_{k=1}^{\infty} \operatorname{Tr}_{2k}^{\text{new}}(\Gamma_0(N), n) x^{k-1}.$$

Similarly, we consider the power series

(1.10) 
$$R(\Gamma_0(N), n; x) := \sum_{k=1}^{\infty} \operatorname{Tr}_{2k}(\Gamma_0(N), n) x^{k-1}.$$

For the forms in (1.8), calculations suggest that these series are rational functions. In particular, for levels 3, 5, and 7,

calculations suggest the following formulas:

$$\begin{split} R^{\text{new}}(\Gamma_0(8),3;x) &= -4x + 20x^2 - 40x^3 + 8x^4 + 20x^5 + \cdots \\ &= \frac{-4x}{27x^3 + 15x^2 + 5x + 1}, \\ R^{\text{new}}(\Gamma_0(8),5;x) &= -2x - 74x^2 + 348x^3 - \cdots \\ &= \frac{-50x^3 - 84x^2 - 2x}{3125x^5 + 625x^4 + 70x^3 + 14x^2 + 5x + 1} \\ R^{\text{new}}(\Gamma_0(8),7;x) &= 24x - 24x^2 - 1680x^3 + \cdots \\ &= \frac{168x^2 + 24x}{2401x^4 + 392x^3 + 78x^2 + 8x + 1}. \end{split}$$

These formulas prove to be correct, and indeed more is true. For generating functions of traces in general, we prove the following result.

**Theorem 1.5.** If N is a positive integer, and if  $n \ge 2$  is prime to N, then  $R^{\text{new}}(\Gamma_0(N), n; x)$  and  $R(\Gamma_0(N), n; x)$  are both rational functions in  $\mathbb{Q}(x)$ . Moreover, their poles are all simple and are algebraic numbers of degree  $\le 2$  over  $\mathbb{Q}$ .

In Section 3, we obtain Theorem 3.3, a result describing a basis of rational functions which are summands for  $R(\Gamma_0(N), n; x)$ . By the Atkin-Lehner theory of newforms, Theorem 1.5 follows as an immediate corollary. The most complicated rational functions appearing in Theorem 3.3 are of the form

$$\frac{nx+1}{n^2x^2 + (2n-s^2)x+1}.$$

Using the well known generating functions for the Gegenbauer (a.k.a. ultraspherical) polynomials  $C_n^{(\lambda)}(r)$ 

$$(1 - 2rx + x^2)^{-\lambda} = \sum_{n=0}^{\infty} C_n^{(\lambda)}(r) x^n$$

(for example, see (6.4.10) of [2]), and the fact that

$$C_n^{(\lambda)}(r) = \frac{(\lambda)_n}{n!} (2r)^n \cdot {}_2F_1 \left( \begin{array}{cc} -n/2, & (1-n)/2 \\ & 1-n-\lambda \end{array} \right| \frac{1}{r^2} \right)$$

(for example, see (6.4.12) of [2]), it is not difficult to deduce that

$$(1.11) \quad \frac{nx+1}{n^2x^2+(2n-s^2)x+1} = 1+nx + \sum_{m=1}^{\infty} (s^2-2n)^m {}_2F_1 \Big( \begin{array}{c} -m/2, \ (1-m)/2 \\ -m \end{array} \Big| \begin{array}{c} \frac{4n^2}{(2n-s^2)^2} \Big) x^m \\ + n \sum_{m=1}^{\infty} (s^2-2n)^m {}_2F_1 \Big( \begin{array}{c} -m/2, \ (1-m)/2 \\ -m \end{array} \Big| \begin{array}{c} \frac{4n^2}{(2n-s^2)^2} \Big) x^{m+1}. \end{array}$$

Consequently, it follows in general that Hecke traces are essentially simple sums of values of Gegenbauer polynomials as in Theorem 1.2.

Theorem 3.3, which is not difficult to prove, follows from an analysis of the intrinsic combinatorial structure of the Eichler-Selberg trace formula for Hecke operators. In Section 2, we recall a formulation of this result, and we make some key observations. In the last section, we derive Theorems 1.1 through 1.4.

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# 2. The Eichler-Selberg Trace formula

Our methods involve reformulating the Eichler-Selberg trace formula for  $\operatorname{Tr}_{2k}(\Gamma_0(N), n)$  (see [3], [4], [13]). We utilize the version of this trace formula due to Hijikata (see [7], [8]). Fix throughout positive integers k, N, and n. Let

(2.1)  $E = \{ s \in \mathbb{Z} \mid s^2 - 4n < 0 \},\$ 

(2.2) 
$$H = \{ s \in \mathbb{Z} \mid \exists t \in \mathbb{Z}^+, \ s^2 - 4n = t^2 \},\$$

(2.3) 
$$P = \{ s \in \mathbb{Z} \mid s^2 - 4n = 0 \}$$

Decompose E into the disjoint union  $E = E' \cup E''$ , where  $s \in E'$  (resp.  $s \in E''$ ) if the discriminant of  $\mathbb{Q}(\sqrt{s^2 - 4n})$  is 1 modulo 4 (resp. 0 modulo 4). For each  $s \in E \cup H \cup P$ , define the non-negative integer t = t(s) by

(2.4) 
$$s^2 - 4n = \begin{cases} mt^2 & \text{if } s \in E', \text{ and } m \text{ is a fund. disc.} \\ 4mt^2 & \text{if } s \in E'', \text{ and } 4m \text{ is a fund. disc.} \\ t^2 & \text{if } s \in H, \\ 0 & \text{if } s \in P. \end{cases}$$

Then define sets of integers

(2.5) 
$$F(s) := \begin{cases} \{f \in \mathbb{Z}^+ \mid f \text{ divides } t(s)\} & \text{if } s \in E \cup H, \\ \{1\} & \text{if } s \in P. \end{cases}$$

Furthermore, for  $s \in E \cup H \cup P$ , define y and  $\overline{y}$  to be the roots of  $X^2 - sX + n = 0$ , and accordingly let

(2.6) 
$$a(s,k,n) := \begin{cases} \frac{1}{2} \cdot \frac{y^{2k-1} - \bar{y}^{2k-1}}{y - \bar{y}} & \text{if } s \in E, \\ \frac{\min\{|y|, |\bar{y}|\}^{2k-1}}{|y - \bar{y}|} & \text{if } s \in H, \\ \frac{1}{4}|y|n^{k-1} & \text{if } s \in P. \end{cases}$$

Finally, let

(2.7) 
$$\delta(k,n) := \begin{cases} \prod_{p|n} \frac{1-p^{\operatorname{ord}_p(n)+1}}{1-p} & \text{if } k = 1, \\ 0 & \text{otherwise}; \end{cases}$$

and if n is a perfect square,

(2.8) 
$$\sigma(k, N, n) := \frac{1}{12} (2k - 1) n^{k-1} N \prod_{\ell \mid N} (1 + 1/\ell);$$

otherwise  $\sigma(k, N, n) := 0$ .

**Theorem 2.1** (Hijikata [7, Thm. 0.1]). If N and n are positive coprime integers, and  $k \ge 1$ , then

$$\operatorname{Tr}_{2k}(\Gamma_0(N), n) = \delta(k, n) + \sigma(k, N, n) - \sum_{s \in E \cup H \cup P} a(s, k, n) \sum_{f \in F(s)} b(s, f, n) c(s, f, N, n),$$

where b(s, f, n), c(s, f, N, n) are rational numbers depending only on s, f, N, and n, and are given explicitly (see [7, §0], [8, §2]).

Remark. The numbers b(s, f, n) in the statement of the theorem are given in terms of class numbers of orders of imaginary quadratic fields if  $s \in E$  and in terms of Euler's  $\phi$ -function if  $s \in H$ . The numbers c(s, f, N, n) are calculated by counting solutions to certain congruences. In both cases the numbers can be calculated explicitly, but for brevity we do not repeat their definitions here. The main observation is that their values are independent of the weight 2k.

# 3. Proof of Theorem 1.5

Throughout this section we fix coprime positive integers nand N, and we recall the definition of the generating function

$$R(\Gamma_0(N), n; x) = \sum_{k=1}^{\infty} \operatorname{Tr}_{2k}(\Gamma_0(N), n) x^{k-1}$$

from (1.10). In this section we explore the combinatorics of the variation of  $\operatorname{Tr}_{2k}(\Gamma_0(N), n)$  in k. By the Atkin-Lehner theory of newforms,  $R^{\operatorname{new}}(\Gamma_0(N), n; x)$  is an integral linear combination of  $R(\Gamma_0(M), n; x)$ , where  $M \mid N$ . Hence it suffices to examine  $R(\Gamma_0(N), n; x)$ . In particular, in Theorem 3.3, a more precise version of Theorem 1.5, we determine an explicit formula for  $R(\Gamma_0(N), n; x)$ .

Continuing with the notation of Section 2, we first make the following observation about the coefficients a(s, k, n) for  $s \in E$ .

**Proposition 3.1.** If  $s \in E$ , then

$$a(s,k,n) = \frac{1}{2} \sum_{j=0}^{k-1} (-1)^j \binom{2k-2-j}{j} n^j s^{2k-2j-2}.$$

*Proof.* From (2.6), when  $s \in E$ ,

(3.1) 
$$a(s,k,n) = \frac{1}{2} \cdot \frac{y^{2k-1} - \bar{y}^{2k-1}}{y - \bar{y}} = \frac{1}{2} \sum_{j=0}^{2k-2} y^j \bar{y}^{2k-2-j}.$$

This sum can be expressed in terms of powers of  $y\bar{y}$  and  $y+\bar{y}$ , using the relation

(3.2) 
$$y^m + \bar{y}^m = \sum_{j=0}^{\lfloor m/2 \rfloor} (-1)^j \frac{m}{m-j} \binom{m-j}{j} (y\bar{y})^j (y+\bar{y})^{m-2j}.$$

Then a straightforward induction, in conjunction with the relations  $y + \bar{y} = s$  and  $y\bar{y} = n$ , yields the desired expression.

We now determine the generating function for the power series with coefficients a(s, k, n), for  $s \in E$ .

**Lemma 3.2.** If  $s \in \mathbb{Z}$  and  $s^2 - 4n < 0$ , then

$$\sum_{k=1}^{\infty} a(s,k,n) x^{k-1} = \frac{1}{2} \cdot \frac{nx+1}{n^2 x^2 + (2n-s^2)x+1}.$$

Proof. The proof follows from Proposition 3.1 and from

(3.3) 
$$\sum_{j=1}^{\infty} (-1)^j \binom{2k+j}{j} x^j = \frac{1}{(1+x)^{2k+1}},$$

which is simply the binomial theorem. More specifically, we have

$$\sum_{k=1}^{\infty} a(s,k,n) x^{k-1} = \frac{1}{2} \sum_{k=1}^{\infty} \sum_{j=0}^{k-1} (-1)^j \binom{2k-2-j}{j} n^j s^{2k-2j-2} x^{k-1},$$
$$= \frac{1}{2} \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} (-1)^j \binom{2k+j}{j} n^j s^{2k} x^{k+j},$$
$$= \frac{1}{2} \sum_{k=0}^{\infty} \frac{s^{2k} x^k}{(nx+1)^{2k+1}},$$

where the first equality follows from Proposition 3.1, the second after reindexing the sums, and the third from (3.3).  $\Box$ 

Now let

(3.4) 
$$S(N,n) := \begin{cases} \frac{N}{12} \prod_{\ell \mid N} (1+1/\ell) & \text{if } n \text{ a perfect square,} \\ 0 & \text{otherwise;} \end{cases}$$

and

(3.5)  

$$\pi(N,n) := \begin{cases} \frac{\sqrt{n}}{2}c\left(2\sqrt{n},1,N,n\right) & \text{if } n \text{ a perfect square,} \\ 0 & \text{otherwise,} \end{cases}$$

where  $c(2\sqrt{n}, 1, N, n)$  is defined as in [7, §0].

**Theorem 3.3.** If N and n are coprime positive integers, then

$$R(\Gamma_0(N), n; x) = \delta(1, n) + S(N, n) \frac{nx + 1}{(nx - 1)^2} + \frac{\pi(N, n)}{nx - 1} + \sum_{\substack{d \mid n \\ d < \sqrt{n}}} \frac{2d^2}{n - d^2} \sum_{f \mid (\frac{n}{d} - d)} \frac{b\left(\frac{n}{d} + d, f, n\right)c\left(\frac{n}{d} + d, f, N, n\right)}{d^2x - 1} - \frac{1}{2} \sum_{\substack{s^2 - 4n < 0}} \sum_{f \mid t(s)} b(s, f, n)c(s, f, N, n) \frac{nx + 1}{n^2x^2 + (2n - s^2)x + 1}.$$

Proof. We proceed by using the trace formula from Theorem 2.1. The first and second terms in the proposed formula for  $R(\Gamma_0(N), n; x)$  follow easily from (2.7) and (2.8). The third term arises from the terms in the trace formula corresponding to  $s \in P$ . (We make use of the fact that b(s, 1, n) = 1 as in [7, §0].) The sum on divisors d of n with  $d < \sqrt{n}$  corresponds to the terms in the trace formula coming from  $s \in H$ . Finally, using Lemma 3.2, the last sum corresponds to the sum on  $s \in E$  in the trace formula.  $\Box$ 

*Remark.* By taking n = 1, Theorem 3.3 provides generating functions for dimensions of spaces of modular forms. For example,

$$\sum_{k=1}^{\infty} \dim S_{2k}(\Gamma_0(25)) x^{k-1} = \frac{x^3 + 4x^2 + 5x}{(x+1)(x-1)^2}$$
$$= 5x + 9x^2 + 15x^3 + \cdots$$

## 4. Combinatorial Theorems

Here we prove Theorems 1.1 through 1.4. These results follow from an analysis of the generating functions described in Theorem 3.3. Using this result, it is straightforward to verify the following proposition.

**Proposition 4.1.** With the notation as in (1.10), we have

$$R(\Gamma_0(3), 2; x) = \frac{2x}{x-1} + \frac{2x}{2x+1}$$
  
=  $-6x^2 + 6x^3 - 18x^4 + \cdots$ ,  
$$R(\Gamma_0(7), 2; x) = 3 + \frac{2}{x-1} - \frac{2x+1}{4x^2+3x+1}$$
  
=  $-x - x^2 - 9x^3 + \cdots$ ,  
$$R(\Gamma_0(4), 3; x) = 4 + \frac{3}{x-1} - \frac{1}{3x+1}$$
  
=  $-12x^2 + 24x^3 - \cdots$ ,  
$$R(\Gamma_0(17), 3; x) = 4 + \frac{2}{x-1} - \frac{6x+2}{9x^2+2x+1}$$
  
=  $-4x + 20x^2 - 28x^3 - \cdots$ .

Proof of Theorem 1.1. By Proposition 4.1, we have that

$$R(\Gamma_0(7), 2; x) = 3 + \frac{2}{x-1} - \frac{2x+1}{4x^2+3x+1}$$
$$= 1 - 2\sum_{n=1}^{\infty} x^n - \frac{2x+1}{4x^2+3x+1}.$$

To prove the theorem, it suffices to show that

$$a(n) = \sum_{j=0}^{n} \binom{n+j}{2j} (-2)^{n-j},$$

where the integers a(n) are defined by

$$\frac{2x+1}{4x^2+3x+1} = \sum_{n=0}^{\infty} a(n)x^n = 1 - x - x^2 + 7x^3 - \cdots$$

This is a straightforward calculation involving recurrence relations.  $\hfill \Box$ 

Proof of Theorem 1.2. By Proposition 4.1, we have

$$R(\Gamma_0(17), 3; x) = 4 + \frac{2}{x-1} - \frac{6x+2}{9x^2+2x+1}$$
$$= 2 - 2\sum_{n=1}^{\infty} x^n - \frac{6x+2}{9x^2+2x+1}$$

The theorem follows from (1.11).

Proof of Theorem 1.3. By Proposition 4.1, we have

$$R(\Gamma_0(3), 2; x) = \frac{2x}{x-1} + \frac{2x}{2x+1} = \frac{6x^2}{2x^2 - x - 1}.$$

By replacing x by -x, we obtain the known recurrence for 6T(n) (see Theorem 1 of [6]).

Proof of Theorem 1.4. By Proposition 4.1, we have

$$R(\Gamma_0(4), 3; x) = 4 + \frac{3}{x-1} - \frac{1}{3x+1} = \frac{12x^2}{3x^2 - 2x - 1}.$$

By replacing x by -x, we obtain the known recurrence for  $12M_a(n)$  (see Propositions 1 and 2 of [14]).

In view of the results presented here, it is natural to revisit the properties of the Hecke operators from a purely combinatorial perspective. For example, it is natural to ask the following question.

**Question.** Are there direct combinatorial proofs of Theorems 1.1 through 1.4 using the theory of modular symbols?

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