

# Compact trie nodes and pointers for random marked involutions

TAOCP exercise 7.2.2.4–205

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## Abstract

For the compact trie of TAOCP exercise 7.2.2.4–204 built from  $n$  i.i.d. random length- $q$  marked involutions, we prove, as  $q \rightarrow \infty$  with  $n \geq 1$  fixed,

$$\begin{aligned} P_{\text{nodes}}(n, q) &= nq + (n-1) - c_n^* \sqrt{q} - d_n^* + O(q^{-1/2}), \\ P_{\text{ptr}}(n, q) &= \frac{n}{6} q^2 - \frac{n}{3} q^{3/2} + A_n q + B_n \sqrt{q} + O(1), \end{aligned}$$

where  $c_j := \int_0^\infty e^{-(j/2)\xi^2 - 2j\xi} d\xi = \sqrt{\pi/(2j)} e^{2j} \operatorname{erfc}(\sqrt{2j})$ , the constants  $c_n^*, d_n^*, B_n$  are explicit (rational +  $\mathbb{Q}$ -linear in  $c_1, \dots, c_n$ ) combinations ( $c_n^*, d_n^*$  involve only  $c_2, \dots, c_n$ ;  $c_1$  enters  $B_n$  via the term  $n c_1$ ), and  $A_n = \frac{5n}{2} + H_n + 2c_n^*$ , a clean closed form mediated by the classical alternating-binomial identity  $\sum_{j=1}^n (-1)^{j+1} \binom{n}{j} / j = H_n$ . For general  $n$  we leave the  $O(1)$  residual of  $P_{\text{ptr}}(n, q)$  implicit (its rational +  $\mathbb{Q}$ -linear-in- $c_j$  structure is captured by Cor. 21); at  $n = 1$  we resolve it to the fifth term:  $P_{\text{ptr}}(1, q) = q^2/6 - q^{3/2}/3 + 7q/2 + (c_1 - 31/12)\sqrt{q} + (17/12 + c_1) + O(q^{-1/2})$ . All closed forms are verified against exact-rational enumeration up through  $(n, q) = (4, 5)$  for  $P_{\text{nodes}}$  and  $(n, q) = (4, 4)$  for  $P_{\text{ptr}}$ , and against log-space float64 evaluation through  $q = 10^4$ . The only non-elementary analytic input is the saddle-point asymptotic of  $T_N$  (the marked-involution count, OEIS A005425), in the form of Knuth’s exercise 7.2.2.4–177.

## 1 Introduction

In the typescript of Pre-Fascicle 8A (8 May 2026 revision), §7.2.2.4 “Hamiltonian paths and cycles: dynamic enumeration”, Knuth introduces *Algorithm E* (DYNHAM), a frontier-based dynamic-programming algorithm that, given a graph  $G$  on  $\{1, \dots, n\}$ , computes the cycle counts  $\text{CYC}[m]$  of every induced subgraph  $G_m = G|\{1, \dots, m\}$  for  $3 \leq m \leq n$ . As Algorithm E advances from level  $m-1$  to level  $m$ , its state is an  $m$ -class — an equivalence class of edge sets satisfying three combinatorial constraints — encoded, by the convention of exercise 178, as a string  $a_1 \dots a_q$  of length  $q = |E_m|$  over the alphabet  $\{\bar{1}, 0, 1, 2, \dots, \lfloor q/2 \rfloor\}$ . Such a string is precisely a marked involution of order  $q$  in the sense of that exercise. The set of  $m$ -classes that arise during the algorithm is stored in a trie keyed by these strings; exercise 204 designs a *compact* version of this trie, in which each node stores only those pointer fields that correspond to feasible extensions consistent with the prefix’s open-pair structure and the remaining length. The construction allocates, at a node of length  $l$  holding TMS (“two-marked-stack”) open pairs — i.e.  $k_p$  in the notation of §3; `tms` is the matching CWEB variable name in DYNHAM —

$$d(l, \text{TMS}) = \begin{cases} \text{TMS} & \text{if } l + \text{TMS} = q, \\ \text{TMS} + 2 & \text{if } l + \text{TMS} = q - 1, \\ \text{TMS} + 3 & \text{otherwise,} \end{cases} \quad (1)$$

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field positions, each holding a pointer to a child or to null (see Knuth’s answer to exercise 204).<sup>1</sup> Throughout the remainder of the paper we write  $k_p$  for the open-pair count (denoted TMS in (1) and `tms` in the CWEB), and abbreviate  $d_p := d(l_p, k_p)$  with  $l_p = |p|$ . The total *pointer count* of the trie is the sum of  $d_p$  over all distinct prefix nodes.

Exercise 205, rated [HM46], asks:

*Analyze the average total number of pointers, when the method of exercise 204 builds a compact trie from  $n$  random keys  $a_1 \dots a_q$  (that is, from  $n$  independently generated marked involutions as in exercise 176, with repetitions allowed).*

The printed answer is a single sentence:

*The simpler problem for  $n$  fixed at 1 should presumably be solved first, with its asymptotics when  $q \rightarrow \infty$ . The average number of trie nodes (distinct prefixes of  $n$  random keys) is also of interest.*

The printed answer references two distinct quantities: the “average total number of pointers”  $P_{\text{ptr}}(n, q)$ , and the “average number of trie nodes”  $P_{\text{nodes}}(n, q)$ . With  $d_p$  defined by (1),

$$P_{\text{ptr}}(n, q) = \mathbf{E} \left[ \sum_{p \in \text{Trie}} d_p \right], \quad P_{\text{nodes}}(n, q) = \mathbf{E} \left[ \sum_{\substack{p \in \text{Trie} \\ |p| \geq 1}} 1 \right],$$

where the expectation is over  $n$  i.i.d. uniform marked involutions of order  $q$ , and Trie is the set of nodes of the compact trie of those keys. We do not count the root in  $P_{\text{nodes}}$ , matching the  $\sum_{l=1}^q$  convention used throughout.

This paper gives closed-form asymptotic expansions of both quantities for every fixed  $n \geq 1$ : a four-term expansion of  $P_{\text{nodes}}(n, q) = nq + (n - 1) - c_n^* \sqrt{q} - d_n^* + O(q^{-1/2})$  (Theorem 13, with  $c_n^*, d_n^*$  explicit inclusion–exclusion combinations of the boundary-layer integrals  $c_j := \int_0^\infty e^{-(j/2)\xi^2 - 2j\xi} d\xi$ ) and a four-term expansion of  $P_{\text{ptr}}(n, q)$  through order  $\sqrt{q}$  (Theorem 19). The trivial-looking case  $n = 1$  already contributes  $P_{\text{nodes}}(1, q) = q$  (one key forms a single path with  $q$  distinct prefixes) but  $P_{\text{ptr}}(1, q) \sim q^2/6$  — on average, each prefix node carries  $\Theta(\sqrt{q})$  field positions, so the total pointer count grows quadratically in  $q$  even for one key. The interesting structure for  $P_{\text{nodes}}$  appears at  $n \geq 2$ , where prefix sharing between keys reduces the count below  $nq$  by a  $-c_n^* \sqrt{q}$  amount.

The generating-function pair attached to marked involutions [1, exercise 7.2.2.4–177] is

$$\sum_{q \geq 0} T_q \frac{z^q}{q!} = \exp \left( 2z + \frac{z^2}{2} \right), \quad (2)$$

where  $T_q := |\{\text{length-}q \text{ marked involutions}\}|$  equals  $a(q)$  of OEIS A005425 and satisfies the recurrence  $T_{N+2} = 2T_{N+1} + (N + 1)T_N$  with initial values  $T_0 = 1, T_1 = 2$ :

<sup>1</sup>Equation (1) encodes exactly what the CWEB section `<Allocate a new node for level 1+1>` in DYNAMHAM [2] computes. The CWEB variable `1` holds the *parent* level, so the new node being analysed sits at level  $l = 1 + 1$  in the paper’s notation; with `TMS = tms` its open-pair count, the three branches of the code map one-to-one onto the three cases of (1):

- `else` branch ( $1 + 1 + \text{tms} \geq q$ , i.e.  $l + \text{TMS} = q$ ): `slots = tms`, total TMS fields (case 1).
- `if`-branch with `1+2+tms==q` (i.e.  $l + \text{TMS} = q - 1$ ): two extra fields plus `slots = tms`, total TMS + 2 fields (case 2).
- `if`-branch with `1+2+tms<q` (i.e.  $l + \text{TMS} \leq q - 2$ ): two extra fields plus `slots = tms + 1`, total TMS + 3 fields (case 3, “otherwise”).

The two extra fields hold the codes `0` and `1`, present whenever there is room beneath the node; the `slots` positive entries `1, \dots, TMS` are augmented by one extra slot in case 3 to accommodate opening a new pair.

$N$	0	1	2	3	4	5	6	7	8	9
$T_N$	1	2	5	14	43	142	499	1850	7193	29186

(verified against OEIS A005425's b-file). The factor  $2z$  is the two-flavour 1-cycle (marked or unmarked), the  $z^2/2$  is the 2-cycle. Compare with the standard (unmarked) involution count  $I_N$  (OEIS A000085; 1, 1, 2, 4, 10, 26, ...), which has EGF  $\exp(z + z^2/2)$  and recurrence  $I_{N+2} = I_{N+1} + (N+1)I_N$ ; the marked variant differs only in the linear factor  $2z$  vs.  $z$  of the EGF, but this changes the Wright asymptotic constant and the boundary-layer profile  $\exp(-\xi^2/2 - 2\xi)$  specific to exercise 205.

Throughout the paper,  $n$  denotes the (fixed) number of random keys of exercise 205, while the running index of the  $T$ -sequence and of Wright's asymptotic is written  $N$  to avoid collision.

*Background reading.* The classical analysis of trie height and pointer count under the uniform i.i.d. model is in Knuth's TAOCP Vol. 3 [5] and Szpankowski [7]; the analytic-combinatorics framework, including Mellin-transform techniques for digital-tree asymptotics, is developed in Flajolet–Régner–Sedgewick [6]; the involution-counting recurrence and EGF (with weight 1 per fixed point) appears in Riordan [8].

## 2 Main results and structure of the paper

*Main results.* For every fixed integer  $n \geq 1$ , as  $q \rightarrow \infty$ ,

$$\begin{aligned} P_{\text{nodes}}(n, q) &= nq + (n-1) - c_n^* \sqrt{q} - d_n^* + O(q^{-1/2}), \\ P_{\text{ptr}}(n, q) &= \frac{n}{6} q^2 - \frac{n}{3} q^{3/2} + A_n q + B_n \sqrt{q} + O(1), \end{aligned}$$

with closed-form coefficients

$$\begin{aligned} c_n^* &= \sum_{j=2}^n (-1)^j \binom{n}{j} c_j, & c_j &:= \int_0^\infty e^{-(j/2)\xi^2 - 2j\xi} d\xi, \\ A_n &= \frac{5n}{2} + H_n + 2c_n^* \quad (\text{Theorem 20}), & B_n &= n(c_1 - \frac{31}{12}) - 3c_n^* + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} d_j^{(k)}. \end{aligned}$$

*Glossary.*  $c_n^* = \sum_{j=2}^n (-1)^j \binom{n}{j} c_j$  (boundary-layer integral combination, appearing in both  $P_{\text{nodes}}$  and  $A_n, B_n$ );  $d_n^* = \sum_{j=2}^n (-1)^j \binom{n}{j} \text{const}_j$  (parallel combination of sub-leading constants);  $c_j^{(k)}, d_j^{(k)}$  are the leading and sub-leading coefficients of  $S_j^{(k)}(q)$  respectively (Lemma 18). All four families are  $\mathbb{Q}$ -linear in  $\{c_j\}$  with rational shifts. The recurrence of  $c_n^*$  across  $P_{\text{nodes}}$ 's  $\sqrt{q}$ -term and  $P_{\text{ptr}}$ 's  $q$ - and  $\sqrt{q}$ -terms — combined with the classical identity  $\sum_{j=1}^n (-1)^{j+1} \binom{n}{j} / j = H_n$  — is what produces the clean  $A_n = 5n/2 + H_n + 2c_n^*$  of Theorem 20. The  $n = 1$  specialisation is  $P_{\text{nodes}}(1, q) = q$  and  $P_{\text{ptr}}(1, q) = \frac{q^2}{6} - \frac{q^{3/2}}{3} + \frac{7q}{2} + (c_1 - \frac{31}{12})\sqrt{q} + (\frac{17}{12} + c_1) + O(q^{-1/2})$ .

*Three building blocks.* Both expansions reduce to asymptotics of three families of sums over a marked involution of size  $q$ :

- the *prefix moments*  $S_j(q) = 1 + \sum_{l \geq 1, k} f(l, k) [h(q-l, k)/T_q]^j$  (the “+1” is the root  $l = 0$  contribution), contributing to  $P_{\text{nodes}}$  at order  $\sqrt{q}$  (Lemma 12:  $S_j = c_j \sqrt{q} + \text{const}_j + O(q^{-1/2})$ );
- the *k-weighted prefix moments*  $S_j^{(k)}(q) = \sum_{l, k} k f(l, k) [h(q-l, k)/T_q]^j$ , contributing to  $P_{\text{ptr}}$  at orders  $q^2, q^{3/2}, q, \sqrt{q}$  (Lemma 14 for  $j = 1$ , Lemma 18 for  $j \geq 2$ );
- the *boundary moments*  $B_j^{(b)}(q)$  collected on the line  $q - l - k = b$ , contributing to  $P_{\text{ptr}}$  at  $\sqrt{q}$  (Lemma 15 for  $j = 1$ , Lemma 17 for  $j \geq 2$  — for fixed  $j \geq 2$  these decay like  $\exp(-(j \log 2)/2 \cdot q(1 + o(1)))$ , the  $j = 2$  term ( $\exp(-q \log 2(1 + o(1)))$ ) dominating the collapse of  $R(n, q)$  to  $n R(1, q)$ ).

The unifying analytical input is the *boundary-layer profile*  $h(q-k, k)/T_q = e^{-\xi^2/2-2\xi}(1+O((\xi^3+1)/\sqrt{q}))$  for  $\xi = k/\sqrt{q}$  on  $k \leq \sqrt{q \log q}$  (Lemma 9), itself derived from the Wright/Hayman saddle-point asymptotic of  $T_N$ .

*Structure of the paper.* The paper splits into two parts.

**Part I (§3–§5):** combinatorial reductions. §3 defines  $f(l, k)$ ,  $h(r, k)$ , and proves their closed forms (Lemmas 2, 3); §3 also derives the keystone identity (Lemma 4) and the closed form for  $S_1^{(k)}$  (Lemma 5). §4 expresses both  $P_{\text{nodes}}$  and  $P_{\text{ptr}}$  as finite linear combinations of  $S_j$ ,  $S_j^{(k)}$ , and  $B_j^{(b)}$  by inclusion–exclusion (Theorems 6, 7), and gives a closed form for  $R(1, q)$  (Proposition 8). Part I is exact: no asymptotics enter until Part II. §5 recapitulates.

**Part II (§6–§10):** asymptotic analysis. §6 establishes the boundary-layer profile (Lemma 9) and the leading  $S_j$  asymptotic (Lemma 12). §7 assembles  $P_{\text{nodes}}$  (Theorem 13). §8 handles the  $n = 1$  pointer count via the asymptotics of  $W(1, q) = S_1^{(k)}(q)$  (Lemma 14) and  $R(1, q)$  (Lemma 15), yielding the four-term expansion of  $P_{\text{ptr}}(1, q)$  (Theorem 16). §9 extends to general  $n$ : the boundary moments collapse (Lemma 17), the  $k$ -weighted moments admit a two-term closed form (Lemma 18), and assembling everything proves Theorem 19. §10 recapitulates the analytical content.

*Verification.* Every claim is checked numerically against either exact-rational enumeration (small  $q$ ) or log-space float64 evaluation of the defining sums (up to  $q = 10^4$ ). Verification tables appear inline after every Lemma, Theorem, and Proposition.

## Part I

# Combinatorial reductions

The first part of this paper develops the algebraic and combinatorial identities that reduce  $P_{\text{nodes}}(n, q)$  and  $P_{\text{ptr}}(n, q)$  to per-prefix moments and boundary sums. Everything in Part I holds as *exact* identities for every  $n \geq 1$  and  $q \geq 0$ ; no asymptotics are used until Part II.

**Verification methodology.** Every closed form in Part I is accompanied by exact-rational verification against direct enumeration, implemented in Rust with the `num-bigint` and `num-rational` crates. The common ground-truth object is the explicit set  $\mathcal{S}_q$  of all length- $q$  marked involutions, built by enumerating pair partitions of  $\{1, \dots, q\}$  and marking each fixed point as  $\bar{1}$  or  $0$  (*without* using the recurrence  $T_{N+2} = 2T_{N+1} + (N+1)T_N$ ), then computing the canonical string of exercise 178 for each. Each verification below states its own specific enumeration method on  $\mathcal{S}_q$ ; the column “closed form” evaluates the formula in `BigInt/BigRational`; ✓ marks digit-for-digit equality.

## 3 Notation and preliminaries

A *marked involution* of order  $q$  is a permutation  $\sigma$  of  $\{1, \dots, q\}$  with  $\sigma^2 = \text{id}$ , in which each fixed point is marked or unmarked. Following Knuth’s exercise 178, we encode it as a string  $a_1 \dots a_q$  with each  $a_j \in \{\bar{1}, 0, 1, 2, \dots, \lfloor q/2 \rfloor\}$ , where  $\bar{1}$  marks a marked 1-cycle,  $0$  an unmarked 1-cycle, and a positive label  $t$  marks the two endpoints of a single 2-cycle (the smaller endpoint receives a fresh label from a strictly increasing reservoir).

**Definition 1** (Prefix counts). For  $0 \leq k \leq l$ , let  $f(l, k)$  be the number of length- $l$  prefixes of marked involutions in which exactly  $k$  pair labels remain *open* (their partner has not yet appeared). For  $0 \leq k \leq r$ , let  $h(r, k)$  be the number of completions of a  $k$ -open prefix into a full marked involution after  $r$  further positions.

**Lemma 2** (Closed form for  $f$ ).  $f(l, k) = \binom{l}{k} T_{l-k}$ .

*Proof.* Figure 1 illustrates the bijection.

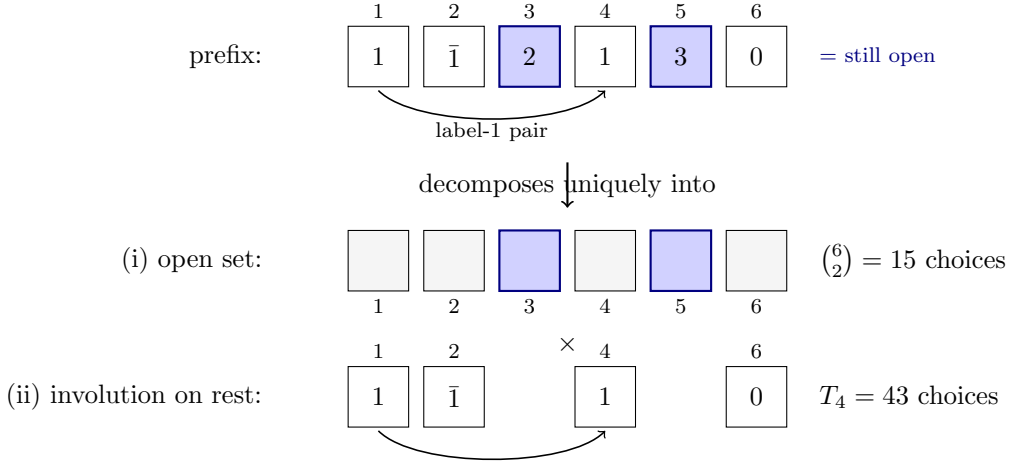


Figure 1: The bijection for Lemma 2: a length- $l$  prefix with  $k$  still-open pairs decomposes uniquely into the *set* of  $k$  open-left-endpoint positions and a marked involution on the remaining  $l - k$  positions. Once these two data are fixed, the canonical encoding rule of exercise 178 forces every label, so no further choice remains. Example shown:  $l = 6$ ,  $k = 2$ , with open positions  $\{3, 5\}$  and the marked involution  $1 \leftrightarrow 4$ ,  $2 = \bar{1}$ ,  $6 = 0$  on  $\{1, 2, 4, 6\}$ . Total:  $\binom{6}{2} \cdot T_4 = 15 \cdot 43 = 645 = f(6, 2)$ .

A length- $l$  prefix with exactly  $k$  open pairs at position  $l$  is uniquely determined by (i) the set of  $k$  positions among  $\{1, \dots, l\}$  that hold the *left* endpoints of the still-open pairs ( $\binom{l}{k}$  choices); and (ii) a marked involution on the remaining  $l - k$  positions, accounting for all closed 2-cycles together with marked and unmarked 1-cycles ( $T_{l-k}$  choices). Once these two data are fixed, the labels at the  $k$  open positions and at the closed-pair endpoints are forced by the canonical encoding rule of exercise 178 (each new opening takes the smallest positive integer not yet appearing in the prefix so far; closed-pair endpoints repeat their opening label), so no further choice remains. Hence  $f(l, k) = \binom{l}{k} T_{l-k}$ .  $\square$

**Enumeration method for  $f(l, k)$  (brute force).** For each row, choose any  $q$  with  $q \geq l + k$  (so every  $k$ -open length- $l$  prefix has at least one extension to a length- $q$  marked involution), enumerate the full set  $\mathcal{S}_q$ , group its elements by length- $l$  prefix, restrict to groups whose prefix has exactly  $k$  open pairs at position  $l$ , and read off the number of such groups (= “distinct  $k$ -open prefixes”) together with the maximum and minimum group size. The distinct count is independent of  $q$  (provided  $q \geq l + k$ ), but the group size scales with  $q$  as  $h(q - l, k)$ . We vary the offset  $q - (l + k) \in \{0, 1, 2\}$  across rows to demonstrate that the verification is not tied to the minimal  $q$ .

**Exact-rational check.** For each row we pick some  $q \geq l + k$  (the slack  $q - (l + k) \in \{0, 1, 2\}$  varies across rows), group  $\mathcal{S}_q$  by length- $l$  prefix, and restrict to groups whose prefix has  $k$  open pairs. We then record the number of such distinct  $k$ -open prefixes (the enumeration value of  $f(l, k)$ ) together with the maximum and minimum group size over them. Two checks pass simultaneously: the count matches  $f(l, k) = \binom{l}{k} T_{l-k}$  (independent of  $q$  once  $q \geq l + k$ ), and  $\max = \min$  at every row – confirming the symmetry that every  $k$ -open length- $l$  prefix has the same number of extensions in  $\mathcal{S}_q$ , namely  $h(q - l, k)$  (varying with  $q$ ).

$(l, k)$	offset	$q$	$ \mathcal{S}_q =T_q$	distinct $k$ -open	$f(l, k)$ closed	max	min	max = min
(3, 1)	0	4	43	15	$\binom{3}{1}T_2=15$	1	1	✓
	1	5	142	15		4	4	✓
	2	6	499	15		15	15	✓
(4, 1)	0	5	142	56	$\binom{4}{1}T_3=56$	1	1	✓
	1	6	499	56		4	4	✓
	2	7	1,850	56		15	15	✓
(4, 2)	0	6	499	30	$\binom{4}{2}T_2=30$	2	2	✓
	1	7	1,850	30		12	12	✓
	2	8	7,193	30		60	60	✓
(5, 2)	0	7	1,850	140	$\binom{5}{2}T_3=140$	2	2	✓
	1	8	7,193	140		12	12	✓
	2	9	29,186	140		60	60	✓
(5, 3)	0	8	7,193	50	$\binom{5}{3}T_2=50$	6	6	✓
	1	9	29,186	50		48	48	✓
	2	10	123,109	50		300	300	✓
(6, 2)	0	8	7,193	645	$\binom{6}{2}T_4=645$	2	2	✓
	1	9	29,186	645		12	12	✓
	2	10	123,109	645		60	60	✓
(6, 3)	0	9	29,186	280	$\binom{6}{3}T_3=280$	6	6	✓
	1	10	123,109	280		48	48	✓
	2	11	538,078	280		300	300	✓
(7, 3)	0	10	123,109	1,505	$\binom{7}{3}T_4=1,505$	6	6	✓
	1	11	538,078	1,505		48	48	✓
	2	12	2,430,355	1,505		300	300	✓
(7, 4)	0	11	538,078	490	$\binom{7}{4}T_3=490$	24	24	✓
	1	12	2,430,355	490		240	240	✓
	2	13	11,317,646	490		1,800	1,800	✓
(8, 4)	0	12	2,430,355	3,010	$\binom{8}{4}T_4=3,010$	24	24	✓
	1	13	11,317,646	3,010		240	240	✓
	2	14	54,229,907	3,010		1,800	1,800	✓

Table 1: Exact-rational verification of  $f(l, k) = \binom{l}{k}T_{l-k}$  (Lemma 2). Each  $(l, k)$  pair is verified at three offsets  $q - (l + k) \in \{0, 1, 2\}$ . “distinct  $k$ -open” is the number of distinct length- $l$  canonical prefixes appearing in  $\mathcal{S}_q$  with  $k$  open pairs at position  $l$ , independent of the offset; “max” and “min” are the maximum/minimum of the group sizes  $|\{\sigma \in \mathcal{S}_q : \sigma \text{ begins with } p\}|$  over those distinct  $k$ -open prefixes  $p$ . The fact that  $\max = \min = h(q - l, k)$  at every row confirms the symmetry: every  $k$ -open length- $l$  prefix has the same number of extensions in  $\mathcal{S}_q$ .

**Lemma 3** (Closed form for  $h$ ).  $h(r, k) = k! \binom{r}{k} T_{r-k}$ .

*Proof.* Figure 2 illustrates the bijection.

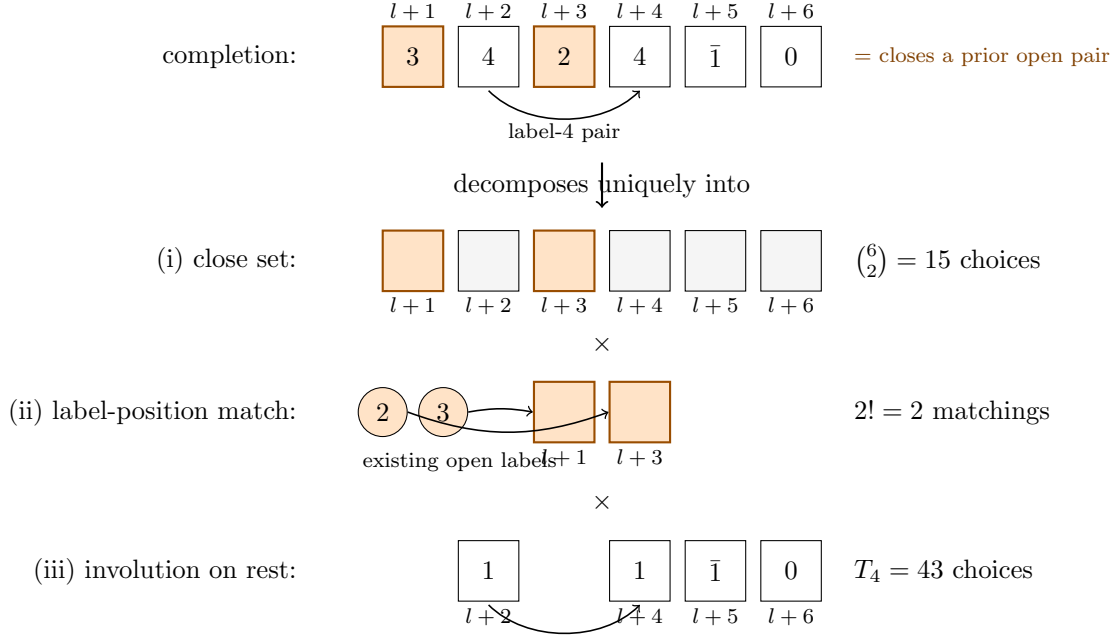


Figure 2: The bijection for Lemma 3: completing a  $k$ -open state over  $r$  further positions decomposes uniquely into (i) the set of  $k$  positions that close existing open pairs, (ii) a matching of the  $k$  pre-existing open labels to those positions, and (iii) a marked involution on the remaining  $r - k$  positions. Example:  $r = 6$ ,  $k = 2$ , continuing the prefix of Figure 1 (existing open labels  $\{2, 3\}$ ). Closing positions  $\{l + 1, l + 3\}$  close labels 3 and 2 respectively; the remaining four positions  $\{l + 2, l + 4, l + 5, l + 6\}$  carry the marked involution  $l + 2 \leftrightarrow l + 4$ ,  $l + 5 = \bar{1}$ ,  $l + 6 = 0$  (the new pair gets label 4 in the global encoding, the smallest integer not yet appearing). The full completion string is 3, 4, 2, 4,  $\bar{1}$ , 0. Total:  $\binom{6}{2} \cdot 2! \cdot T_4 = 15 \cdot 2 \cdot 43 = 1,290 = h(6, 2)$ .

A completion of a  $k$ -open state over  $r$  further positions is determined by (i) the set of  $k$  positions among the  $r$  that close the existing open pairs ( $\binom{r}{k}$  choices); (ii) the matching between the  $k$  pre-existing open labels and these  $k$  chosen positions ( $k!$  ordered bijections); and (iii) a fresh marked involution on the remaining  $r - k$  positions ( $T_{r-k}$  choices). Hence  $h(r, k) = k! \binom{r}{k} T_{r-k}$ .  $\square$

**Enumeration method for  $h(r, k)$  (brute force).** For each row pick some  $q \geq k + r$  (the slack  $q - (k + r) \in \{0, 1, 2\}$  varies across rows), set  $l = q - r$  (so  $l \in \{k, k + 1, k + 2\}$ ), enumerate the full set  $\mathcal{S}_q$ , group by length- $l$  prefix, restrict to groups whose prefix has  $k$  open pairs. The number of such groups equals  $f(l, k)$  (varies with  $l$ ; already verified in Table 1); the maximum and minimum group sizes are both  $h(r, k)$ , since every  $k$ -open length- $l$  prefix has exactly  $h(r, k)$  completions in  $\mathcal{S}_{l+r}$  by symmetry. The offset-0 case ( $l = k$ ,  $f(l, k) = 1$ ) is the original single-prefix enumeration; the offset-1, 2 cases give the same  $h(r, k)$  over  $f(l, k) > 1$  distinct prefixes.

**Exact-rational check.** For each row of Table 2 we group  $\mathcal{S}_q$  (with  $q = l + r$ ) by length- $l$  prefix and restrict to  $k$ -open groups; the number of such groups equals  $f(l, k)$  (column “distinct  $k$ -open”), and the maximum and minimum group size are recorded. Two checks pass simultaneously:  $\max = \min$  at every row (the symmetry that all  $k$ -open length- $l$  prefixes have the same number of completions), and the common value equals  $h(r, k) = k! \binom{r}{k} T_{r-k}$  independently of the choice of  $l$  within  $\{k, k + 1, k + 2\}$  (the  $h(r, k)$  value is shared down each  $(r, k)$  block of three rows).

$(r, k)$	offset	$l$	$q=l+r$	$ \mathcal{S}_q =T_q$	distinct $k$ -open	max	min	max = min = $h(r, k)$
(3, 1)	0	1	4	43	1	15	15	$h(3, 1)=15$
	1	2	5	142	4	15	15	
	2	3	6	499	15	15	15	
(4, 1)	0	1	5	142	1	56	56	$h(4, 1)=56$
	1	2	6	499	4	56	56	
	2	3	7	1,850	15	56	56	
(4, 2)	0	2	6	499	1	60	60	$h(4, 2)=60$
	1	3	7	1,850	6	60	60	
	2	4	8	7,193	30	60	60	
(5, 2)	0	2	7	1,850	1	280	280	$h(5, 2)=280$
	1	3	8	7,193	6	280	280	
	2	4	9	29,186	30	280	280	
(5, 3)	0	3	8	7,193	1	300	300	$h(5, 3)=300$
	1	4	9	29,186	8	300	300	
	2	5	10	123,109	50	300	300	
(6, 2)	0	2	8	7,193	1	1,290	1,290	$h(6, 2)=1,290$
	1	3	9	29,186	6	1,290	1,290	
	2	4	10	123,109	30	1,290	1,290	
(6, 3)	0	3	9	29,186	1	1,680	1,680	$h(6, 3)=1,680$
	1	4	10	123,109	8	1,680	1,680	
	2	5	11	538,078	50	1,680	1,680	
(7, 3)	0	3	10	123,109	1	9,030	9,030	$h(7, 3)=9,030$
	1	4	11	538,078	8	9,030	9,030	
	2	5	12	2,430,355	50	9,030	9,030	
(7, 4)	0	4	11	538,078	1	11,760	11,760	$h(7, 4)=11,760$
	1	5	12	2,430,355	10	11,760	11,760	
	2	6	13	11,317,646	75	11,760	11,760	
(8, 4)	0	4	12	2,430,355	1	72,240	72,240	$h(8, 4)=72,240$
	1	5	13	11,317,646	10	72,240	72,240	
	2	6	14	54,229,907	75	72,240	72,240	

Table 2: Exact-rational verification of  $h(r, k) = k! \binom{r}{k} T_{r-k}$  (Lemma 3). Each  $(r, k)$  pair is verified at three offsets  $q - (k + r) \in \{0, 1, 2\}$ , giving  $l = q - r \in \{k, k + 1, k + 2\}$ . “distinct  $k$ -open” is the number of distinct length- $l$  canonical  $k$ -open prefixes (equals  $f(l, k)$ ; varies with  $l$ ). The fact that max = min at every row, all three equal to  $h(r, k)$  independently of  $l$ , confirms the symmetry: every  $k$ -open length- $l$  prefix has the same number of completions in  $\mathcal{S}_{l+r}$ , namely  $h(r, k)$ .

**Lemma 4** (Keystone identity). For  $0 \leq l \leq q$ ,

$$\sum_{k=0}^l f(l, k) h(q - l, k) = T_q. \quad (3)$$

*Proof.* Figure 3 illustrates the partition.

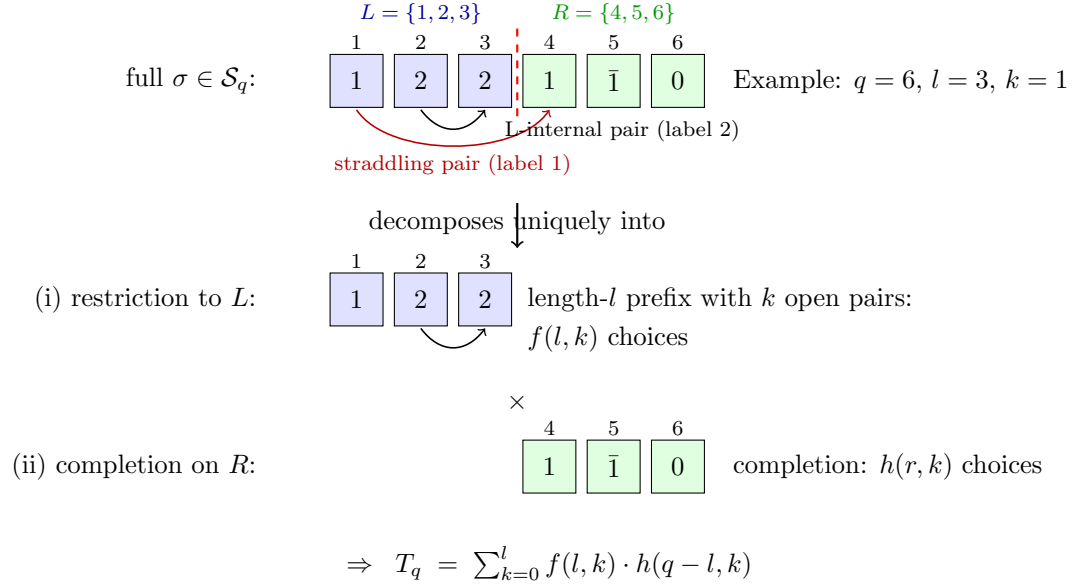


Figure 3: The partition for Lemma 4: a length- $q$  marked involution decomposes by the number  $k$  of pairs that straddle the boundary  $L \cup R$  ( $|L| = l, |R| = r = q - l$ ), into (i) a length- $l$  prefix with  $k$  open pairs (contributing  $f(l, k)$  choices for each  $k$ ) and (ii) a completion of that  $k$ -open state over  $r$  further positions (contributing  $h(r, k)$ ). Example shown:  $\sigma = 1221\bar{1}0$  in  $\mathcal{S}_6$  with  $l = 3, k = 1$  (one straddling pair labeled 1, one L-internal closed pair labeled 2, two R-internal fixed points). Summing over  $k$  gives  $T_q$ .

Setting  $r := q - l$ , we partition marked involutions of order  $l + r$  by the number  $k$  of pairs that *straddle* the boundary between  $L := \{1, \dots, l\}$  and  $R := \{l + 1, \dots, l + r\}$  (i.e. have one endpoint in  $L$  and the other in  $R$ ).

A marked involution with exactly  $k$  straddling pairs is determined by two independent data:

- Its restriction to  $L$ , which is a length- $l$  prefix in which the  $k$  left endpoints of the straddling pairs are precisely the positions that are *still open* at the end of the prefix; this contributes  $f(l, k)$  choices.
- A completion of that  $k$ -open state into a full marked involution by filling the  $r$  further positions of  $R$ : this is counted by  $h(r, k)$ .

Summing over  $k$  gives  $\sum_{k=0}^l f(l, k)h(r, k) = T_q$ . □

**Exact-rational check.** For every  $q \in \{2, 3, 4, 5, 6\}$  and every  $l \in \{0, 1, \dots, q\}$  we compute the sum  $\sum_{k=0}^l f(l, k)h(q-l, k)$  from the closed forms of Lemmas 2 and 3 and compare with  $T_q$ ; all  $3 + 4 + 5 + 6 + 7 = 25$  entries match (Table 3 below).

$q$	$l$	$\sum_{k=0}^l f(l, k)h(q-l, k)$	$T_q$	match
2	0	5	5	✓
	1	5	5	✓
	2	5	5	✓
3	0	14	14	✓
	1	14	14	✓
	2	14	14	✓
	3	14	14	✓
4	0	43	43	✓
	1	43	43	✓
	2	43	43	✓
	3	43	43	✓
	4	43	43	✓
5	0	142	142	✓
	1	142	142	✓
	2	142	142	✓
	3	142	142	✓
	4	142	142	✓
	5	142	142	✓
6	0	499	499	✓
	1	499	499	✓
	2	499	499	✓
	3	499	499	✓
	4	499	499	✓
	5	499	499	✓
	6	499	499	✓

Table 3: Exact-rational verification of the keystone identity  $\sum_{k=0}^l f(l, k)h(q-l, k) = T_q$  (Lemma 4). All  $(q, l)$  with  $2 \leq q \leq 6$  and  $0 \leq l \leq q$  are checked exhaustively; all 25 entries match.

Substituting the closed forms of Lemmas 2 and 3 into (3) yields the equivalent Vandermonde-style algebraic identity

$$T_{l+r} = \sum_{k \geq 0} \binom{l}{k} \binom{r}{k} k! T_{l-k} T_{r-k}, \quad (4)$$

a classical identity for the EGF  $e^{2z+z^2/2}$  recorded as an exercise in Riordan [8].

For a fixed length- $l$  prefix  $p$  of order  $q$  with  $k_p$  open pairs, the probability that a uniformly random marked involution of order  $q$  begins with  $p$  is  $\pi_p := h(q-l, k_p)/T_q$ .

The trie-node and pointer counts of §4 are averages over  $n$  i.i.d. keys, so each reduces by inclusion–exclusion on the event “prefix  $p$  appears in the trie” = “at least one of the  $n$  keys begins with  $p$ ”. The indicator of this event has expectation  $1 - (1 - \pi_p)^n = \sum_{j \geq 1} (-1)^{j+1} \binom{n}{j} \pi_p^j$ , so its  $j$ -th term contributes the sum  $\sum_p \pi_p^j$  over prefixes. The node count is just  $\sum_p \mathbf{1}[p \text{ in trie}]$ , so it reduces to the *unweighted* moments  $\sum_p \pi_p^j$ . The pointer count is  $\sum_p d_p \mathbf{1}[p \text{ in trie}]$  with  $d_p = k_p + 3$  by (1) except on two thin boundary lines where it drops by 1 or 3, so it reduces to a linear combination of the unweighted moments and the *TMS-weighted* moments  $\sum_p k_p \pi_p^j$ . We therefore define

$$S_j(q) := 1 + \sum_{l=1}^q \sum_{p:|p|=l} \pi_p^j = 1 + \sum_{l=1}^q \sum_{k=0}^l f(l, k) \left( \frac{h(q-l, k)}{T_q} \right)^j, \quad (5)$$

$$S_j^{(k)}(q) := \sum_{l=1}^q \sum_{p:|p|=l} k_p \pi_p^j = \sum_{l=1}^q \sum_{k=0}^l k f(l, k) \left( \frac{h(q-l, k)}{T_q} \right)^j. \quad (6)$$

The leading “1” in  $S_j$  is the contribution of the root prefix  $p = \varepsilon$  at level  $l = 0$ , which has  $\pi_\varepsilon = 1$  and so contributes  $1^j = 1$  for every  $j$ ; the same root contributes  $k_\varepsilon \cdot 1 = 0$  to  $S_j^{(k)}$  (no open pairs at the root), which is why no such “1+” appears there.

The second equality in each of (5) and (6) deserves a quick justification:  $\pi_p = h(q - |p|, k_p)/T_q$  depends on the prefix  $p$  only through its length  $|p|$  and its open-pair count  $k_p$ . So if we group the length- $l$  prefixes by their open-pair count, the number of  $p$  with  $|p| = l$  and  $k_p = k$  is exactly  $f(l, k)$  (Lemma 2), each contributing  $\pi_p^j = (h(q - l, k)/T_q)^j$  (respectively  $k_p \pi_p^j = k (h(q - l, k)/T_q)^j$  for  $S_j^{(k)}$ ). Replacing  $\sum_{p:|p|=l}$  by  $\sum_{k=0}^l f(l, k)$  gives the two  $(l, k)$ -cell forms.

At  $j = 1$ ,  $\sum_{p:|p|=l} \pi_p = 1$  at every level  $l$  by (3), so  $S_1(q) = 1 + q$ .

**Lemma 5** ( $S_1^{(k)}$  in closed form). *For all  $q \geq 2$ ,*

$$S_1^{(k)}(q) = \frac{T_{q-2}}{T_q} \cdot \frac{q^3 - q}{6}. \quad (7)$$

(For  $q \in \{0, 1\}$  the sum is empty,  $S_1^{(k)}(q) = 0$ .)

*Proof.* At fixed level  $l$ , using  $k \binom{l}{k} = l \binom{l-1}{k-1}$  and the matching identity  $(m+1)! \binom{q-l}{m+1} = (q-l) m! \binom{q-l-1}{m}$  on the  $h$ -factor, then shifting the summation index  $k \rightarrow m+1$ ,

$$\begin{aligned} \sum_k k f(l, k) h(q-l, k) &= \sum_{k \geq 1} k \binom{l}{k} T_{l-k} \cdot k! \binom{q-l}{k} T_{q-l-k} \\ &= \sum_{m \geq 0} l \binom{l-1}{m} T_{l-1-m} \cdot (q-l) m! \binom{q-l-1}{m} T_{q-l-1-m} \\ &= l(q-l) \sum_{m \geq 0} \binom{l-1}{m} \binom{q-l-1}{m} m! T_{l-1-m} T_{q-l-1-m} \\ &= l(q-l) T_{q-2} \end{aligned}$$

by the keystone identity (3) applied at total length  $(l-1) + (q-l-1) = q-2$ . Summing over  $l = 1, \dots, q$  and dividing by  $T_q$  gives (7), since  $\sum_{l=1}^q l(q-l) = (q^3 - q)/6$ .  $\square$

**Exact-rational check.** For each  $q \in \{3, 4, \dots, 10\}$  we compute  $S_1^{(k)}(q)$  via two *separate closed-form expressions* and check agreement: (i) the definition unwound via Lemmas 2 and 3,

$$S_1^{(k)}(q) = \sum_{l=1}^q \sum_{k=0}^l k f(l, k) h(q-l, k)/T_q,$$

evaluated as a `BigRational`; (ii) the Lemma 5 closed form  $T_{q-2}/T_q \cdot (q^3 - q)/6$ . Both are pure formula evaluations; this is not a brute-force enumeration check but an algebraic agreement test.

$q$	by definition (i)	by Lemma 5 (ii)	match
3	4/7	4/7	✓
4	50/43	50/43	✓
5	140/71	140/71	✓
6	1505/499	1505/499	✓
7	3976/925	3976/925	✓
8	41,916/7,193	41,916/7,193	✓
9	111,000/14,593	111,000/14,593	✓
10	1,186,845/123,109	1,186,845/123,109	✓

Table 4: Verification of Lemma 5 by computing  $S_1^{(k)}(q)$  via two separate closed-form expressions: (i) the definition  $\sum_{l,k} k f(l,k) h(q-l,k)/T_q$  from Lemmas 2, 3, and (ii) the Lemma 5 closed form  $T_{q-2}/T_q \cdot (q^3 - q)/6$ . The two formulas produce the same `BigRational` at every  $q$  tested.

## 4 Reductions

Two reductions, one for the node count, one for the pointer count.

**Theorem 6** (Reduction for  $P_{\text{nodes}}$ ). *For all integers  $n \geq 1$  and  $q \geq 0$ ,*

$$P_{\text{nodes}}(n, q) = nq + (n - 1) - \sum_{j=2}^n (-1)^j \binom{n}{j} S_j(q). \quad (8)$$

*Proof.* By definition  $P_{\text{nodes}}(n, q) = \sum_{l=1}^q \sum_{p:|p|=l} (1 - (1 - \pi_p)^n)$ , the inner sum running over the (finitely many) length- $l$  prefixes of order- $q$  marked involutions and  $(1 - (1 - \pi_p)^n)$  being the probability that at least one of the  $n$  random keys begins with  $p$ . Expanding  $1 - (1 - x)^n = \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} x^j$  in the coordinate  $x = \pi_p$  and exchanging summation order,

$$P_{\text{nodes}}(n, q) = \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} \sum_{l=1}^q \sum_{p:|p|=l} \pi_p^j = \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} (S_j(q) - 1).$$

For  $j = 1$ ,  $S_1(q) - 1 = q$  by (3); this contributes  $nq$ . The constant offset coming from  $-\sum_{j \geq 2} (-1)^{j+1} \binom{n}{j} \cdot 1 = \sum_{j=2}^n (-1)^j \binom{n}{j} = n - 1$  (since  $\sum_{j=0}^n (-1)^j \binom{n}{j} = 0$  for  $n \geq 1$ , so the  $j \geq 2$  tail equals  $-[(-1)^0 \binom{n}{0} + (-1)^1 \binom{n}{1}] = n - 1$ ).  $\square$

**Exact-rational check.** We verify (8) at small  $(n, q)$  by two independent computations: (i) “enumeration”: enumerate all  $T_q^n$  ordered  $n$ -tuples of length- $q$  marked involutions, build the compact trie of each tuple, count its distinct non-root nodes, and average as a `BigRational` (this code path uses no  $f, h$  formulas, only the trie construction); (ii) “closed form”: compute  $S_j(q)$  for  $j = 2, \dots, n$  from  $S_j(q) = 1 + \sum_{(l,k)} f(l,k) (h(q-l,k)/T_q)^j$  using Lemmas 2 and 3, then plug into  $P_{\text{nodes}}(n, q) = nq + (n - 1) - \sum_{j=2}^n (-1)^j \binom{n}{j} S_j(q)$ . If Theorem 6 holds, both columns must agree digit by digit; Table 5 confirms this.

$(n, q)$	$T_q^n$ tuples	enumeration	closed form	match
(2, 4)	1,849	13868/1849	13868/1849	✓
(2, 5)	20,164	95899/10082	95899/10082	✓
(2, 6)	249,001	2865678/249001	2865678/249001	✓
(3, 4)	79,507	844810/79507	844810/79507	✓
(3, 5)	2,863,288	19561753/1431644	19561753/1431644	✓
(3, 6)	124,251,499	2070484608/124251499	2070484608/124251499	✓
(4, 4)	3,418,801	46024640/3418801	46024640/3418801	✓
(4, 5)	406,586,896	3566149555/203293448	3566149555/203293448	✓

Table 5: Verification of Theorem 6 by two independent computations of  $P_{\text{nodes}}(n, q)$ : “enumeration” (build the compact trie of every ordered  $n$ -tuple, count nodes, average) and “closed form” (apply (8) with  $S_j(q)$  computed from  $f, h$ ). Both columns match digit for digit at every tested  $(n, q)$ .

**Theorem 7** (Reduction for  $P_{\text{ptr}}$ ). *For all integers  $n \geq 1$  and  $q \geq 2$  (so that the root’s  $l = k = 0$  satisfies  $l + k = 0 \leq q - 2$ , placing it in the “otherwise” branch of (1) with  $d(0, 0) = 0 + 3 = 3$ ),*

$$P_{\text{ptr}}(n, q) = 3P_{\text{nodes}}(n, q) + 3 + W(n, q) + R(n, q), \quad (9)$$

where the additive  $+3$  is the root contribution ( $d_{\text{root}} = 3$ , not counted in  $P_{\text{nodes}}$ ), and

$$W(n, q) = \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} S_j^{(k)}(q), \quad R(n, q) = \mathbf{E} \left[ \sum_{p \in \text{Trie}} r_p \right],$$

with  $r_p \in \{-3, -1, 0\}$  the per-node correction  $d_p - (k_p + 3)$  from (1) (so  $r_p = -1$  at the “tight =  $q - 1$ ” boundary  $l_p + k_p = q - 1$ ,  $r_p = -3$  at the “tight =  $q$ ” boundary  $l_p + k_p = q$ , and  $r_p = 0$  elsewhere). The two boundary lines  $l_p + k_p \in \{q - 1, q\}$  each carry  $\Theta(q)$  candidate cells, but the probability-weighted contribution  $\mathbf{E}[\sum_p \mathbf{1}[p \text{ on boundary, in trie}]]$  scales like  $\sqrt{q}$  (a  $1/\sqrt{q}$  saturation density times  $\Theta(q)$  length), so  $R(n, q)$  is not a bounded  $O(1)$  quantity; in fact  $R(1, q) = (c_1 - 2)\sqrt{q} + O(1)$  with  $c_1 := \int_0^\infty e^{-\xi^2/2 - 2\xi} d\xi \approx 0.42136923$  (§9 below), and  $R(n, q) = n R(1, q)$  up to an exponentially small remainder  $O(e^{-q \log^2(1+o(1))})$ , by Lemma 17.

*Proof.* The pointer count sums  $d_p$  over internal nodes  $p$  of the trie (levels  $0 \leq l_p \leq q - 1$ ); the leaf level  $l_p = q$  holds the terminal involution data (the “WordTable” of exercise 204) and contributes no  $d$ . Equivalently, since  $d(q, 0) = 0$  in the tight branch of (1), we may include the leaf level without changing the value, and separate out the root:

$$P_{\text{ptr}}(n, q) = \mathbf{E} \left[ \sum_{p \in \text{Trie}} d_p \right] = d(0, 0) + \mathbf{E} \left[ \sum_{\substack{p \in \text{Trie} \\ |p| \geq 1}} d_p \right].$$

The root is in the trie deterministically, so the second sum collapses to one over  $(l, k)$  cells with  $1 \leq l \leq q$ ,  $0 \leq k \leq l$ . Each such cell contains  $f(l, k)$  candidate prefixes, all sharing the same probability  $\pi_{l,k} := h(q - l, k)/T_q$  that a random key begins with any one of them; the probability that the trie contains a given such prefix is  $1 - (1 - \pi_{l,k})^n$ . Hence

$$P_{\text{ptr}}(n, q) = 3 + \sum_{l=1}^q \sum_{k=0}^l d(l, k) f(l, k) (1 - (1 - \pi_{l,k})^n),$$

using  $d_{\text{root}} = d(0, 0) = 3$ .

We decompose  $d(l, k)$  into a baseline plus two boundary corrections:

$$d(l, k) = (k + 3) - \mathbf{1}[l + k = q - 1] - 3\mathbf{1}[l + k = q], \quad (10)$$

which one checks against (1) case by case (at  $l + k = q$ :  $k + 3 - 0 - 3 = k$ ; at  $l + k = q - 1$ :  $k + 3 - 1 - 0 = k + 2$ ; otherwise:  $k + 3 - 0 - 0 = k + 3$ ). Substituting (10) into the  $P_{\text{ptr}}$ -expression splits the double sum into three pieces:

$$\begin{aligned} P_{\text{ptr}}(n, q) - 3 &= \sum_{l, k} (k + 3) f(l, k) (1 - (1 - \pi_{l, k})^n) \\ &\quad - \sum_{l, k} \mathbf{1}[l + k = q - 1] f(l, k) (1 - (1 - \pi_{l, k})^n) \\ &\quad - 3 \sum_{l, k} \mathbf{1}[l + k = q] f(l, k) (1 - (1 - \pi_{l, k})^n). \end{aligned}$$

Expand each  $(1 - (1 - \pi_{l, k})^n)$  via the binomial identity  $1 - (1 - x)^n = \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} x^j$  and exchange the  $j$ -sum with the  $(l, k)$ -sums. For the first piece, the inner  $j$ -th term is

$$\sum_{l=1}^q \sum_{k=0}^l (k + 3) f(l, k) \pi_{l, k}^j = \underbrace{\sum_{l, k} k f(l, k) \pi_{l, k}^j}_{= S_j^{(k)}(q)} + 3 \underbrace{\sum_{l, k} f(l, k) \pi_{l, k}^j}_{= S_j(q-1)},$$

by (5) and (6) (the “ $-1$ ” is the root term  $\pi_{0,0}^j = 1$  in  $S_j$ ). For the second and third pieces, define the *boundary moments*

$$B_j^{(b)}(q) := \sum_{(l, k): q-l-k=b} f(l, k) \pi_{l, k}^j \quad (b = 0, 1), \quad (11)$$

so the inner  $j$ -th terms are  $B_j^{(1)}(q)$  and  $B_j^{(0)}(q)$  respectively. Combining,

$$P_{\text{ptr}}(n, q) = 3 + \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} [S_j^{(k)}(q) + 3(S_j(q) - 1) - B_j^{(1)}(q) - 3B_j^{(0)}(q)].$$

The  $3(S_j - 1)$  sum reduces to  $3P_{\text{nodes}}(n, q)$  by Theorem 6; the  $S_j^{(k)}$  sum is  $W(n, q)$  by definition; the  $B_j^{(b)}$  sums assemble into  $-R(n, q)$  via  $R(n, q) := -\sum_{j=1}^n (-1)^{j+1} \binom{n}{j} [B_j^{(1)}(q) + 3B_j^{(0)}(q)]$ , which is the inclusion–exclusion expansion of  $\mathbf{E}[\sum_p r_p]$  with  $r_p = d_p - (k_p + 3)$  from (10). This yields (9).  $\square$

**Exact-rational check.** We verify (9) at small  $(n, q)$  by two independent computations: (i) “enumeration”: enumerate all  $T_q^n$  ordered  $n$ -tuples, build the compact trie of each, sum the  $d_p$  rule (1) over distinct nodes, and average as a **BigRational** (this code path uses no  $f, h$  formulas, only the trie construction and the  $d_p$  rule); (ii) “closed form”: for each  $(l, k)$  cell compute  $d(l, k) f(l, k) (1 - (1 - \pi_{l, k})^n)$  from Lemmas 2, 3 with  $\pi_{l, k} = h(q - l, k)/T_q$ , plus the root term  $d(0, 0) = 3$ , and sum. If Theorem 7 holds (which is equivalent to the displayed sum (9) after the  $d$ -decomposition (10)), both columns must agree digit for digit; Table 6 confirms this.

$(n, q)$	$T_q^n$ tuples	enumeration	closed form	match
(1, 3)	14	54/7	54/7	✓
(1, 4)	43	471/43	471/43	✓
(1, 6)	499	9064/499	9064/499	✓
(2, 5)	20,164	122042/5041	122042/5041	✓
(3, 4)	79,507	1810095/79507	1810095/79507	✓
(3, 5)	2,863,288	23488091/715822	23488091/715822	✓
(4, 4)	3,418,801	93409173/3418801	93409173/3418801	✓

Table 6: Verification of Theorem 7 by two independent computations of  $P_{\text{ptr}}(n, q)$ : “enumeration” (build the compact trie of every ordered  $n$ -tuple, sum the  $d_p$  rule over distinct nodes, average) and “closed form” (sum  $d(l, k)f(l, k)(1 - (1 - h(q - l, k)/T_q)^n)$  over  $(l, k)$  cells using Lemmas 2, 3). Both columns match digit for digit at every tested  $(n, q)$ .

**Proposition 8** (Closed form of  $R(1, q)$ ). *For  $q \geq 2$ ,*

$$R(1, q) = - \sum_{c=0}^{\lfloor (q-1)/2 \rfloor} \binom{q-1-c}{c} T_{q-1-2c} \frac{2(c+1)!}{T_q} - 3 \sum_{c=0}^{\lfloor q/2 \rfloor} \binom{q-c}{c} T_{q-2c} \frac{c!}{T_q}.$$

The first sum tracks the “ $\text{TMS}_l = q - 1 - l$ ” boundary line ( $r_p = -1$ ); the second tracks the “ $\text{TMS}_l = q - l$ ” boundary ( $r_p = -3$ ). Each term is a probability that a random length- $q$  marked involution hits the corresponding boundary at some level  $l$ .

*Proof.* For  $n = 1$  the trie is a path: a length- $l$  prefix  $p$  belongs to the trie precisely when it equals the length- $l$  prefix of the single random key, which happens with probability  $q_{l, k_p} = h(q - l, k_p)/T_q$ . Linearity of expectation therefore gives, summing  $r_p$  over all  $(l, k)$  cells,

$$R(1, q) = \sum_{l, k} r_{l, k} f(l, k) \pi_{l, k} = -B_1^{(1)}(q) - 3B_1^{(0)}(q), \quad (12)$$

using  $r_{l, k} = -1$  on the line  $l+k = q-1$ ,  $r_{l, k} = -3$  on  $l+k = q$ , and  $r_{l, k} = 0$  elsewhere (from (10)); the two boundary moments  $B_1^{(b)}(q) = \sum_{(l, k): q-l-k=b} f(l, k) \pi_{l, k}$  are the  $j = 1$  specializations of (11). We now turn each boundary moment into the stated single sum.

*First sum (line  $l + k = q - 1$ ,  $r = -1$ ).* On this line set  $c := q - 1 - l$ , so  $k = c$  and  $l = q - 1 - c$ . The constraint  $0 \leq k \leq l$  becomes  $0 \leq c \leq \lfloor (q - 1)/2 \rfloor$ . The closed forms of Lemmas 2 and 3 give

$$f(l, k) = \binom{q-1-c}{c} T_{q-1-2c},$$

$$h(q-l, k) = h(c+1, c) = c! \binom{c+1}{c} T_1 = 2(c+1)!$$

(using  $T_1 = 2$ , the two markings of a single 1-cycle), so  $f(l, k) \pi_{l, k} = \binom{q-1-c}{c} T_{q-1-2c} \cdot 2(c+1)!/T_q$  and

$$B_1^{(1)}(q) = \sum_{c=0}^{\lfloor (q-1)/2 \rfloor} \binom{q-1-c}{c} T_{q-1-2c} \frac{2(c+1)!}{T_q}.$$

*Second sum (line  $l + k = q$ ,  $r = -3$ ).* Set  $c := q - l$ , so  $k = c$  and  $l = q - c$ . The constraint  $0 \leq k \leq l$  becomes  $0 \leq c \leq \lfloor q/2 \rfloor$ . Now

$$f(l, k) = \binom{q-c}{c} T_{q-2c}, \quad h(q-l, k) = h(c, c) = c! \binom{c}{c} T_0 = c!,$$

so

$$B_1^{(0)}(q) = \sum_{c=0}^{\lfloor q/2 \rfloor} \binom{q-c}{c} T_{q-2c} \frac{c!}{T_q}.$$

Substituting these two sums into (12) yields the stated formula.  $\square$

**Exact-rational check.** For each  $q \in \{3, 4, 5, 6, 7\}$  we compute  $R(1, q)$  by three independent methods and check they all agree:

(i) the direct definition (= Theorem 7 specialized to  $n = 1$ , expanded via Lemmas 2, 3):

$$R(1, q) = \sum_{(l,k): l+k \in \{q-1, q\}} r_{l,k} f(l, k) h(q-l, k) / T_q,$$

with  $r_{l,k} = -1$  on  $l+k = q-1$  and  $r_{l,k} = -3$  on  $l+k = q$  (pure formula evaluation);

(ii) the Proposition 8 closed form (two single sums over  $c$ , pure formula evaluation);

(iii) true enumeration: for each  $\sigma \in \mathcal{S}_q$ , walk its canonical string, compute  $\sum_{l=0}^q r(l, \text{TMS}_l(\sigma))$  with  $r$  from (10), and average over  $\sigma$  as a **BigRational**. This method touches neither  $f$  nor  $h$  nor Proposition 8.

$q$	by definition (i)	by Prop. 8 (ii)	by enumeration (iii)	match
3	-34/7	-34/7	-34/7	✓
4	-224/43	-224/43	-224/43	✓
5	-394/71	-394/71	-394/71	✓
6	-2920/499	-2920/499	-2920/499	✓
7	-5678/925	-5678/925	-5678/925	✓

Table 7: Verification of Proposition 8 by three independent computations of  $R(1, q)$ : (i) direct definition as a sum over boundary-line  $(l, k)$  cells; (ii) the Proposition 8 closed form as two sums over  $c$ ; (iii) true enumeration – iterate over every  $\sigma \in \mathcal{S}_q$ , sum  $r(l, \text{TMS}_l(\sigma))$  over all  $q+1$  positions, and average. All three columns produce the same **BigRational**.

## 5 Summary of Part I

The reductions of Part I express both  $P_{\text{nodes}}(n, q)$  and  $P_{\text{ptr}}(n, q)$  as finite, exact linear combinations of the per-prefix moments

$$S_j(q) = 1 + \sum_{l=1}^q \sum_{k=0}^l f(l, k) \left( \frac{h(q-l, k)}{T_q} \right)^j, \quad S_j^{(k)}(q) = \sum_{l=1}^q \sum_{k=0}^l k f(l, k) \left( \frac{h(q-l, k)}{T_q} \right)^j,$$

the boundary moments

$$B_j^{(b)}(q) = \sum_{(l,k): q-l-k=b} f(l, k) \left( \frac{h(q-l, k)}{T_q} \right)^j \quad (b = 0, 1),$$

and the keystone identity  $\sum_k f(l, k) h(q-l, k) = T_q$ . Specifically:

$$P_{\text{nodes}}(n, q) = nq + (n-1) - \sum_{j=2}^n (-1)^j \binom{n}{j} S_j(q), \quad (13)$$

$$P_{\text{ptr}}(n, q) = 3P_{\text{nodes}}(n, q) + 3 + W(n, q) + R(n, q), \quad (14)$$

with

$$W(n, q) = \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} S_j^{(k)}(q), \quad R(n, q) = - \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} [B_j^{(1)}(q) + 3B_j^{(0)}(q)].$$

To turn (13)–(14) into closed-form asymptotic expansions, Part II will establish exactly three asymptotic facts about the building blocks:

- (A) *Leading constant for  $S_j$*  (Lemma 12):  $S_j(q) = c_j \sqrt{q} + \text{const}_j + O(q^{-1/2})$  for every fixed  $j \geq 2$ , where  $c_j = \int_0^\infty \exp(-\frac{j}{2}\xi^2 - 2j\xi) d\xi$ ,  $\text{const}_j = \frac{1}{2} + \frac{j-2}{2}(\frac{1}{j} - 2c_j)$  for  $j \geq 3$ , with the  $j = 2$  case  $\text{const}_2 = \frac{3}{2} - 4c_2$  differing from the general formula's  $j = 2$  specialisation (which would give  $\frac{1}{2}$ ) by  $1 - 4c_2$ , arising from the off-diagonal  $a = 1$  slice contribution (see Case  $j = 2$  in the proof of Lemma 12).
- (B) *Asymptotic of  $\rho(q) := T_{q-1}/T_q$*  (Lemma 14): bootstrapped from the recurrence  $\rho(q)[2 + (q-1)\rho(q-1)] = 1$ , used to develop  $T_{q-2}/T_q$  and hence  $S_1^{(k)}(q) = (q^3 - q)T_{q-2}/(6T_q)$  to four orders.
- (C) *Asymptotic of  $B_j^{(b)}$  and  $S_j^{(k)}$*  (§9):  $B_j^{(b)}(q)$  is exponentially small for  $j \geq 2$ , with rate  $-(j \log 2)/2$  per unit  $q$  (so  $R(n, q) = nR(1, q) + O(e^{-q \log 2 \cdot (1+o(1))})$ ), and  $S_j^{(k)}(q) = c_j^{(k)} q + d_j^{(k)} \sqrt{q} + O(1)$  with explicit rational +  $c_j$ -linear coefficients.

The Wright saddle-point asymptotic for  $T_N$  (eq. 15 below) is the sole external analytical input.

## Part II

# Asymptotic analysis

The second part turns the exact reductions of Part I into closed-form asymptotic expansions as  $q \rightarrow \infty$ . The analytical input comprises Stirling's formula, the saddle-point asymptotic of  $T_N$  ((15), due to Hayman's admissibility method), and a boundary-layer expansion in the scaled variable  $\xi := k/\sqrt{q}$ . Special-function content enters through the family  $c_j := \int_0^\infty e^{-(j/2)\xi^2 - 2j\xi} d\xi$ .

## 6 Leading constant $c_j$ for $S_j$

The analytical input is the marked-involution saddle-point asymptotic of the Hayman-admissibility framework [3]; equivalently, this is the specialisation to  $H(z) = e^{2z+z^2/2}$  of the saddle-point method for  $H$ -admissible functions developed by Hayman [3] (see also [4, Thm. VIII.4, Example VIII.5], with fixed-point weight 2). The  $O(N^{-1/2})$  remainder in the form below is Wright's:

$$\log T_N = \frac{N}{2} \log N - \frac{N}{2} + 2\sqrt{N} - \frac{1}{4} + \log C + r(N), \quad (15)$$

for an explicit positive constant  $C$ , with remainder  $r(N) \rightarrow 0$  as  $N \rightarrow \infty$  and the uniform bound  $|r(N)| \leq K_0$  for all  $N \geq 1$  ( $K_0 \leq 1$  suffices; explicit derivation in §A.4):

$$r(N) \rightarrow 0 \quad (N \rightarrow \infty), \quad |r(N)| \leq K_0 \quad \text{for all } N \geq 1. \quad (16)$$

The  $-\frac{1}{4} + \log C$  piece cancels in every ratio  $h(q-l, k)/T_q$  we form, so only the structural shape of (15) enters.

*An aside on the complementary error function.* The constants  $c_j$  defined in the abstract,

$$c_j := \int_0^\infty e^{-(j/2)\xi^2 - 2j\xi} d\xi,$$

admit an elementary closed form via the complementary error function  $\text{erfc}(x) := \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2} du$ : completing the square  $\xi^2/2 + 2\xi = (\xi + 2)^2/2 - 2$  and substituting  $u = \sqrt{j/2}(\xi + 2)$  gives

$$c_j = \sqrt{\pi/(2j)} e^{2j} \text{erfc}(\sqrt{2j}), \quad j \geq 1, \quad (17)$$

which we will use occasionally for numerical evaluation. Numerically (to six digits):  $c_1 \approx 0.421369$ ,  $c_2 \approx 0.226339$ ,  $c_3 \approx 0.155304$ ,  $c_4 \approx 0.118326$ ,  $c_5 \approx 0.095609$ ,  $c_6 \approx 0.080224$ ,  $c_7 \approx 0.069111$ ,  $c_8 \approx 0.060706$ ,  $c_9 \approx 0.054126$ ,  $c_{10} \approx 0.048834$ .

The single analytical workhorse for both the  $c_j \sqrt{q}$  asymptotic of  $S_j$  (Lemma 12 below) and the asymptotic of the boundary moments  $B_1^{(b)}$  that drive Lemma 15 is the following uniform expansion of the all-open prefix probability  $h(q-k, k)/T_q$ .

**Lemma 9** (Boundary-layer profile). *There exist absolute constants  $C^* \leq 4$  and  $q^* = 20$  such that for all  $q \geq q^*$  and all integers  $k$  with  $0 \leq k \leq \sqrt{q \log q}$ , setting  $\xi := k/\sqrt{q}$ :*

$$\left| \frac{h(q-k, k)}{T_q} - e^{-\xi^2/2 - 2\xi} \right| \leq C^* e^{-\xi^2/2 - 2\xi} \cdot \frac{\xi^3 + 1}{\sqrt{q}}. \quad (18)$$

(The bound  $C^* \leq 4$  comes from  $|P(\xi)| \leq 2(1 + \xi^3)$  (§A) plus the exponentiation step. With  $X := P(\xi)/\sqrt{q} + O((\xi^4 + 1)/q + q^{-1/2})$  from (59), on the boundary layer  $|X| \leq o(1)$ , so  $|e^X - 1| \leq |X| + |X|^2/2 + \dots \leq 2|X|$ , giving  $|h/T_q - \varphi(\xi)| = \varphi(\xi)|e^X - 1| \leq 2\varphi(\xi)|P(\xi)|/\sqrt{q} + O(\dots) \leq 4\varphi(\xi)(1 + \xi^3)/\sqrt{q}$ . Sharper constants are possible but not needed; the value  $C^* \leq 4$  suffices below.) Outside the boundary layer, for  $\sqrt{q \log q} < k \leq q/2$ ,  $h(q-k, k)/T_q \leq e^{-\xi^2/2}$  uniformly (see Figure 4), and consequently  $\sum_{k > \sqrt{q \log q}}^{\lfloor q/2 \rfloor} h(q-k, k)/T_q \leq 2/\sqrt{\log q}$ .

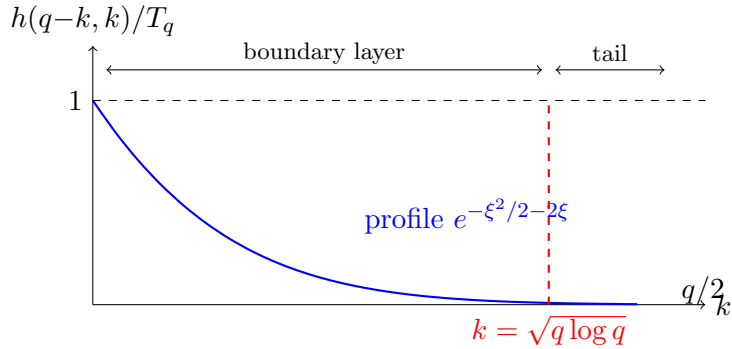


Figure 4: Decay regions in Lemma 9 (schematic; coefficients chosen to match  $q = 16$  so that  $1/(2q) \approx 0.031$  and  $2/\sqrt{q} = 0.5$  both appear consistently). Inside the boundary layer ( $k \leq \sqrt{q \log q}$ ) the multiplicative profile  $e^{-\xi^2/2 - 2\xi}$  approximates  $h(q-k, k)/T_q$  to relative error  $O((\xi^3 + 1)/\sqrt{q})$ . In the tail only the cruder upper bound  $h(q-k, k)/T_q \leq e^{-\xi^2/2}$  is needed, and the contribution of the entire tail is  $O(1/\sqrt{\log q})$ .

*Proof.* By Stirling on factorials and Wright on  $T_q, T_{q-2k}$ , then Taylor expanding in  $\xi = k/\sqrt{q}$ , the leading  $q \log q$ ,  $\xi \sqrt{q} \log q$ ,  $\xi \sqrt{q}$ ,  $\frac{1}{2} \log q$  contributions all cancel (forced by  $h(q-k, k)/T_q \leq 1$ ). What survives is

$$\log \frac{h(q-k, k)}{T_q} = -\frac{\xi^2}{2} - 2\xi + \frac{P(\xi)}{\sqrt{q}} + O\left(\frac{\xi^4 + 1}{q}\right) + O(q^{-1/2}), \quad P(\xi) := -\frac{\xi^3}{2} - \xi^2 + \frac{\xi}{2}$$

Exponentiation on the boundary layer ( $\xi \leq \sqrt{\log q}$ ) yields (18). For the tail ( $\sqrt{q \log q} < k \leq q/2$ ): splitting at  $\xi = q^{1/4}$ , both the Taylor truncation regime ( $\xi \leq q^{1/4}$ ) and the non-truncated entropy regime ( $\xi > q^{1/4}$ , using  $E(u) := (1-u) \log(1-u) - \frac{1-2u}{2} \log(1-2u) \leq -u^2/2$  for  $u \in [0, 1/2)$ , proved by series expansion in §A.2) give  $h(q-k, k)/T_q \leq e^{-\xi^2/2}$  uniformly; the boundary endpoint  $k = \lfloor q/2 \rfloor$  is  $\leq 2^{-q/2} e^{O(\sqrt{q})}$  by direct Stirling+Wright. Riemann summation + Mills ratio yield  $\sum_{\sqrt{q \log q} < k < q/2} h(q-k, k)/T_q \leq 2/\sqrt{\log q}$ .

Full Stirling+Wright bookkeeping for both regimes is in §A.1–§A.2.  $\square$

Table 8: Numerical verification of Lemma 9 (boundary-layer profile) at five representative  $k$  for each  $q \in \{10, 100, 1000, 10000\}$ . “Exact” is  $h(q - k, k)/T_q = k! \binom{q-k}{k} T_{q-2k}/T_q$  in exact rational arithmetic; “Profile” is  $e^{-\xi^2/2-2\xi}$  with  $\xi = k/\sqrt{q}$ ; “Ratio” is Exact/Profile (should approach 1 on the boundary layer  $\xi \leq \sqrt{\log q}$ , and diverges from 1 outside it since the true decay is faster than  $e^{-\xi^2/2-2\xi}$ ). The middle column  $k = \lfloor \sqrt{q \log q} \rfloor$  is the upper boundary of the layer where Lemma 9 guarantees  $(1 + O((\xi^3 + 1)/\sqrt{q}))$  accuracy. Entries written as “ $< 10^{-300}$ ” indicate underflow below `float64` range; the corresponding Ratio is reported as “ $\approx 0$ ” rather than computed.

$q$	$k$	$\xi$	Exact	Profile	Ratio
10	0	0.0000	1.0000	1.0000	1.0000
10	1	0.3162	$5.2585 \times 10^{-1}$	$5.0537 \times 10^{-1}$	1.0405
10	4	1.2649	$1.4621 \times 10^{-2}$	$3.5799 \times 10^{-2}$	0.4084
10	4	$(\lfloor \sqrt{q \log q} \rfloor = 4)$			
10	5	1.5811	$9.7475 \times 10^{-4}$	$1.2128 \times 10^{-2}$	0.0804
100	0	0.0000	1.0000	1.0000	1.0000
100	1	0.1000	$8.1855 \times 10^{-1}$	$8.1465 \times 10^{-1}$	1.0048
100	21	2.1000	$6.0174 \times 10^{-4}$	$1.6533 \times 10^{-3}$	0.3640
100	21	$(\lfloor \sqrt{q \log q} \rfloor = 21)$			
100	49	4.9000	$1.4706 \times 10^{-20}$	$3.3901 \times 10^{-10}$	$\approx 0$
100	50	5.0000	$1.1534 \times 10^{-22}$	$1.6919 \times 10^{-10}$	$\approx 0$
1000	0	0.0000	1.0000	1.0000	1.0000
1000	1	0.0316	$9.3871 \times 10^{-1}$	$9.3824 \times 10^{-1}$	1.0005
1000	83	2.6247	$1.0114 \times 10^{-4}$	$1.6761 \times 10^{-4}$	0.6034
1000	83	$(\lfloor \sqrt{q \log q} \rfloor = 83)$			
1000	499	15.78	$< 10^{-300}$	$< 10^{-50}$	$\approx 0$
1000	500	15.81	$< 10^{-300}$	$< 10^{-50}$	$\approx 0$
10000	0	0.0000	1.0000	1.0000	1.0000
10000	1	0.0100	$9.8020 \times 10^{-1}$	$9.8015 \times 10^{-1}$	1.0000
10000	303	3.0300	$1.8959 \times 10^{-5}$	$2.3690 \times 10^{-5}$	0.8003
10000	303	$(\lfloor \sqrt{q \log q} \rfloor = 303)$			
10000	4999	49.99	$< 10^{-300}$	$< 10^{-300}$	–
10000	5000	50.00	$< 10^{-300}$	$< 10^{-300}$	–

*Reading the table.* For each  $q$ , the ratio  $\rightarrow 1$  as  $k \rightarrow 0$  (small  $\xi$ , well inside the boundary layer where  $(\xi^3 + 1)/\sqrt{q}$  is negligible), starts departing as  $\xi$  approaches  $\sqrt{\log q}$  (the  $O((\xi^3 + 1)/\sqrt{q})$  correction becomes visible), and collapses far outside the layer as the true profile decays faster than  $e^{-\xi^2/2-2\xi}$  (cf. the entropy-function bound in the “outside-the-boundary-layer” part of the proof of Lemma 9). For  $k \in \{q/2 - 1, q/2\}$ , both Exact and Profile are sub-poly small, so their numerical ratio is dominated by arithmetic precision; the multiplicative form  $h(q - k, k)/T_q \leq e^{-\xi^2/2}$  is what is actually used in Lemma 9’s tail bound, and it holds with room to spare.

### The diagonal asymptotic — a shared engine

Both  $S_j$  (§6, leading to  $P_{\text{nodes}}$ ) and  $S_j^{(k)}$  (§9, leading to  $W(n, q)$  for  $n \geq 2$ ) reduce to a sum over the diagonal  $\{a = 0\}$  of the  $(a, k)$ -triangle, scaled by a power of  $k$ . We isolate the shared analytical work in one lemma below.

**Lemma 10** (Diagonal asymptotic). *For each fixed integer  $j \geq 1$  and  $\alpha \in \{0, 1\}$ ,*

$$\sum_{k \geq 1} k^\alpha \left[ \frac{h(q - k, k)}{T_q} \right]^j = q^{(\alpha+1)/2} M_\alpha^{(j)} - \mathbf{1}[\alpha = 0] \cdot \frac{1}{2} + q^{\alpha/2} j \int_0^\infty \xi^\alpha P(\xi) e^{-j\xi^2/2 - 2j\xi} d\xi + O(q^{(\alpha-1)/2}), \quad (19)$$

where  $P(\xi) := -\xi^3/2 - \xi^2 + \xi/2$  is the profile correction from Lemma 9 and the moments are

$$M_n^{(j)} := \int_0^\infty \xi^n e^{-j\xi^2/2-2j\xi} d\xi, \quad M_0^{(j)} = c_j, \quad M_1^{(j)} = \frac{1}{j} - 2c_j.$$

*Proof.* Inside the boundary layer ( $1 \leq k \leq \sqrt{q \log q}$ ), Lemma 9 gives, with  $\xi = k/\sqrt{q}$ ,

$$[h(q-k, k)/T_q]^j = e^{-j\xi^2/2-2j\xi} \left[ 1 + \frac{jP(\xi)}{\sqrt{q}} + O((\xi^6 + 1)/q) \right].$$

The contribution beyond the boundary layer is super-polynomially small (again Lemma 9, tail bound). Apply Euler–Maclaurin (trapezoidal rule with step  $\Delta\xi = 1/\sqrt{q}$ ) to  $\sum_{k \geq 0} k^\alpha e^{-j\xi_k^2/2-2j\xi_k}$ . Since  $k = \sqrt{q} \xi_k$ , the integrand at  $\xi = 0$  has value  $\mathbf{1}[\alpha = 0]$ :

$$\sum_{k \geq 0} k^\alpha e^{-j\xi_k^2/2-2j\xi_k} = q^{(\alpha+1)/2} \int_0^\infty \xi^\alpha e^{-j\xi^2/2-2j\xi} d\xi + \frac{1}{2} \mathbf{1}[\alpha = 0] + O(q^{(\alpha-1)/2}).$$

The first term is  $q^{(\alpha+1)/2} M_\alpha^{(j)}$ . The multiplicative  $jP(\xi)/\sqrt{q}$  correction contributes

$$q^{\alpha/2} j \int_0^\infty \xi^\alpha P(\xi) e^{-j\xi^2/2-2j\xi} d\xi + O(q^{(\alpha-1)/2})$$

(the trapezoidal endpoint at  $\xi = 0$  vanishes since  $P(0) = 0$ ).

The unified  $O(q^{(\alpha-1)/2})$  remainder absorbs three sources, each of that order: (i) the second-order Euler–Maclaurin endpoint term  $(\Delta\xi/12) \cdot f'(0) \cdot q^{\alpha/2}$  where  $\Delta\xi = 1/\sqrt{q}$ ; (ii) the boundary-layer-tail contribution  $\sum_{k > \sqrt{q \log q}}$ , which by Mills' ratio gives  $O(q^{\alpha/2}/\sqrt{\log q})$ , in particular  $O(q^{(\alpha-1)/2})$  for any fixed power; and (iii) the  $O((\xi^3 + 1)/\sqrt{q})$  multiplicative profile error from Lemma 9, which contributes  $q^{\alpha/2} \cdot O(1/\sqrt{q}) = O(q^{(\alpha-1)/2})$  after integration. Subtracting the  $k = 0$  term (value  $\mathbf{1}[\alpha = 0]$ ) yields (19).  $\square$

**Remark 11.** Specialisation to  $\alpha = 0$  gives  $\Sigma_{a=0}^{(0)} = c_j \sqrt{q} - \frac{1}{2} + j \int P e^{-j\xi^2/2-2j\xi} d\xi + o(1)$  (used in Lemma 12). Specialisation to  $\alpha = 1$  gives  $\Sigma_{a=0}^{(1)} = qM_1^{(j)} + \sqrt{q} j \int \xi P e^{-j\xi^2/2-2j\xi} d\xi + o(\sqrt{q})$  (used in Lemma 18). The two profile integrals evaluate via the moment recurrence  $M_{n+1}^{(j)} = nM_{n-1}^{(j)}/j - 2M_n^{(j)}$  (using  $[\xi^n e^{-j\xi^2/2-2j\xi}]_0^\infty = 0$  for  $n \geq 1$ ):

$$\begin{aligned} j \int_0^\infty P(\xi) e^{-j\xi^2/2-2j\xi} d\xi &= \frac{j-2}{2} M_1^{(j)}, \\ j \int_0^\infty \xi P(\xi) e^{-j\xi^2/2-2j\xi} d\xi &= \frac{(j-3)[(4j+1)c_j - 2]}{2j}. \end{aligned}$$

**Lemma 12** (Leading asymptotic of  $S_j$ ). *For each integer  $j \geq 2$ , as  $q \rightarrow \infty$ ,*

$$S_j(q) = c_j \sqrt{q} + \text{const}_j + O(q^{-1/2}), \quad c_j := \int_0^\infty e^{-(j/2)\xi^2-2j\xi} d\xi. \quad (20)$$

*Numerically,  $c_1 \approx 0.42136923$ ,  $c_2 \approx 0.22634$ ,  $c_3 \approx 0.15530$ ,  $c_4 \approx 0.11833$ ; the constants  $\text{const}_j$  are also explicit:*

$$\text{const}_2 = \frac{3}{2} - 4c_2 \approx 0.5946, \quad \text{const}_j = \frac{1}{2} + \frac{j-2}{2} M_1^{(j)} = \frac{1}{2} + \frac{j-2}{2} \left( \frac{1}{j} - 2c_j \right) \quad \text{for } j \geq 3,$$

*where  $M_1^{(j)} := \int_0^\infty \xi e^{-(j/2)\xi^2-2j\xi} d\xi = 1/j - 2c_j$ . Numerically:  $\text{const}_3 \approx 0.5114$ ,  $\text{const}_4 \approx 0.5133$ ,  $\text{const}_5 \approx 0.5132$ . The remainder beyond  $c_j \sqrt{q} + \text{const}_j$  is  $O(q^{-1/2})$  for all  $j \geq 2$ .*

*Proof of Lemma 12.* The proof reduces, via the boundary-layer profile (Lemma 9), to a Riemann sum plus an explicit accounting of off-diagonal slices.

*Setup.* By the second equality of (5), with the closed forms  $f(l, k) = \binom{l}{k} T_{l-k}$  (Lemma 2) and  $h(q-l, k) = k! \binom{q-l}{k} T_{q-l-k}$  (Lemma 3), reparametrise the  $(l, k)$  sum by  $a := l - k \geq 0$  (so  $l = a + k$ ,  $q - l - k = q - a - 2k$ ):

$$S_j(q) - 1 = \sum_{\substack{a, k \geq 0 \\ a+2k \leq q \\ (a, k) \neq (0, 0)}} \binom{a+k}{k} T_a \left[ \frac{k! \binom{q-a-k}{k} T_{q-a-2k}}{T_q} \right]^j. \quad (21)$$

We split the sum by  $a$ : *diagonal* ( $a = 0$ ),  $k = 0$  *column*, and *off-diagonal slices* ( $a, k \geq 1$ ).

*Diagonal*  $a = 0, k \geq 1$ . On  $a = 0$ ,  $\binom{k}{k} T_0 = 1$ , and the summand is  $[h(q-k, k)/T_q]^j$ . Apply Lemma 10 with  $\alpha = 0$  and substitute the profile integral evaluation  $j \int P e^{-j\xi^2/2 - 2j\xi} d\xi = (j-2)M_1^{(j)}/2$  from Remark 11:

$$\Sigma_{a=0} := \sum_{k \geq 1} \left[ \frac{h(q-k, k)}{T_q} \right]^j = c_j \sqrt{q} - \frac{1}{2} + \frac{j-2}{2} M_1^{(j)} + o(1), \quad (22)$$

which is  $c_j \sqrt{q} - \frac{1}{2} + o(1)$  for  $j = 2$  and  $c_j \sqrt{q} - \frac{1}{2} + \frac{j-2}{2}(1/j - 2c_j) + o(1)$  for  $j \geq 3$ .

$k = 0$  *column* ( $a \geq 1$ ). On  $k = 0$ ,  $\binom{a}{0} T_a = T_a$  and  $h(q-a, 0)/T_q = T_{q-a}/T_q$ . Directly from Wright's asymptotic (15),  $\log(T_{q-a}/T_q) = \frac{q-a}{2} \log(q-a) - \frac{q}{2} \log q + (a/2) + 2(\sqrt{q-a} - \sqrt{q}) + O(1) = -(a/2) \log q + O(1)$ , so  $T_{q-a}/T_q = O(q^{-a/2})$  uniformly for each fixed  $a$ . Hence

$$\Sigma_{k=0} := \sum_{a \geq 1} T_a [T_{q-a}/T_q]^j = O(q^{-j/2}),$$

since the  $a = 1$  term dominates ( $T_1 \cdot q^{-j/2} = 2q^{-j/2}$ ),  $a = 2$  contributes  $O(q^{-j})$ , and higher  $a$  even less. So for  $j \geq 2$ ,  $\Sigma_{k=0} = o(1)$ .

*Off-diagonal*  $a = 1, k \geq 1$ . With  $\binom{1+k}{k} T_1 = 2(k+1)$ , the  $a = 1$  summand is  $2(k+1) \cdot [h(q-1-k, k)/T_q]^j$ . Factor through size  $q-1$ :  $h(q-1-k, k)/T_q = \rho(q) \cdot h(q-1-k, k)/T_{q-1}$ , where the inner ratio is the size- $(q-1)$  profile (apply Lemma 9 at size  $q-1$ ). Apply Lemma 10 at size  $q-1$  with  $\alpha = 1$  then  $\alpha = 0$ :

$$\sum_{k \geq 1} (k+1) \left[ \frac{h(q-1-k, k)}{T_{q-1}} \right]^j = q M_1^{(j)} + c_j \sqrt{q} + O(\sqrt{q} + q^{(1-j)/2}) = q M_1^{(j)} + O(\sqrt{q}),$$

using  $M_1^{(j)} = 1/j - 2c_j$  from Remark 11. Multiplying by  $2\rho(q)^j = 2q^{-j/2}(1 + O(q^{-1/2}))$ :

$$\Sigma_{a=1} = 2M_1^{(j)} \cdot q^{1-j/2} + O(q^{(1-j)/2}). \quad (23)$$

For  $j = 2$ :  $\Sigma_{a=1} = 2M_1^{(2)} + o(1) = 1 - 4c_2 + o(1)$ . For  $j \geq 3$ :  $\Sigma_{a=1} = o(1)$ .

*Off-diagonal*  $a \geq 2, k \geq 1$ . By the same  $T_{q-a}/T_q$  factoring,  $[h(q-a-k, k)/T_q]^j = \rho(q)^{aj} \cdot [h(q-a-k, k)/T_{q-a}]^j (1 + o(1))$  on the boundary layer. So  $\Sigma_{a \geq 2} = O(q^{(a+1-aj)/2})$  summed over  $a \geq 2$ ; the dominant  $a = 2$  term is  $O(q^{(3-2j)/2})$ , which for  $j \geq 2$  is  $O(q^{-1/2}) = o(1)$ .

*Combining.*  $S_j(q) - 1 = \Sigma_{a=0} + \Sigma_{k=0} + \Sigma_{a=1} + \Sigma_{a \geq 2}$ . With (22),  $\Sigma_{k=0} = o(1)$ ,  $\Sigma_{a \geq 2} = o(1)$ , and (23):

- For  $j \geq 3$ : the  $a = 1$  slice is  $o(1)$ , so

$$S_j(q) = 1 + c_j \sqrt{q} - \frac{1}{2} + \frac{j-2}{2} M_1^{(j)} + o(1) = c_j \sqrt{q} + \frac{1}{2} + \frac{j-2}{2} M_1^{(j)} + o(1),$$

$$\text{i.e., } \text{const}_j = \frac{1}{2} + \frac{j-2}{2} M_1^{(j)} = \frac{1}{2} + \frac{j-2}{2}(1/j - 2c_j).$$

- For  $j = 2$ : the diagonal correction vanishes ( $(j-2)/2 = 0$ ), and the  $a = 1$  slice contributes  $1 - 4c_2$ :

$$S_2(q) = 1 + c_2\sqrt{q} - \frac{1}{2} + 0 + (1 - 4c_2) + o(1) = c_2\sqrt{q} + \frac{3}{2} - 4c_2 + o(1),$$

$$\text{i.e., } \text{const}_2 = \frac{3}{2} - 4c_2.$$

This completes the proof.  $\square$

Table 9: Exact  $S_j(q)$  vs. a leading two-term estimate “est” =  $c_j\sqrt{q} + \text{const}$ , where  $\text{const} = 3/2 - 4c_2$  for  $j = 2$  (the full  $\text{const}_2$  from Lemma 12) and  $\text{const} = 1/2$  for  $j \geq 3$  (the leading  $\Sigma_{a=0} + (a, k) = (0, 0)$  contribution alone, omitting the refinement  $\frac{j-2}{2}M_1^{(j)}$  which is  $\approx 0.011$  for  $j = 3$  and  $\approx 0.013$  for  $j = 4$  — this refinement appears as the dominant  $O(1)$  part of the residual  $S_j(q) - \text{est}$ ). Also shown: the contributions of five disjoint cells of the  $(a, k)$ -triangle (which sum to  $S_j(q) - 1$ ):  $\Sigma_{a=0,1,2}$  are the rows  $a \in \{0, 1, 2\}$  within  $\{a + 2k \leq q/2\}$  (these are the dominant boundary-layer terms);  $\Sigma_{a \geq 3}$  collects rows  $a \geq 3$  within  $\{a + 2k \leq q/2\}$ ;  $\Sigma_{a+2k > q/2}$  collects everything in the upper half of the triangle (bulk + large- $a$  tail). Computed in log-space float64 via the  $T$ -recurrence and Lemmas 2, 3; all 12 row sums verify  $(S_j(q) - 1) = \Sigma_{a=0} + \Sigma_{a=1} + \Sigma_{a=2} + \Sigma_{a \geq 3} + \Sigma_{a+2k > q/2}$ .

$q$	$j$	$S_j(q)$	Est	$\Sigma_{a=0}$	$\Sigma_{a=1}$	$\Sigma_{a=2}$	$\Sigma_{a \geq 3}$	$\Sigma_{a+2k > q/2}$
10	2	1.56091	1.31039	0.32804	0.18430	0.02914	$6.74 \times 10^{-3}$	$1.27 \times 10^{-2}$
10	3	1.19325	0.99111	0.15710	0.03428	0.00134	$6.92 \times 10^{-5}$	$4.56 \times 10^{-4}$
10	4	1.08640	0.87418	0.07912	0.00719	0.00007	$8.54 \times 10^{-7}$	$2.96 \times 10^{-5}$
100	2	2.93159	2.85803	1.80424	0.12079	0.00619	$3.62 \times 10^{-4}$	$2.64 \times 10^{-9}$
100	3	2.12538	2.05304	1.11894	0.00642	0.00002	$9.64 \times 10^{-8}$	$2.43 \times 10^{-14}$
100	4	1.76612	1.68326	0.76571	0.00041	0.00000	$3.78 \times 10^{-11}$	$4.95 \times 10^{-19}$
1000	2	7.77488	7.75210	6.67068	0.10257	0.00161	$2.74 \times 10^{-5}$	$\sim 0$
1000	3	5.44180	5.41114	4.44018	0.00162	0.00000	$2.20 \times 10^{-10}$	$\sim 0$
1000	4	4.27764	4.24180	3.27761	0.00003	0.00000	$2.59 \times 10^{-15}$	$\sim 0$
10000	2	23.23565	23.22850	22.13806	0.09711	0.00048	$2.50 \times 10^{-6}$	$\sim 0$
10000	3	16.04785	16.03039	15.04738	0.00047	0.00000	$6.20 \times 10^{-13}$	$\sim 0$
10000	4	12.35312	12.33262	11.35312	0.00000	0.00000	$2.25 \times 10^{-19}$	$\sim 0$
100000	2	72.17143	72.16917	71.07586	0.09542	0.00015	$2.43 \times 10^{-7}$	$\sim 0$
100000	3	49.62469	49.61140	48.62455	0.00015	0.00000	$1.89 \times 10^{-15}$	$\sim 0$
100000	4	37.93364	37.91803	36.93364	0.00000	0.00000	$2.15 \times 10^{-23}$	$\sim 0$

## 7 Combined: $P_{\text{nodes}}$

**Theorem 13** ( $P_{\text{nodes}}$ , four-term expansion). *For every integer  $n \geq 1$ , as  $q \rightarrow \infty$ ,*

$$P_{\text{nodes}}(n, q) = nq + (n-1) - c_n^* \sqrt{q} - d_n^* + O(q^{-1/2}), \quad (24)$$

where

$$c_n^* := \sum_{j=2}^n (-1)^j \binom{n}{j} c_j = \int_0^\infty [(1 - \varphi(\xi))^n + n\varphi(\xi) - 1] d\xi, \quad (25)$$

$$d_n^* := \sum_{j=2}^n (-1)^j \binom{n}{j} \text{const}_j, \quad (26)$$

in perfect symmetry with  $c_n^*$ , so that the  $\sqrt{q}$  and  $O(1)$  corrections combine to  $c_n^*\sqrt{q} + d_n^* = \sum_{j=2}^n (-1)^j \binom{n}{j} (c_j\sqrt{q} + \text{const}_j)$ , with  $\varphi(\xi) := \exp(-\xi^2/2 - 2\xi)$  and  $c_j, \text{const}_j$  from Lemma 12. The  $j = 2$  case is anomalous: the off-diagonal  $a = 1$  slice contributes at the same order and gives  $\text{const}_2 = 3/2 - 4c_2$  rather than the naive  $j = 2$  value  $1/2$  from the general formula. The  $O(q^{-1/2})$  remainder is inherited from the worst-case ( $j = 2$ ) residual in Lemma 12; at  $n = 1$  it vanishes identically because  $P_{\text{nodes}}(1, q) = q$  exactly. The first two coefficients  $nq$  and  $(n-1)$  are exact (from the keystone identity at every level and from  $\sum_{j=2}^n (-1)^j \binom{n}{j} = n-1$ ); the  $-c_n^*\sqrt{q}$  correction reflects the boundary-layer prefix-coincidence effect; the constant  $-d_n^*$  absorbs the sub-leading  $\text{const}_j$  contributions hidden inside the original  $O(1)$  remainder.

*Proof.* Combine Theorem 6

$$P_{\text{nodes}}(n, q) = nq + (n-1) - \sum_{j=2}^n (-1)^j \binom{n}{j} S_j(q)$$

with the three-term expansion  $S_j(q) = c_j\sqrt{q} + \text{const}_j + R_j(q)$  (Lemma 12, where  $R_j(q) = O(q^{-1/2})$  for  $j \in \{2, 3\}$  and  $O(q^{(2-j)/2})$  for  $j \geq 4$ ; both  $j = 2$  and  $j = 3$  give the same  $q^{-1/2}$  rate,  $j \geq 4$  strictly faster). Substituting:

$$\begin{aligned} P_{\text{nodes}}(n, q) &= nq + (n-1) \\ &\quad - \sqrt{q} \sum_{j=2}^n (-1)^j \binom{n}{j} c_j \\ &\quad - \sum_{j=2}^n (-1)^j \binom{n}{j} \text{const}_j \\ &\quad - \sum_{j=2}^n (-1)^j \binom{n}{j} R_j(q), \end{aligned}$$

which identifies the three coefficient sums as  $-c_n^*\sqrt{q}$ ,  $-d_n^*$ , and  $-R_n(q)$ . The dominant residual comes from  $j \in \{2, 3\}$  both at rate  $O(q^{-1/2})$  (with  $j \geq 4$  contributing  $O(q^{(2-j)/2})$ , strictly faster).

*Integral form for  $c_n^*$ .* By Lemma 12,  $c_j = \int_0^\infty \varphi(\xi)^j d\xi$  with  $\varphi(\xi) = e^{-\xi^2/2 - 2\xi}$ . Interchange sum and integral (the sum is finite, no convergence issue):

$$c_n^* = \sum_{j=2}^n (-1)^j \binom{n}{j} \int_0^\infty \varphi^j d\xi = \int_0^\infty \left[ \sum_{j=2}^n (-1)^j \binom{n}{j} \varphi^j \right] d\xi.$$

The bracketed sum is the binomial  $(1-\varphi)^n = \sum_{j=0}^n (-1)^j \binom{n}{j} \varphi^j$  with the  $j = 0, 1$  terms removed:

$$\sum_{j=2}^n (-1)^j \binom{n}{j} \varphi^j = (1-\varphi)^n - \underbrace{\binom{n}{0}}_{=1} + \underbrace{\binom{n}{1}\varphi}_{=n\varphi} = (1-\varphi)^n + n\varphi - 1.$$

Substituting back yields the integral form  $c_n^* = \int_0^\infty [(1-\varphi)^n + n\varphi - 1] d\xi$  recorded in (25). Split:  $c_n^* = n c_1 + \int_0^\infty [(1-\varphi)^n - 1] d\xi$ . On the second integrand,  $(1-\varphi)^n \rightarrow 0$  when  $n\varphi \gg 1$  and  $(1-\varphi)^n \rightarrow 1$  when  $n\varphi \ll 1$ . The crossover happens at  $\varphi(\xi^*) = (\log 2)/n$ , i.e. at the solution of  $\xi^{*2}/2 + 2\xi^* = \log n - \log \log 2$ ; since the quadratic term dominates for large  $n$ ,  $\xi^* = \sqrt{2 \log n} - 2 + O((\log n)^{-1/2})$ . Hence

$$\int_0^\infty [(1-\varphi)^n - 1] d\xi = -\xi^* + O(1) = -\sqrt{2 \log n} + O(1),$$

giving  $c_n^* = n c_1 - \sqrt{2 \log n} + O(1)$  as  $n \rightarrow \infty$  —  $c_n^*$  grows *linearly* in  $n$  with slope  $c_1 \approx 0.42136923$ , shifted down by a  $\sqrt{2 \log n}$  correction. Numerically at  $n = 1000$ :  $1000 c_1 - \sqrt{2 \log 1000} \approx 417.65$  versus actual  $c_{1000}^* \approx 419.02$  (consistent with an  $O(1)$  residual  $\approx 1.4$ ).

*Derivation of the closed form (26).* By Lemma 12,  $\text{const}_j = \frac{1}{2} + \frac{j-2}{2} M_1^{(j)}$  for  $j \geq 3$  (and the same formula at  $j = 2$  would give  $\frac{1}{2}$ ; the actual  $\text{const}_2 = \frac{3}{2} - 4c_2$  differs by the  $a = 1$  off-diagonal contribution  $1 - 4c_2$ ). Separating out  $j = 2$ :

$$d_n^* = \binom{n}{2} \text{const}_2 + \sum_{j=3}^n (-1)^j \binom{n}{j} \left( \frac{1}{2} + \frac{j-2}{2} M_1^{(j)} \right).$$

which is precisely the symmetric form (26). For  $n = 3$  this evaluates to  $d_3^* = 3 \text{const}_2 - \text{const}_3 = 3(\frac{3}{2} - 4c_2) - (\frac{2}{3} - c_3) = \frac{23}{6} - 12c_2 + c_3 \approx 1.273$ .  $\square$

Table 10: Verification of Theorem 13 for  $n = 1, 2, 3$  and  $q = 10, 100, 1000, 10000$ . “Exact” is computed via Theorem 6  $P_{\text{nodes}}(n, q) = nq + (n-1) - \sum_{j=2}^n (-1)^j \binom{n}{j} S_j(q)$  with  $S_j$  from the brute-force  $(a, k)$  sum (Table 9). “Est” is  $nq + (n-1) - c_n^* \sqrt{q} - d_n^*$ . The residual Exact – Est decays at rate  $O(q^{-1/2})$  as expected. For  $n = 1$  the columns  $c_n^*$  and  $d_n^*$  are 0 by convention (the empty sums  $\sum_{j=2}^1$ ).

$n$	$q$	$P_{\text{nodes}}(n, q)$	exact	est	residual	$c_n^*$	$d_n^*$
1	10		10.00000	10.00000	0.00000	0	0
1	100		100.00000	100.00000	0.00000	0	0
1	1000		1000.00000	1000.00000	0.00000	0	0
1	10000		10000.00000	10000.00000	0.00000	0	0
2	10		19.43909	19.68961	-0.25052	0.22634	0.59465
2	100		198.06841	198.14197	-0.07356	0.22634	0.59465
2	1000		1993.22512	1993.24790	-0.02278	0.22634	0.59465
2	10000		19977.76435	19977.77150	-0.00716	0.22634	0.59465
3	10		28.51051	29.07122	-0.56071	0.52371	1.27258
3	100		295.33062	295.49032	-0.15970	0.52371	1.27258
3	1000		2984.11716	2984.16639	-0.04923	0.52371	1.27258
3	10000		29948.34089	29948.35642	-0.01553	0.52371	1.27258

*Coefficients used.*  $c_2 \approx 0.22634$ ,  $c_3 \approx 0.15530$ . Then

$$c_2^* = c_2, \quad c_3^* = 3c_2 - c_3 \approx 0.52371,$$

$$d_2^* = \text{const}_2 \approx 0.59465, \quad d_3^* = 3 \text{const}_2 - \text{const}_3 = \frac{23}{6} - 12c_2 + c_3 \approx 1.27258,$$

using  $\text{const}_3 = \frac{1}{2} + \frac{1}{2}(\frac{1}{3} - 2c_3) = \frac{2}{3} - c_3 \approx 0.51136$ . The residuals shrink by  $\sqrt{10}$  each time  $q$  scales by 10, confirming the  $O(q^{-1/2})$  rate of  $R_n(q)$ .

## 8 Combined: $P_{\text{ptr}}(1, q)$

By Theorem 7,

$$P_{\text{ptr}}(n, q) = 3P_{\text{nodes}}(n, q) + 3 + W(n, q) + R(n, q),$$

where the general formulas are

$$W(n, q) = \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} S_j^{(k)}(q), \quad R(n, q) = \mathbf{E} \left[ \sum_{p \in \text{Trie}} r_p \right]$$

with  $r_p \in \{-3, -1, 0\}$  the per-node correction from (1). For  $n = 1$ , each piece simplifies:

- $P_{\text{nodes}}(1, q) = q$  is exact (one key gives a path of  $q$  distinct prefixes; Theorem 13 at  $n = 1$ ).
- $W(1, q) = \binom{1}{1} S_1^{(k)}(q) = S_1^{(k)}(q)$ , which has the exact closed form (Lemma 5):

$$W(1, q) = S_1^{(k)}(q) = \frac{T_{q-2}}{T_q} \cdot \frac{q^3 - q}{6}.$$

- $R(1, q)$  has the exact closed form (Proposition 8):

$$R(1, q) = - \sum_{c=0}^{\lfloor (q-1)/2 \rfloor} \binom{q-1-c}{c} T_{q-1-2c} \frac{2(c+1)!}{T_q} - 3 \sum_{c=0}^{\lfloor q/2 \rfloor} \binom{q-c}{c} T_{q-2c} \frac{c!}{T_q},$$

the first sum from the  $\text{TMS}_l = q-1-l$  boundary line ( $r_p = -1$ ) and the second from  $\text{TMS}_l = q-l$  ( $r_p = -3$ ).

All the asymptotic content of  $P_{\text{ptr}}(1, q)$  is therefore captured by the expansions of  $W(1, q)$  (Lemma 14 below) and of  $R(1, q)$  (Lemma 15).

**Lemma 14** (Asymptotic of  $W(1, q)$ ). *As  $q \rightarrow \infty$ ,*

$$W(1, q) = S_1^{(k)}(q) = \frac{q^2}{6} - \frac{q^{3/2}}{3} + \frac{q}{2} - \frac{7\sqrt{q}}{12} + \frac{5}{12} + O(q^{-1/2}). \quad (27)$$

*Proof.* By Lemma 5,  $W(1, q) = S_1^{(k)}(q) = \frac{q^3 - q}{6} \cdot \frac{T_{q-2}}{T_q}$ , so the proof reduces to expanding  $T_{q-2}/T_q$  to five orders. Setting  $\rho(q) := T_{q-1}/T_q$ , division of the recurrence  $T_q = 2T_{q-1} + (q-1)T_{q-2}$  by  $T_q$  gives

$$\rho(q)[2 + (q-1)\rho(q-1)] = 1, \quad \frac{T_{q-2}}{T_q} = \frac{1 - 2\rho(q)}{q-1}. \quad (28)$$

Wright's asymptotic guarantees  $\rho(q)$  has a full asymptotic series  $\rho(q) = \sum_{k \geq 1} a_k q^{-k/2}$ , and (28) identifies the coefficients via dominant-balance coefficient matching. The computation (see §A.5) gives

$$\begin{aligned} \rho(q) &= q^{-1/2} - q^{-1} + \frac{3}{4}q^{-3/2} - \frac{1}{4}q^{-2} - \frac{7}{32}q^{-5/2} + O(q^{-3}), \\ \frac{T_{q-2}}{T_q} &= \frac{1}{q} - \frac{2}{q^{3/2}} + \frac{3}{q^2} - \frac{7}{2q^{5/2}} + \frac{7}{2q^3} + O(q^{-7/2}). \end{aligned}$$

Multiplying  $T_{q-2}/T_q$  by  $(q^3 - q)/6$ : the  $q^0$  term comes from  $(q^3/6) \cdot (7/2)q^{-3} - (q/6) \cdot q^{-1} = 7/12 - 1/6 = 5/12$ , yielding (27).  $\square$

Table 11: Verification of Lemma 14 for  $q \in \{10, 100, 1000, 10000\}$ . “Exact” is  $W(1, q) = \frac{q^3 - q}{6} \cdot T_{q-2}/T_q$  computed in exact rational arithmetic. “Est” is the four-term estimate  $q^2/6 - q^{3/2}/3 + q/2 - 7\sqrt{q}/12$  (without the  $+5/12$  constant). The residual Exact – Est converges to  $5/12 \approx 0.4167$ , the explicit  $O(1)$  constant of (27).

$q$	$W(1, q)$ exact	est (4-term)	residual
10	9.640603	9.281079	0.359524
100	1,377.898643	1,377.500000	0.398643
1000	156,607.705541	156,607.294513	0.411028
10000	16,338,275.414892	16,338,275.000000	0.414892

**Lemma 15** (Asymptotic of  $R(1, q)$ ). *As  $q \rightarrow \infty$ ,*

$$R(1, q) = (c_1 - 2)\sqrt{q} + (c_1 - 2) + O(q^{-1/2}), \quad (29)$$

where  $c_1 := \int_0^\infty e^{-\xi^2/2 - 2\xi} d\xi \approx 0.42136923$ .

*Proof.* By Proposition 8,  $R(1, q) = -B_1^{(1)}(q) - 3B_1^{(0)}(q)$  where

$$B_1^{(0)}(q) = \sum_{k=0}^{\lfloor q/2 \rfloor} \frac{h(q-k, k)}{T_q}, \quad B_1^{(1)}(q) = 2 \sum_{k=0}^{\lfloor (q-1)/2 \rfloor} \frac{(k+1)h(q-1-k, k)}{T_q}.$$

*Asymptotic of  $B_1^{(0)}$ .* The  $k=0$  term equals 1; for  $k \geq 1$ , apply Lemma 10 at  $j=1, \alpha=0$  and Remark 11 (giving  $j \int P e^{-\xi^2/2-2\xi} d\xi = -M_1^{(1)}/2 = -(1-2c_1)/2$  at  $j=1$ ):

$$\sum_{k \geq 1} h(q-k, k)/T_q = c_1 \sqrt{q} - \frac{1}{2} - \frac{1-2c_1}{2} + o(1) = c_1 \sqrt{q} + O(1).$$

Tracking the constant explicitly, the  $k=0$  contribution gives +1, the Euler–Maclaurin boundary half-correction at  $k=0$  gives  $-1/2$ , and the profile sub-leading  $P(\xi)/\sqrt{q}$  integrated against  $e^{-\xi^2/2-2\xi}$  multiplied by  $\sqrt{q}$  gives  $\int_0^\infty P(\xi) e^{-\xi^2/2-2\xi} d\xi = -(1-2c_1)/2 \cdot 1 = c_1 - 1/2$  (using  $M_1^{(1)} = 1 - 2c_1$  and the Remark 11 identity at  $j=1$ ). Summing:  $1 - 1/2 + (c_1 - 1/2) = c_1$ , so

$$B_1^{(0)}(q) = c_1 \sqrt{q} + c_1 + o(1). \quad (30)$$

*Asymptotic of  $B_1^{(1)}$ .* Factor  $h(q-1-k, k)/T_q = \rho(q) \cdot h(q-1-k, k)/T_{q-1}$ , where the inner ratio is the size- $(q-1)$  profile (Lemma 9 at size  $q-1$ ) and  $\rho(q) = q^{-1/2} - q^{-1} + O(q^{-3/2})$  (Lemma 14). At size  $N := q-1$ , apply Lemma 10 with the  $\sqrt{N}$ -coefficient supplied by Remark 11's identity  $j \int \xi P(\xi) e^{-j\xi^2/2-2j\xi} d\xi = (j-3)[(4j+1)c_j - 2]/(2j)$  which at  $j=1$  gives  $2 - 5c_1$ :

$$\begin{aligned} \sum_{k \geq 1} k \cdot \frac{h(N-k, k)}{T_N} &= NM_1^{(1)} + \sqrt{N}(2 - 5c_1) + o(\sqrt{N}) = N(1 - 2c_1) + \sqrt{N}(2 - 5c_1) + o(\sqrt{N}), \\ \sum_{k \geq 0} \frac{h(N-k, k)}{T_N} &= c_1 \sqrt{N} + c_1 + o(1) \quad (\text{as for } B_1^{(0)} \text{ at size } N). \end{aligned}$$

Adding:

$$\sum_{k \geq 0} (k+1) \frac{h(N-k, k)}{T_N} = N(1 - 2c_1) + \sqrt{N}(2 - 4c_1) + c_1 + o(\sqrt{N}).$$

Multiplying by  $2\rho(q) = 2q^{-1/2} - 2q^{-1} + O(q^{-3/2})$ , with  $N = q-1$  (so  $\sqrt{N} = \sqrt{q} - 1/(2\sqrt{q}) + O(q^{-3/2})$ ):

$$\begin{aligned} 2\rho(q) \cdot N(1 - 2c_1) &= 2(1 - 2c_1)[(q-1)q^{-1/2} - (q-1)q^{-1} + O(q^{-3/2}) \cdot q] \\ &= 2(1 - 2c_1)[\sqrt{q} - 1 - q^{-1/2} + O(1) \cdot q^{-1}] \\ &= 2(1 - 2c_1)\sqrt{q} - 2(1 - 2c_1) + O(q^{-1/2}), \\ 2\rho(q) \cdot \sqrt{N}(2 - 4c_1) &= 2(2 - 4c_1)[1 + O(q^{-1/2})] = (4 - 8c_1) + O(q^{-1/2}). \end{aligned}$$

The  $2\rho(q) \cdot c_1$  contributes  $O(q^{-1/2})$ . Summing:

$$B_1^{(1)}(q) = 2(1 - 2c_1)\sqrt{q} + (2 - 4c_1) + O(q^{-1/2}), \quad (31)$$

where the constant collects  $-2(1 - 2c_1) + (4 - 8c_1) = (2 - 4c_1)$ .

*Combine.*  $R(1, q) = -B_1^{(1)}(q) - 3B_1^{(0)}(q) = -[2(1 - 2c_1)\sqrt{q} + (2 - 4c_1)] - 3[c_1 \sqrt{q} + c_1] + O(q^{-1/2}) = (c_1 - 2)\sqrt{q} + (c_1 - 2) + O(q^{-1/2})$  (both coefficients collapse to  $c_1 - 2$ ).  $\square$

Table 12: Verification of Lemma 15 for  $q \in \{10, 100, 1000, 10000\}$ . “Exact” is  $R(1, q) = -B_1^{(1)}(q) - 3B_1^{(0)}(q)$  from Proposition 8, evaluated in exact rational arithmetic by summing  $h(q-l, k)/T_q$  term by term. “Est” is the leading estimate  $(c_1 - 2)\sqrt{q}$  with  $c_1 \approx 0.42136923$ . The residual Exact – Est converges to a finite  $O(1)$  constant  $c_1 - 2 \approx -1.579$ , as predicted by (29).

$q$	$R(1, q)$ exact	est $((c_1 - 2)\sqrt{q})$	residual
10	-6.899707	-4.992069	-1.907638
100	-17.479101	-15.786308	-1.692793
1000	-51.536354	-49.920688	-1.615666
10000	-159.453508	-157.863077	-1.590431

**Theorem 16** ( $P_{\text{ptr}}(1, q)$ , four leading orders). As  $q \rightarrow \infty$ ,

$$P_{\text{ptr}}(1, q) = \frac{q^2}{6} - \frac{q^{3/2}}{3} + \frac{7q}{2} + \left(c_1 - \frac{31}{12}\right)\sqrt{q} + \left(\frac{17}{12} + c_1\right) + O(q^{-1/2}). \quad (32)$$

*Proof.* By Theorem 7 and  $P_{\text{nodes}}(1, q) = q$ ,  $P_{\text{ptr}}(1, q) = 3q + 3 + W(1, q) + R(1, q)$ . Substituting  $W(1, q)$  from (27) (which carries through the constant  $5/12$  from  $W(1, q) = q^2/6 - q^{3/2}/3 + q/2 - 7\sqrt{q}/12 + 5/12 + O(q^{-1/2})$ ) and  $R(1, q)$  from (29),

$$\begin{aligned} P_{\text{ptr}}(1, q) &= 3q + 3 + \left[\frac{q^2}{6} - \frac{q^{3/2}}{3} + \frac{q}{2} - \frac{7\sqrt{q}}{12} + \frac{5}{12}\right] + [(c_1 - 2)\sqrt{q} + (c_1 - 2)] + O(q^{-1/2}) \\ &= \frac{q^2}{6} - \frac{q^{3/2}}{3} + \frac{7q}{2} + \left(c_1 - \frac{31}{12}\right)\sqrt{q} + \left(\frac{17}{12} + c_1\right) + O(q^{-1/2}), \end{aligned}$$

where the  $q$  coefficient collects  $3 + \frac{1}{2} = \frac{7}{2}$ , the  $\sqrt{q}$  coefficient combines  $-\frac{7}{12} + (c_1 - 2) = c_1 - \frac{31}{12}$ , and the constant collects  $3 + \frac{5}{12} + (c_1 - 2) = \frac{17}{12} + c_1 \approx 1.83803$ .  $\square$

Table 13: Verification of Theorem 16 for  $q \in \{10, 100, 1000, 10000\}$ . “Exact” is  $P_{\text{ptr}}(1, q) = 3q + 3 + W(1, q) + R(1, q)$  in exact rational arithmetic, with  $W(1, q) = \frac{q^3 - q}{6} \cdot T_{q-2}/T_q$  and  $R(1, q) = -B_1^{(1)}(q) - 3B_1^{(0)}(q)$  summed term by term over  $k$ . “Est” is the four-term estimate  $q^2/6 - q^{3/2}/3 + 7q/2 + (c_1 - \frac{31}{12})\sqrt{q}$  with  $c_1 \approx 0.42136923$ . The residual Exact – Est converges to  $C^* = \frac{17}{12} + c_1 \approx 1.83803$ , as predicted by (32).

$q$	$P_{\text{ptr}}(1, q)$ exact	est (4-term)	residual
10	35.740896	34.289010	1.451886
100	1,663.419542	1,661.713692	1.705850
1000	159,559.169187	159,557.373825	1.795362
10000	16,368,118.961384	16,368,117.136923	1.824461

## 9 Combined: $P_{\text{ptr}}(n, q)$ for general $n$

We close the general- $n$  pointer count by carrying the boundary-layer machinery of §6 through to two new families of sums: the  $k$ -weighted moments  $S_j^{(k)}(q)$  and the boundary moments  $B_j^{(b)}(q)$  that make up  $R(n, q)$ . The decisive input is that the latter collapse to the  $j = 1$  term, so that  $R(n, q) = nR(1, q)$  up to an exponentially small remainder of rate  $-q \log 2$ .

## Boundary moments collapse for $j \geq 2$

**Lemma 17** ( $B_j^{(b)}$  exponential bound). *For  $b \in \{0, 1\}$  and each fixed  $j \geq 2$ , the boundary moment*

$$B_j^{(b)}(q) := \sum_{(l,k): q-l-k=b} f(l,k) \left( \frac{h(q-l,k)}{T_q} \right)^j \quad (33)$$

is exponentially small in  $q$ :

$$\log B_j^{(b)}(q) \leq -\frac{j \log 2}{2} q - 2j\sqrt{q} + O(\log q), \quad (34)$$

equivalently  $B_j^{(b)}(q) \leq \exp(-\frac{j \log 2}{2} q (1 + O((\log q)/q)))$ . Consequently,

$$R(n, q) = n \cdot R(1, q) + O(e^{-q \log 2 (1 + O((\log q)/q))}). \quad (35)$$

*Proof. Setup.* On the boundary line  $\{q-l-k=b\}$ ,  $l = q-b-k$  and  $h(q-l, k) = k! \binom{b+k}{k} T_b$  ( $= k!$  for  $b=0$ ,  $= 2(k+1)!$  for  $b=1$ ). Substituting into (33):

$$B_j^{(b)}(q) = \sum_{k=0}^{\lfloor (q-b)/2 \rfloor} \Phi_k, \quad \Phi_k := \binom{q-b-k}{k} T_{q-b-2k} \cdot (h(b+k, k)/T_q)^j.$$

*Quantitative bound (full details in §A.3; ratio-monotonicity approach).* The consecutive ratio  $\varrho_k := \Phi_{k+1}/\Phi_k$  (for  $b=0$ ) simplifies via the recurrence  $T_N = 2T_{N-1} + (N-1)T_{N-2}$  to

$$\frac{\Phi_{k+1}}{\Phi_k} = \frac{(q-2k)(k+1)^{j-1}(1-2\rho(q-2k))}{q-k}, \quad \rho(N) := T_{N-1}/T_N \leq 1/\sqrt{N}.$$

A three-regime case analysis (left endpoint  $k=1$ , right endpoint  $k = \lfloor q/2 \rfloor - 2$ , interior) shows  $\varrho_k \geq 1$  for  $1 \leq k \leq \lfloor q/2 \rfloor - 2$  and  $q \geq 20$ , so  $\Phi_1 \leq \Phi_2 \leq \dots \leq \Phi_{\lfloor q/2 \rfloor - 1}$ . At the edges the ratio can dip slightly below 1 ( $\Phi_1/\Phi_0 = 1 - 2\rho(q) < 1$ , and for  $j=2$  also  $\Phi_{q/2}/\Phi_{q/2-1} \rightarrow 2/5 < 1$ ), so the global maximum sits at  $k^* \in \{\lfloor q/2 \rfloor - 1, \lfloor q/2 \rfloor\}$  with  $\Phi_{k^*} \leq \frac{5}{2} \Phi_{\lfloor q/2 \rfloor} (1 + o(1))$  (worst-case constant from  $j=2, q$  even). Direct Stirling+Wright evaluation of  $\Phi_{\lfloor q/2 \rfloor}$  (where  $\binom{q/2}{q/2} T_0 = 1$ , so  $\Phi_{q/2} = ((q/2)!/T_q)^j$ ) gives  $\log \Phi_{\lfloor q/2 \rfloor} = -(jq \log 2)/2 - 2j\sqrt{q} + O(\log q)$ . Hence

$$B_j^{(0)}(q) \leq (q/2 + 1) \cdot \max_k \Phi_k \leq e^{-(j \log 2/2)q(1+o(1))},$$

which is (34) for  $b=0$ . The case  $b=1$  reduces to  $b=0$  via the multiplicative identity  $\Phi_k^{(1)}(q) = (2(k+1)\rho(q))^j \Phi_k^{(0)}(q-1)$ , giving the same bound.

*Inclusion-exclusion.* By the derivation of  $R(n, q)$  at (11) (just before Theorem 7):

$$R(n, q) = - \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} [B_j^{(1)}(q) + 3B_j^{(0)}(q)].$$

The  $j=1$  term gives  $-n[B_1^{(1)} + 3B_1^{(0)}] = nR(1, q)$  by Proposition 8. The  $j \geq 2$  terms each have  $|B_j^{(b)}(q)| \leq e^{-(j \log 2/2)q(1+o(1))}$ , the sum dominated by  $j=2$ :

$$\sum_{j=2}^n (-1)^{j+1} \binom{n}{j} [B_j^{(1)} + 3B_j^{(0)}] = O(2^n \cdot e^{-q \log 2 (1+o(1))}) = O(e^{-q \log 2 (1+o(1))}),$$

yielding (35). □

Table 14: Verification of Lemma 17 for  $j \in \{2, 3\}$ ,  $b \in \{0, 1\}$ ,  $q \in \{10, 100, 1000, 10000\}$ . “ $\log_{10} B_j^{(b)}$ ” is the actual value, computed in log-space float64 from (33). “Bound” is the  $\log_{10}$  of the upper bound  $\exp(-j(\log 2/2)q)$  in (34) (taking the  $(1 + o(1))$  factor as 1, so the actual bound with sub-leading corrections is yet smaller). Both  $b = 0$  and  $b = 1$  columns show actual values well below the bound, with empirical decay rate slightly faster than  $j \log 2/2$  due to the additional  $-2j\sqrt{q}$  contribution from Wright’s  $e^{2\sqrt{q}}$  factor in  $T_q$ .

$q$	$j$	$\log_{10} B_j^{(0)}$	$\log_{10} B_j^{(1)}$	$\log_{10}$ bound
10	2	-4.63	-3.88	-3.01
10	3	-8.74	-7.03	-4.52
100	2	-43.05	-40.79	-30.10
100	3	-65.79	-62.90	-45.15
1000	2	-350.52	-347.24	-301.03
1000	3	-526.98	-523.08	-451.55
10000	2	-3177.57	-3173.28	-3010.30
10000	3	-4767.54	-4762.63	-4515.45

### The $k$ -weighted moments $S_j^{(k)}$ for $j \geq 2$

Let  $M_n^{(j)} := \int_0^\infty \xi^n \exp(-(j/2)\xi^2 - 2j\xi) d\xi$  denote the  $n$ -th moment of  $[h(q-k, k)/T_q]^j$ ’s leading profile  $e^{-j\xi^2/2-2j\xi}$  (so  $M_0^{(j)} = c_j$  and  $M_1^{(j)} = 1/j - 2c_j$  via integration by parts of  $d[e^{-j\xi^2/2-2j\xi}] = -(j\xi + 2j)e^{-j\xi^2/2-2j\xi} d\xi$ ). The boundary-layer machinery of §6 now applies with the extra  $k$ -weight in the sum (giving an extra factor  $k = \sqrt{q}\xi$  inside the Riemann integrand), yielding:

**Lemma 18** ( $S_j^{(k)}$  closed form). *For each fixed integer  $j \geq 2$ , as  $q \rightarrow \infty$ ,*

$$S_j^{(k)}(q) = c_j^{(k)} q + d_j^{(k)} \sqrt{q} + O(1),$$

with

$$c_j^{(k)} = \frac{1}{j} - 2c_j \quad (j \geq 2),$$

$$d_j^{(k)} = \frac{(j-3)((4j+1)c_j - 2)}{2j} \quad (j \geq 4), \quad d_3^{(k)} = 0, \quad d_2^{(k)} = \frac{27}{4}c_2 - \frac{3}{2}.$$

*Proof of Lemma 18. Setup.* By definition,

$$S_j^{(k)}(q) = \sum_{l=1}^q \sum_{k=0}^l k f(l, k) \left( \frac{h(q-l, k)}{T_q} \right)^j.$$

Reparametrise via  $a := l - k \geq 0$  (so  $l = a + k$ ); the  $k = 0$  rows contribute 0 (factor of  $k$ ):

$$S_j^{(k)}(q) = \sum_{\substack{a, k \geq 0 \\ a+2k \leq q \\ k \geq 1}} k \binom{a+k}{k} T_a \left[ \frac{k! \binom{q-a-k}{k} T_{q-a-2k}}{T_q} \right]^j.$$

Split by  $a$ : *diagonal*  $a = 0$  and *off-diagonal slices*  $a \geq 1$ .

*Diagonal*  $a = 0, k \geq 1$ . On  $a = 0$ ,  $\binom{k}{k} T_0 = 1$  and the summand reduces to  $k \cdot [h(q-k, k)/T_q]^j$ . Apply Lemma 10 with  $\alpha = 1$  and substitute the profile integral evaluation  $j \int \xi P e^{-j\xi^2/2-2j\xi} d\xi = (j-3)[(4j+1)c_j - 2]/(2j)$  from Remark 11:

$$\Sigma_{a=0}^{(k)} := \sum_{k \geq 1} k \left[ \frac{h(q-k, k)}{T_q} \right]^j = \left( \frac{1}{j} - 2c_j \right) q + \frac{(j-3)[(4j+1)c_j - 2]}{2j} \sqrt{q} + o(\sqrt{q}).$$

Off-diagonal  $a = 1, k \geq 1$ . On  $a = 1$ ,  $\binom{1+k}{k} T_1 = 2(k+1)$ , and using the identity  $h(q-1-k, k)/T_q = \varrho_{1,k} \cdot h(q-k, k)/T_q$  where

$$\varrho_{1,k} := \frac{\binom{q-1-k}{k} T_{q-1-2k}}{\binom{q-k}{k} T_{q-2k}} = \frac{q-2k}{q-k} \cdot \rho(q-2k) = \frac{1}{\sqrt{q}} \left( 1 - \frac{1}{\sqrt{q}} + O\left(\frac{\xi^2+1}{q}\right) \right)$$

on the boundary layer (cancellation of the linear-in- $u$  piece of  $(1-2u)^{1/2}/(1-u)$  leaves  $1-u^2/2 + O(u^3)$  for the leading- $\rho$  part, while the  $-N^{-1}$  correction of  $\rho(q-2k)$  contributes the  $-1/\sqrt{q}$  shift; here  $u = \xi/\sqrt{q}$ ,  $\xi = k/\sqrt{q}$ ). Hence  $\varrho_{1,k}^j = q^{-j/2}(1 + O(q^{-1/2}))$  uniformly on the boundary layer (since on  $\xi \leq \sqrt{\log q}$ ,  $(\xi^2+1)/q \leq (\log q+1)/q \ll q^{-1/2}$ ), in particular  $q^{-j/2}(1 + o(1))$ .

$$\begin{aligned} \Sigma_{a=1}^{(k)} &= 2 \sum_{k \geq 1} k(k+1) \cdot \varrho_{1,k}^j \left[ \frac{h(q-k, k)}{T_q} \right]^j \\ &= \frac{2}{q^{j/2}} \sum_{k \geq 1} k(k+1) e^{-j\xi^2/2-2j\xi} (1 + o(1)) \\ &= \frac{2}{q^{j/2}} \cdot [q^{3/2} M_2^{(j)} + O(q)] = 2M_2^{(j)} q^{(3-j)/2} + O(q^{1-j/2}), \end{aligned}$$

where the Riemann-sum step uses  $k(k+1) = k^2 + k$  and (with  $\xi_k = k/\sqrt{q}$ ,  $\Delta\xi = 1/\sqrt{q}$ , Euler–Maclaurin error  $O(1)$ ):

$$\begin{aligned} \sum_{k \geq 1} k^2 e^{-j\xi^2/2-2j\xi} &= q \sum_{k \geq 1} \xi_k^2 e^{\dots} = q \cdot (\sqrt{q} M_2^{(j)} + O(1)) = q^{3/2} M_2^{(j)} + O(q), \\ \sum_{k \geq 1} k e^{-j\xi^2/2-2j\xi} &= \sqrt{q} \sum_{k \geq 1} \xi_k e^{\dots} = \sqrt{q} \cdot (\sqrt{q} M_1^{(j)} + O(1)) = q M_1^{(j)} + O(\sqrt{q}), \end{aligned}$$

so  $\sum_k k(k+1)e^{\dots} = q^{3/2} M_2^{(j)} + q M_1^{(j)} + O(\sqrt{q}) = q^{3/2} M_2^{(j)} + O(q)$ .

Off-diagonal  $a \geq 2$ . By the analogous computation, for fixed  $a$ :  $\varrho_{a,k} = \prod_{i=0}^{a-1} (q-2k-i)\rho(q-2k-i)/(q-k-i) = O(q^{-a/2})$ , so  $\varrho_{a,k}^j = O(q^{-aj/2})$ , and the prefactor  $k \binom{a+k}{k} T_a = O_a(k^{a+1})$  (with constant depending on  $a$  through  $T_a/a!$ ). Riemann-summing gives each slice  $O_a(q^{(a+2-aj)/2})$ . For  $j \geq 2$  and  $a \geq 2$ :  $(a+2-aj)/2 = (a(1-j)+2)/2 \leq (2-a)/2$ , so the slice is  $O_a(q^{(2-a)/2})$ , geometric decay in  $a$ :

$$\sum_{a \geq 2} \Sigma_a^{(k)} = \Sigma_{a=2}^{(k)} (1 + O(q^{-1/2}) + O(q^{-1}) + \dots) = \Sigma_{a=2}^{(k)} (1 + o(1)) = O(1).$$

The large- $a$  tail (where  $a+2k$  approaches the boundary  $q$ ) is dominated by the boundary moments  $B_j^{(b)}(q)$  (Lemma 17), which are exponentially small in  $q$ ; hence the tail contribution is negligible. Thus  $\Sigma_{a \geq 2}^{(k)} = O(1) = o(\sqrt{q})$ .

Combining.  $S_j^{(k)}(q) = \Sigma_{a=0}^{(k)} + \Sigma_{a=1}^{(k)} + \Sigma_{a \geq 2}^{(k)}$ .

Case  $j \geq 4$ :  $\Sigma_{a=1}^{(k)} = 2M_2^{(j)} q^{(3-j)/2} = O(q^{-1/2}) = o(\sqrt{q})$ , and  $\Sigma_{a \geq 2}^{(k)} = o(\sqrt{q})$ . Hence  $S_j^{(k)}(q) = \Sigma_{a=0}^{(k)} + o(\sqrt{q})$ , i.e.

$$c_j^{(k)} = \frac{1}{j} - 2c_j, \quad d_j^{(k)} = \frac{(j-3)[(4j+1)c_j - 2]}{2j}.$$

Case  $j = 3$ :  $\Sigma_{a=1}^{(k)} = 2M_2^{(3)} q^0 + O(q^{-1/2}) = 2M_2^{(3)} + O(q^{-1/2})$ , which is  $O(1)$ , not affecting the  $\sqrt{q}$ -coefficient. The diagonal  $\sqrt{q}$  coefficient  $(j-3)[(4j+1)c_j - 2]/(2j) = 0$  at  $j = 3$ . Hence  $d_3^{(k)} = 0$ . (A pleasant algebraic coincidence: the  $(j-3)$  factor in the diagonal  $\sqrt{q}$ -coefficient

vanishes at exactly the same  $j$  for which  $\Sigma_{a=1}^{(k)}$  drops to  $O(1)$ , so two independent mechanisms agree on  $d_3^{(k)} = 0$ .)

**Case  $j = 2$ :**  $\Sigma_{a=1}^{(k)} = 2M_2^{(2)}\sqrt{q} + O(1)$ , which contributes to the  $\sqrt{q}$ -coefficient. With  $M_2^{(2)} = 9c_2/2 - 1$ :

$$\Sigma_{a=1}^{(k)}|_{\sqrt{q}\text{-part}} = 2(9c_2/2 - 1) = 9c_2 - 2.$$

The diagonal  $\sqrt{q}$  coefficient at  $j = 2$ :  $(j-3)[(4j+1)c_j - 2]/(2j) = (-1)(9c_2 - 2)/4 = (2 - 9c_2)/4$ . Adding:

$$d_2^{(k)} = \frac{2 - 9c_2}{4} + (9c_2 - 2) = \frac{2 - 9c_2 + 36c_2 - 8}{4} = \frac{27c_2 - 6}{4} = \frac{27}{4}c_2 - \frac{3}{2}.$$

This completes the proof.  $\square$

Table 15: Verification of Lemma 18 for  $j \in \{2, 3, 4, 5\}$  and  $q \in \{10, 100, 1000, 10000\}$ . “Exact” is  $S_j^{(k)}(q)$  computed in log-space float64 from (6). “Est” is  $c_j^{(k)}q + d_j^{(k)}\sqrt{q}$  with the closed-form coefficients from Lemma 18 (using  $c_2 \approx 0.22634$ ,  $c_3 \approx 0.15530$ ,  $c_4 \approx 0.11833$ ,  $c_5 \approx 0.09561$ ). The residual converges to a finite  $O(1)$  constant for each  $j$ .

$j$	$q$	$S_j^{(k)}(q)$ exact	est	residual
2	10	0.512268	0.561094	-0.048825
2	100	4.981249	5.010145	-0.028896
2	1000	48.178072	48.201590	-0.023519
2	10000	475.986128	476.008005	-0.021876
3	10	0.178807	0.227256	-0.048449
3	100	2.220460	2.272556	-0.052096
3	1000	22.672972	22.725557	-0.052585
3	10000	227.202953	227.255569	-0.052616
4	10	0.082772	0.138040	-0.055268
4	100	1.279381	1.349193	-0.069812
4	1000	13.321245	13.393254	-0.072009
4	10000	133.548204	133.620487	-0.072282
5	10	0.041524	0.092748	-0.051225
5	100	0.821375	0.893832	-0.072457
5	1000	8.756335	8.831894	-0.075559
5	10000	87.906545	87.982412	-0.075867

### Assembled closed form for $P_{\text{ptr}}(n, q)$

**Theorem 19** ( $P_{\text{ptr}}(n, q)$  for general  $n$ ). For each integer  $n \geq 1$ , as  $q \rightarrow \infty$ ,

$$P_{\text{ptr}}(n, q) = \frac{n}{6}q^2 - \frac{n}{3}q^{3/2} + A_n q + B_n \sqrt{q} + O(1),$$

with closed-form coefficients

$$A_n = \frac{7n}{2} + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} \left( \frac{1}{j} - 2c_j \right), \quad (36)$$

$$B_n = n \left( c_1 - \frac{31}{12} \right) - 3c_n^* + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} d_j^{(k)}, \quad (37)$$

where  $c_n^* = \sum_{j=2}^n (-1)^j \binom{n}{j} c_j$  (see Theorem 13, eq. (25)). The two leading coefficients  $n/6$  and  $-n/3$  are linear in  $n$  and rational; the  $c_j$ -dependent content first appears at order  $q$  (through  $c_j$  in  $A_n$ ) and then at order  $\sqrt{q}$  (through  $c_n^*$  and  $d_j^{(k)}$ ).

*Proof.* By Theorem 7,  $P_{\text{ptr}}(n, q) = 3P_{\text{nodes}}(n, q) + 3 + W(n, q) + R(n, q)$ . We assemble the four-term expansion piece by piece.

*Piece 1:*  $3P_{\text{nodes}}(n, q) + 3$ . By Theorem 13,  $P_{\text{nodes}}(n, q) = nq + (n-1) - c_n^* \sqrt{q} - d_n^* + O(q^{-1/2})$ , so

$$3P_{\text{nodes}}(n, q) + 3 = 3nq + 3n - 3c_n^* \sqrt{q} - 3d_n^* + O(q^{-1/2}) = 3nq + 3n - 3c_n^* \sqrt{q} + O(1), \quad (38)$$

using  $3(n-1) + 3 = 3n$  and absorbing the explicit constant  $-3d_n^*$  into  $O(1)$ . This contributes 0 at  $q^2$  and  $q^{3/2}$ ,  $3n$  at  $q$ ,  $-3c_n^*$  at  $\sqrt{q}$ .

*Piece 2:*  $W(n, q)$ . By the inclusion–exclusion formula for  $W(n, q)$  derived in Theorem 7,  $W(n, q) = \sum_{j=1}^n (-1)^{j+1} \binom{n}{j} S_j^{(k)}(q)$ . Split into  $j=1$  and  $j \geq 2$  contributions.

$j=1$  piece:  $n \cdot S_1^{(k)}(q)$ . By Lemma 5,  $S_1^{(k)}(q) = (q^3 - q)/6 \cdot T_{q-2}/T_q$ ; and by Lemma 14's expansion  $W(1, q) = S_1^{(k)}(q) = q^2/6 - q^{3/2}/3 + q/2 - 7\sqrt{q}/12 + O(1)$ . Hence

$$n S_1^{(k)}(q) = \frac{n}{6} q^2 - \frac{n}{3} q^{3/2} + \frac{n}{2} q - \frac{7n}{12} \sqrt{q} + O(1). \quad (39)$$

$j \geq 2$  pieces: by Lemma 18,  $S_j^{(k)}(q) = (\frac{1}{j} - 2c_j)q + d_j^{(k)} \sqrt{q} + O(1)$ . So

$$\sum_{j=2}^n (-1)^{j+1} \binom{n}{j} S_j^{(k)}(q) = \left[ \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} \left( \frac{1}{j} - 2c_j \right) \right] q + \left[ \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} d_j^{(k)} \right] \sqrt{q} + O(1). \quad (40)$$

Adding (39) and (40):

$$W(n, q) = \frac{n}{6} q^2 - \frac{n}{3} q^{3/2} + \left[ \frac{n}{2} + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} \left( \frac{1}{j} - 2c_j \right) \right] q + \left[ -\frac{7n}{12} + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} d_j^{(k)} \right] \sqrt{q} + O(1). \quad (41)$$

*Piece 3:*  $R(n, q)$ . By the collapse identity (35) (Lemma 17), and Lemma 15 giving  $R(1, q) = (c_1 - 2)\sqrt{q} + O(1)$ . Hence

$$R(n, q) = n(c_1 - 2)\sqrt{q} + O(1). \quad (42)$$

*Combine.* Summing (38), (41), (42):

$$P_{\text{ptr}}(n, q) = \frac{n}{6} q^2 - \frac{n}{3} q^{3/2} + A_n q + B_n \sqrt{q} + O(1),$$

where collecting the  $q$  and  $\sqrt{q}$  coefficients:

$$A_n = 3n + \frac{n}{2} + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} \left( \frac{1}{j} - 2c_j \right) = \frac{7n}{2} + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} \left( \frac{1}{j} - 2c_j \right),$$

$$B_n = -3c_n^* - \frac{7n}{12} + n(c_1 - 2) + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} d_j^{(k)} = n\left(c_1 - \frac{31}{12}\right) - 3c_n^* + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} d_j^{(k)},$$

using  $c_1 - 2 - 7/12 = c_1 - 31/12$ . These match (36), (37).  $\square$

**Theorem 20** (Simplified form of  $A_n$ ). *The  $q$ -coefficient  $A_n$  of Theorem 19 admits the remarkably clean closed form*

$$\boxed{A_n = \frac{5n}{2} + H_n + 2c_n^*}, \quad (43)$$

where  $H_n := \sum_{k=1}^n 1/k$  is the  $n$ -th harmonic number and  $c_n^* := \sum_{j=2}^n (-1)^j \binom{n}{j} c_j$  is the same constant appearing in Theorem 13. The appearance of  $H_n$  reveals an entropy-like structure: the  $q$ -order term of  $P_{ptr}(n, q)$  decomposes as a rational  $\frac{5n}{2} + H_n$  (uniform expansion fed by the keystone identity) plus twice the boundary-layer prefix-coincidence cost  $c_n^*$ .

*Proof.* The classical identity  $\sum_{j=1}^n (-1)^{j+1} \binom{n}{j} / j = H_n$  (equivalently,  $\int_0^1 (1 - (1-x)^n) / x \, dx = H_n$  by expanding  $(1-x)^n$  binomially) splits off the  $j = 1$  term to give  $\sum_{j=2}^n (-1)^{j+1} \binom{n}{j} / j = H_n - n$ . Substituting into (36):

$$A_n = \frac{7n}{2} + (H_n - n) - 2 \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} c_j = \frac{5n}{2} + H_n + 2c_n^*,$$

since  $\sum_{j=2}^n (-1)^{j+1} \binom{n}{j} c_j = -c_n^*$ .  $\square$

**Corollary 21** (Closed form for  $B_n$ ). *The  $\sqrt{q}$ -coefficient  $B_n$  in Theorem 19 admits the closed form*

$$\boxed{B_n = nc_1 + 3H_n + n^2 - \frac{67n}{12} - 1 - \frac{39}{4} \binom{n}{2} c_2 + 3 \binom{n}{3} c_3 + \sum_{j=4}^n (-1)^{j+1} \binom{n}{j} \frac{4j^2 - 5j - 3}{2j} c_j.} \quad (44)$$

Equivalently,  $B_n = nc_1 + B_n^{\text{rat}} + \sum_{j=2}^n \gamma_j(n) c_j$ , with  $B_n^{\text{rat}} := 3H_n + n^2 - 67n/12 - 1$ , and weights

$$\gamma_2(n) = -\frac{39}{4} \binom{n}{2}, \quad \gamma_3(n) = 3 \binom{n}{3}, \quad \gamma_j(n) = (-1)^{j+1} \binom{n}{j} \frac{4j^2 - 5j - 3}{2j} \quad (j \geq 4).$$

Unlike  $A_n$  (Theorem 20), the  $c_j$ -dependent sum does not telescope to a single transcendental combination — the weights  $(4j^2 - 5j - 3)/(2j) = 2j - 5/2 - 3/(2j)$  mix  $j$ ,  $1$ ,  $1/j$  contributions, and we are unaware of a further reduction. The  $j = 2$  coefficient  $\gamma_2(n)$  acquires an extra  $-9 \binom{n}{2} c_2$  relative to the general formula (giving the apparent weight  $-39/4$  in place of  $(2 \cdot 2 - 5/2 - 3/4) = 3/4$ ): the source is the off-diagonal  $a = 1$  slice contribution  $2M_2^{(2)} = 9c_2 - 2$  to  $d_2^{(k)}$  (cf. Lemma 18, Case  $j = 2$ ), which is multiplied by  $(-1)^{j+1} \binom{n}{j} = -\binom{n}{2}$  in the sum defining  $B_n$ .

*Proof.* From Theorem 19,  $B_n = n(c_1 - 31/12) - 3c_n^* + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} d_j^{(k)}$ .

*Rational part.* The rational part of  $d_j^{(k)}$  (from Lemma 18) is  $-3/2$  at  $j = 2$ ,  $0$  at  $j = 3$ , and  $-(j-3)/j = -1 + 3/j$  for  $j \geq 4$ . Writing  $\sum_{j=2}^n (-1)^{j+1} \binom{n}{j} = 1 - n$  (from  $\sum_{j=0}^n (-1)^j \binom{n}{j} = 0$ , subtracting  $j = 0, 1$ ) and using the classical identity  $\sum_{j=2}^n (-1)^{j+1} \binom{n}{j} / j = H_n - n$  (used in Theorem 20):

$$\sum_{j=2}^n (-1)^{j+1} \binom{n}{j} [\text{rat}(d_j^{(k)})] = 3H_n + n^2 - 3n - 1,$$

which combines with  $-31n/12$  from  $n(c_1 - 31/12)$  to give  $B_n^{\text{rat}} = 3H_n + n^2 - 67n/12 - 1$ .

*$c_j$  coefficients.* For each  $j \geq 2$ , sum the  $c_j$  contributions from  $-3c_n^*$  and from  $(-1)^{j+1} \binom{n}{j} d_j^{(k)}$ :

- $j = 2$ :  $-3 \binom{n}{2} + (-\binom{n}{2}) \cdot \frac{27}{4} = -(3 + \frac{27}{4}) \binom{n}{2} = -\frac{39}{4} \binom{n}{2}$ .
- $j = 3$ :  $3 \binom{n}{3} + 0 = 3 \binom{n}{3}$  (using  $d_3^{(k)} = 0$ ).
- $j \geq 4$ :  $3(-1)^{j+1} \binom{n}{j} + (-1)^{j+1} \binom{n}{j} \cdot \frac{(j-3)(4j+1)}{2j} = (-1)^{j+1} \binom{n}{j} \cdot \frac{6j+(j-3)(4j+1)}{2j} = (-1)^{j+1} \binom{n}{j} \cdot \frac{4j^2 - 5j - 3}{2j}$ .

The  $c_1$  contribution is  $nc_1$  from  $n(c_1 - 31/12)$  alone (neither  $c_n^*$  nor any  $d_j^{(k)}$  involves  $c_1$ ). Assembling all parts yields (44).  $\square$

**Example 22** (Worked  $n = 1, 2, 3$ ). Using  $c_1 \approx 0.42136923$ ,  $c_2 \approx 0.22634$ ,  $c_3 \approx 0.15530$ ,  $d_2^{(k)} = \frac{27}{4}c_2 - \frac{3}{2} \approx 0.02780$ ,  $d_3^{(k)} = 0$ :

- $n = 1$ :  $c_1^* = 0$  (the  $\sum_{j=2}^n$  sums are empty when  $n = 1$ ),  $A_1 = \frac{7}{2} = 3.5$ ,  $B_1 = c_1 - \frac{31}{12} \approx -2.1620$ .

(Recovers Theorem 16.)

- $n = 2$ :  $c_2^* = c_2$ ,  $\binom{2}{2}(\frac{1}{2} - 2c_2) = \frac{1}{2} - 2c_2$   
 $A_2 = 7 - (\frac{1}{2} - 2c_2) = \frac{13}{2} + 2c_2 \approx 6.9527$ ,  $B_2 = 2(c_1 - \frac{31}{12}) - 3c_2 - d_2^{(k)} \approx -5.0308$ .
- $n = 3$ :  $c_3^* = 3c_2 - c_3 \approx 0.5237$ ,  $d_3^{(k)} = 0$   
 $A_3 = \frac{21}{2} - 3(\frac{1}{2} - 2c_2) + (\frac{1}{3} - 2c_3) \approx 10.3808$ ,  $B_3 = 3(c_1 - \frac{31}{12}) - 3(3c_2 - c_3) - 3d_2^{(k)} \approx -8.1405$ .

Substituting into the boxed display of Theorem 19, e.g. for  $n = 3$ :

$$P_{\text{ptr}}(3, q) \approx \frac{1}{2}q^2 - q^{3/2} + 10.3808q - 8.1405\sqrt{q} + O(1),$$

matching Table 16 at every  $q$  to  $O(1)$ .

Table 16: Verification of Theorem 19 for  $n \in \{1, 2, 3\}$  and  $q \in \{10, 100, 1000, 10000\}$ . “Numeric” is  $P_{\text{ptr}}(n, q) = 3P_{\text{nodes}}(n, q) + 3 + W(n, q) + R(n, q)$  computed in log-space `float64` from (9); at  $q = 10000$  this loses about  $10^{-3}$  of absolute precision relative to the exact rational value (compare Table 13’s 16,368,118.961384 versus the entry 16,368,118.962003 below). “Est” is  $\frac{n}{6}q^2 - \frac{n}{3}q^{3/2} + A_nq + B_n\sqrt{q}$  with  $A_n, B_n$  from (36)–(37). The residual converges to a finite  $O(1)$  constant ( $\approx 1.8245$  for  $n = 1$ ,  $\approx 1.83$  for  $n = 2$ ,  $\approx 1.62$  for  $n = 3$  as  $q$  grows).

$n$	$q$	$P_{\text{ptr}}(n, q)$ numeric	est	residual
1	10	35.740896	34.289010	1.4519
1	100	1,663.419542	1,661.713692	1.7058
1	1000	159,559.169187	159,557.373825	1.7954
1	10000	16,368,118.962003	16,368,117.136923	1.8251
2	10	66.286984	65.869691	0.4173
2	100	3,313.063072	3,311.627083	1.4360
2	1000	319,046.835662	319,045.073702	1.7620
2	10000	32,735,692.230917	32,735,690.364284	1.8666
3	10	95.396820	96.442641	-1.0458
3	100	4,957.527195	4,956.671846	0.8553
3	1000	478,501.997783	478,500.558608	1.4392
3	10000	49,102,995.153242	49,102,993.528818	1.6244

## 10 Summary of Part II

Part II established four-term asymptotic expansions for both  $P_{\text{nodes}}(n, q)$  and  $P_{\text{ptr}}(n, q)$ , with all coefficients in closed form (rational +  $\mathbb{Q}$ -linear combinations of the  $c_j := \int_0^\infty e^{-(j/2)\xi^2 - 2j\xi} d\xi$ ):

$$P_{\text{nodes}}(n, q) = nq + (n - 1) - c_n^*\sqrt{q} - d_n^* + O(q^{-1/2}), \quad \text{Theorem 13,}$$

$$P_{\text{ptr}}(1, q) = \frac{q^2}{6} - \frac{q^{3/2}}{3} + \frac{7q}{2} + (c_1 - \frac{31}{12})\sqrt{q} + O(1), \quad \text{Theorem 16,}$$

$$P_{\text{ptr}}(n, q) = \frac{n}{6}q^2 - \frac{n}{3}q^{3/2} + A_nq + B_n\sqrt{q} + O(1), \quad \text{Theorem 19.}$$

The coefficients are

$$c_n^* = \sum_{j=2}^n (-1)^j \binom{n}{j} c_j, \quad A_n = \frac{7n}{2} + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} (\frac{1}{j} - 2c_j),$$

$$d_n^* = \binom{n}{2} (\text{const}_2 - \frac{1}{2}) + \frac{n-1}{2} + \sum_{j=3}^n (-1)^j \binom{n}{j} \frac{j-2}{2} M_1^{(j)}, \quad B_n = n(c_1 - \frac{31}{12}) - 3c_n^* + \sum_{j=2}^n (-1)^{j+1} \binom{n}{j} d_j^{(k)};$$

the latter admits an explicit closed form  $B_n = nc_1 + 3H_n + n^2 - 67n/12 - 1 + \sum_{j=2}^n \gamma_j(n)c_j$  with rational weights  $\gamma_j(n)$  (Corollary 21).

The proofs reduced to three asymptotic facts about the building blocks of Part I:

- (A) *Leading constants of  $S_j$*  (Lemma 12):  $S_j(q) = c_j \sqrt{q} + \text{const}_j + O(q^{-1/2})$ , with  $\text{const}_2 = \frac{3}{2} - 4c_2$  and  $\text{const}_j = \frac{1}{2} + \frac{j-2}{2}(\frac{1}{j} - 2c_j)$  for  $j \geq 3$ .
- (B) *Asymptotic of  $\rho(q) = T_{q-1}/T_q$*  (Lemma 14): bootstrapped from the recurrence  $\rho(q)[2 + (q-1)\rho(q-1)] = 1$  to  $\rho(q) = q^{-1/2} - q^{-1} + \frac{3}{4}q^{-3/2} + O(q^{-2})$ , yielding  $T_{q-2}/T_q$  to four orders and hence  $W(1, q)$  via the closed form  $S_1^{(k)}(q) = (q^3 - q)T_{q-2}/(6T_q)$  (Lemma 5).
- (C) *Boundary-layer machinery*: the profile lemma (Lemma 9) gives

$$h(q-k, k)/T_q = e^{-\xi^2/2 - 2\xi} (1 + O((\xi^3 + 1)/\sqrt{q}))$$

uniformly on the boundary layer  $k \leq \sqrt{q \log q}$ ; this is the single analytical workhorse driving (A), the  $R(1, q)$  asymptotic (Lemma 15), and the  $S_j^{(k)}$  closed form (Lemma 18). The boundary moments  $B_j^{(b)}(q)$  for  $j \geq 2$  are exponentially small (Lemma 17), so (35) reduces the general- $n$  pointer count to the  $n = 1$  case.

The Wright saddle-point asymptotic for  $T_N$  (eq. (15)) is the sole external analytical input. Wright's constant  $C$  cancels in every ratio  $h(q-l, k)/T_q$  formed in this analysis, so the closed-form  $c_j, c_j^{(k)}, d_j^{(k)}$  are independent of its value.

Each result was verified numerically in its own section (Tables 8, 10, 11, 12, 13, 14, 15, 16).

## A Stirling–Wright Bookkeeping

This appendix collects every Stirling-and-Wright manipulation extracted from the main paper, written out at full detail: each cancellation is performed term by term, each Taylor expansion to as many orders as needed, each  $\log q$  coefficient verified by explicit arithmetic. The main paper states its Lemmas and Theorems and uses their consequences; readers wanting the bookkeeping come here.

*Conventions.*  $q$  is the key length,  $k$  the open-pair count of a prefix, with  $\xi = k/\sqrt{q}$  and  $u = k/q$ . The marked-involution count  $T_N = |\{\text{length-}N \text{ marked involutions}\}|$  (OEIS A005425) satisfies the EGF  $\sum_{N \geq 0} T_N z^N / N! = e^{2z + z^2/2}$  and the recurrence  $T_{N+2} = 2T_{N+1} + (N+1)T_N$ . We use Stirling's formula

$$\log m! = (m + \frac{1}{2}) \log m - m + \frac{1}{2} \log(2\pi) + O(1/m) \quad (45)$$

and Wright's saddle-point asymptotic

$$\log T_N = \frac{N}{2} \log N - \frac{N}{2} + 2\sqrt{N} - \frac{1}{4} + \log C + r(N), \quad (46)$$

where  $C$  is an absolute positive constant and the remainder  $r(N)$  satisfies  $r(N) \rightarrow 0$  as  $N \rightarrow \infty$ , with the uniform bound  $|r(N)| \leq K_0$  for all  $N \geq 1$  ( $K_0 \leq 1$  suffices; numerical value  $\approx 0.54$ ).

*Quantity expanded.* The recurring object is  $h(q-k, k)/T_q = k! \binom{q-k}{k} T_{q-2k}/T_q$ , the probability (under Hayman's measure) that the first  $k$  canonical-prefix positions of a random marked involution are all "open new pair".

## A.1 Boundary-layer expansion of $h(q-k, k)/T_q$

### A.1.1 Stirling+Wright decomposition

By the closed form  $h(q-k, k) = k! \binom{q-k}{k} T_{q-2k}$ :

$$\log \frac{h(q-k, k)}{T_q} = \log k! + \log \binom{q-k}{k} + \log T_{q-2k} - \log T_q.$$

Expanding  $\binom{q-k}{k} = (q-k)!/(k!(q-2k)!)$  cancels the  $\log k!$ :

$$\log \frac{h(q-k, k)}{T_q} = \log \frac{(q-k)!}{(q-2k)!} + \log T_{q-2k} - \log T_q. \quad (47)$$

On the boundary layer  $1 \leq k \leq \sqrt{q \log q}$ ,  $q-2k \geq q-2\sqrt{q \log q} \geq q/2$  for  $q$  large enough that  $4\sqrt{\log q} \leq \sqrt{q}$  (i.e.  $q \geq$  absolute constant), so Stirling applied to  $(q-k)!$  and  $(q-2k)!$  has  $O(1/q)$  remainder, and Wright applied to  $T_{q-2k}, T_q$  has  $O(q^{-1/2})$  remainder. Apply Stirling to each factorial:

$$\begin{aligned} \log(q-k)! &= (q-k + \tfrac{1}{2}) \log(q-k) - (q-k) + \tfrac{1}{2} \log(2\pi) + O(q^{-1}), \\ \log(q-2k)! &= (q-2k + \tfrac{1}{2}) \log(q-2k) - (q-2k) + \tfrac{1}{2} \log(2\pi) + O(q^{-1}). \end{aligned}$$

Subtracting:

$$\begin{aligned} \log \frac{(q-k)!}{(q-2k)!} &= (q-k + \tfrac{1}{2}) \log(q-k) - (q-2k + \tfrac{1}{2}) \log(q-2k) \\ &\quad - [(q-k) - (q-2k)] + [\tfrac{1}{2} \log(2\pi) - \tfrac{1}{2} \log(2\pi)] + O(q^{-1}) \\ &= (q-k + \tfrac{1}{2}) \log(q-k) - (q-2k + \tfrac{1}{2}) \log(q-2k) - k + O(q^{-1}), \end{aligned} \quad (48)$$

the two  $\frac{1}{2} \log(2\pi)$  pieces cancelling. Apply Wright to  $T_{q-2k}, T_q$ :

$$\begin{aligned} \log T_{q-2k} &= \frac{q-2k}{2} \log(q-2k) - \frac{q-2k}{2} + 2\sqrt{q-2k} - \frac{1}{4} + \log C + r(q-2k), \\ \log T_q &= \frac{q}{2} \log q - \frac{q}{2} + 2\sqrt{q} - \frac{1}{4} + \log C + r(q). \end{aligned}$$

Subtracting:

$$\begin{aligned} \log T_{q-2k} - \log T_q &= \frac{q-2k}{2} \log(q-2k) - \frac{q}{2} \log q \\ &\quad - [\frac{q-2k}{2} - \frac{q}{2}] + [2\sqrt{q-2k} - 2\sqrt{q}] \\ &\quad + [-\frac{1}{4} + \frac{1}{4}] + [\log C - \log C] + [r(q-2k) - r(q)] \\ &= \frac{q-2k}{2} \log(q-2k) - \frac{q}{2} \log q + k + 2(\sqrt{q-2k} - \sqrt{q}) + O(q^{-1/2}), \end{aligned} \quad (49)$$

the  $-\frac{1}{4}$  pieces and the  $\log C$  pieces cancelling, and the remainders bounded by  $|r(q-2k)| + |r(q)| \leq 2K_0$  (which is  $O(q^{-1/2})$  since for  $q-2k \geq q/2$  we have  $r(q-2k) = O(q^{-1/2})$  via Wright's expansion).

Now add (48) and (49) via (47). The  $-k$  from (48) cancels the  $+k$  from (49):

$$[-k] + [+k] = 0.$$

The two  $\log(q-2k)$ -terms combine:

$$\underbrace{-(q-2k + \tfrac{1}{2}) \log(q-2k)}_{\text{from (48)}} + \underbrace{\frac{q-2k}{2} \log(q-2k)}_{\text{from (49)}} = [-(q-2k + \tfrac{1}{2}) + \frac{q-2k}{2}] \log(q-2k).$$

The bracket simplifies:  $-(q - 2k + \frac{1}{2}) + \frac{q-2k}{2} = -(q - 2k) - \frac{1}{2} + \frac{q-2k}{2} = -\frac{q-2k}{2} - \frac{1}{2}$ . Hence

$$-(q - 2k + \frac{1}{2}) \log(q - 2k) + \frac{q-2k}{2} \log(q - 2k) = -\frac{q-2k}{2} \log(q - 2k) - \frac{1}{2} \log(q - 2k).$$

Putting it all together:

$$\begin{aligned} \log \frac{h(q-k, k)}{T_q} &= (q - k + \frac{1}{2}) \log(q - k) - \frac{q-2k}{2} \log(q - 2k) \\ &\quad - \frac{1}{2} \log(q - 2k) - \frac{q}{2} \log q + 2(\sqrt{q-2k} - \sqrt{q}) + O(q^{-1/2}). \end{aligned} \quad (50)$$

### A.1.2 Taylor expansion of the components

Let  $\xi = k/\sqrt{q}$ , so  $k = \xi\sqrt{q}$  and  $u = k/q = \xi/\sqrt{q}$ . We need three Taylor series; the standard ones are

$$\begin{aligned} \log(1 - v) &= -v - \frac{v^2}{2} - \frac{v^3}{3} - \frac{v^4}{4} - O(v^5), \\ \sqrt{1 - v} &= 1 - \frac{v}{2} - \frac{v^2}{8} - \frac{v^3}{16} - \frac{5v^4}{128} - O(v^5). \end{aligned}$$

Applied with  $v = u = \xi/\sqrt{q}$  to  $\log(q - k) = \log q + \log(1 - u)$ :

$$\log(q - k) = \log q - \frac{\xi}{\sqrt{q}} - \frac{\xi^2}{2q} - \frac{\xi^3}{3q^{3/2}} - \frac{\xi^4}{4q^2} - O(\xi^5/q^{5/2}). \quad (51)$$

With  $v = 2u = 2\xi/\sqrt{q}$  to  $\log(q - 2k) = \log q + \log(1 - 2u)$ :

$$\log(q - 2k) = \log q - \frac{2\xi}{\sqrt{q}} - \frac{2\xi^2}{q} - \frac{8\xi^3}{3q^{3/2}} - \frac{4\xi^4}{q^2} - O(\xi^5/q^{5/2}). \quad (52)$$

With  $v = 2u$  to  $\sqrt{q - 2k} = \sqrt{q} \sqrt{1 - 2u}$ :

$$\sqrt{q - 2k} = \sqrt{q} - \xi - \frac{\xi^2}{2\sqrt{q}} - \frac{\xi^3}{2q} - \frac{5\xi^4}{8q^{3/2}} - O(\xi^5/q^2). \quad (53)$$

On the boundary layer ( $\xi \leq \sqrt{\log q}$ ), each Taylor remainder is dominated by any negative power of  $q$  (i.e.  $o(q^{-a})$  for every  $a > 0$ ), so all are  $o(1/\sqrt{q})$ .

### A.1.3 Multiplying by prefactors (Pieces 1–5)

We now substitute (51), (52), (53) into (50), mark the five summands as Pieces 1–5, and expand each.

*Piece 1:*  $(q - k + \frac{1}{2}) \log(q - k) = (q - \xi\sqrt{q} + \frac{1}{2}) \log(q - k)$ . Distribute across the three subfactors  $q$ ,  $-\xi\sqrt{q}$ ,  $\frac{1}{2}$ :

$$\begin{aligned} q \cdot (51) &= q \log q - \frac{q\xi}{\sqrt{q}} - \frac{q\xi^2}{2q} - \frac{q\xi^3}{3q^{3/2}} - \frac{q\xi^4}{4q^2} + O(\xi^5/q^{3/2}) \\ &= q \log q - \xi\sqrt{q} - \frac{\xi^2}{2} - \frac{\xi^3}{3\sqrt{q}} - \frac{\xi^4}{4q} + O(\xi^5/q^{3/2}), \\ -\xi\sqrt{q} \cdot (51) &= -\xi\sqrt{q} \log q + \frac{\xi^2\sqrt{q}}{\sqrt{q}} + \frac{\xi^3\sqrt{q}}{2q} + \frac{\xi^4\sqrt{q}}{3q^{3/2}} + \frac{\xi^5\sqrt{q}}{4q^2} + O(\xi^6/q^2) \\ &= -\xi\sqrt{q} \log q + \xi^2 + \frac{\xi^3}{2\sqrt{q}} + \frac{\xi^4}{3q} + O(\xi^5/q^{3/2}), \\ \frac{1}{2} \cdot (51) &= \frac{1}{2} \log q - \frac{\xi}{2\sqrt{q}} - \frac{\xi^2}{4q} + O(\xi^3/q^{3/2}). \end{aligned}$$

Summing the three rows term-by-term:

$$\begin{aligned} (q - k + \frac{1}{2}) \log(q - k) &= \underbrace{q \log q}_{(\dagger)} - \underbrace{\xi\sqrt{q} \log q}_{(\ddagger)} - \underbrace{\xi\sqrt{q}}_{(\S)} + \underbrace{\frac{1}{2} \log q}_{(*)} \\ &\quad + \xi^2(-\frac{1}{2} + 1) + \frac{\xi^3}{\sqrt{q}}(-\frac{1}{3} + \frac{1}{2}) - \frac{\xi}{2\sqrt{q}} \\ &\quad + O\left(\frac{\xi^4+1}{q}\right) \\ &= (\dagger) - (\ddagger) - (\S) + (*) + \frac{\xi^2}{2} + \frac{\xi^3}{6\sqrt{q}} - \frac{\xi}{2\sqrt{q}} + O\left(\frac{\xi^4+1}{q}\right). \end{aligned} \quad (54)$$

Piece 2:  $-\frac{q-2k}{2} \log(q-2k) = (-\frac{q}{2} + \xi\sqrt{q}) \log(q-2k)$ .

$$\begin{aligned} -\frac{q}{2} \cdot (52) &= -\frac{q}{2} \log q + \frac{q\xi}{\sqrt{q}} + \frac{q\xi^2}{q} + \frac{4q\xi^3}{3q^{3/2}} + \frac{2q\xi^4}{q^2} + O(\xi^5/q^{3/2}) \\ &= -\frac{q}{2} \log q + \xi\sqrt{q} + \xi^2 + \frac{4\xi^3}{3\sqrt{q}} + \frac{2\xi^4}{q} + O(\xi^5/q^{3/2}), \\ \xi\sqrt{q} \cdot (52) &= \xi\sqrt{q} \log q - \frac{2\xi^2\sqrt{q}}{\sqrt{q}} - \frac{2\xi^3\sqrt{q}}{q} - \frac{8\xi^4\sqrt{q}}{3q^{3/2}} + O(\xi^5/q^2) \\ &= \xi\sqrt{q} \log q - 2\xi^2 - \frac{2\xi^3}{\sqrt{q}} - \frac{8\xi^4}{3q} + O(\xi^5/q^{3/2}). \end{aligned}$$

Summing:

$$\begin{aligned} -\frac{q-2k}{2} \log(q-2k) &= \underbrace{-\frac{q}{2} \log q}_{(\dagger)} + \underbrace{\xi\sqrt{q} \log q}_{(\ddagger)} + \underbrace{\xi\sqrt{q}}_{(\S)} \\ &\quad + \xi^2(1-2) + \frac{\xi^3}{\sqrt{q}}(\frac{4}{3}-2) + O(\frac{\xi^4+1}{q}) \\ &= (\dagger) + (\ddagger) + (\S) - \xi^2 - \frac{2\xi^3}{3\sqrt{q}} + O(\frac{\xi^4+1}{q}). \end{aligned} \tag{55}$$

Piece 3:  $-\frac{1}{2} \log(q-2k)$ . Multiply (52) by  $-\frac{1}{2}$ :

$$-\frac{1}{2} \log(q-2k) = \underbrace{-\frac{1}{2} \log q}_{(*)} + \frac{\xi}{\sqrt{q}} + \frac{\xi^2}{q} + O(\xi^3/q^{3/2}). \tag{56}$$

Piece 4:  $-\frac{q}{2} \log q$ . No expansion needed:

$$-\frac{q}{2} \log q = \underbrace{-\frac{q}{2} \log q}_{(\dagger)}. \tag{57}$$

Piece 5:  $2(\sqrt{q-2k} - \sqrt{q})$ . Multiply (53) by 2, then subtract  $2\sqrt{q}$ :

$$2(\sqrt{q-2k} - \sqrt{q}) = -2\xi - \frac{\xi^2}{\sqrt{q}} - \frac{\xi^3}{q} - \frac{5\xi^4}{4q^{3/2}} - O(\xi^5/q^2). \tag{58}$$

#### A.1.4 Cancellation of the four leading groups

Add Pieces 1–5 (and the  $O(q^{-1/2})$  Wright remainder from (50)). The four marked groups  $(\dagger)$ ,  $(\ddagger)$ ,  $(\S)$ ,  $(*)$  cancel pair-wise:

$$(\dagger): \text{ from Pieces 1, 2, 4: } q \log q - \frac{q}{2} \log q - \frac{q}{2} \log q = (1 - \frac{1}{2} - \frac{1}{2}) q \log q = 0.$$

$$(\ddagger): \text{ from Pieces 1, 2: } -\xi\sqrt{q} \log q + \xi\sqrt{q} \log q = 0.$$

$$(\S): \text{ from Pieces 1, 2: } -\xi\sqrt{q} + \xi\sqrt{q} = 0.$$

$$(*): \text{ from Pieces 1, 3: } \frac{1}{2} \log q - \frac{1}{2} \log q = 0.$$

The cancellations are mandatory:  $h(q-k, k)/T_q \leq 1$  (it is a probability), so  $\log[h/T_q] \leq 0$  uniformly, and any unbounded  $q$ -growth in any of the four groups would violate this.

#### A.1.5 Collecting surviving terms by order

After the four cancellations, the surviving contributions are:

*Order  $\xi^0$  (constant):* None of the Pieces contribute a  $\xi^0$  constant; all surviving terms have a positive power of  $\xi$ . So contribution is 0.

*Order  $\xi^1$  (linear in  $\xi$ ):* Piece 5 contributes  $-2\xi$ . No other Piece contributes at this order (the  $\frac{\xi}{2\sqrt{q}}$  in Piece 1 is at order  $\xi/\sqrt{q}$ , not  $\xi$ ). Total:  $-2\xi$ .

*Order  $\xi^2$  (constant prefactor):*

- Piece 1 contributes  $+\frac{\xi^2}{2}$  (coefficient  $-\frac{1}{2} + 1 = +\frac{1}{2}$ ).
- Piece 2 contributes  $-\xi^2$  (coefficient  $1 - 2 = -1$ ).
- Pieces 3, 4, 5: no  $\xi^2$  contribution.

Total:  $\frac{1}{2} - 1 = -\frac{1}{2}$ , i.e.  $-\frac{\xi^2}{2}$ .

Order  $\xi^3/\sqrt{q}$ :

- Piece 1 contributes  $\frac{\xi^3}{6\sqrt{q}}$  (coefficient  $-\frac{1}{3} + \frac{1}{2} = \frac{1}{6}$ ).
- Piece 2 contributes  $-\frac{2\xi^3}{3\sqrt{q}}$  (coefficient  $\frac{4}{3} - 2 = -\frac{2}{3}$ ).

Total:  $\frac{1}{6} - \frac{2}{3} = -\frac{1}{2}$ , i.e.  $-\frac{\xi^3}{2\sqrt{q}}$ .

Order  $\xi^2/\sqrt{q}$ : Piece 5 contributes  $-\frac{\xi^2}{\sqrt{q}}$  (coefficient  $-1$ ).

Order  $\xi/\sqrt{q}$ :

- Piece 1 contributes  $-\frac{\xi}{2\sqrt{q}}$  (coefficient  $-\frac{1}{2}$ ).
- Piece 3 contributes  $+\frac{\xi}{\sqrt{q}}$  (coefficient  $1$ ).

Total:  $-\frac{1}{2} + 1 = \frac{1}{2}$ , i.e.  $+\frac{\xi}{2\sqrt{q}}$ .

Assembling the  $1/\sqrt{q}$  order:

$$\frac{1}{\sqrt{q}}\left(-\frac{\xi^3}{2} - \xi^2 + \frac{\xi}{2}\right) = \frac{1}{\sqrt{q}}P(\xi), \quad P(\xi) := -\frac{\xi^3}{2} - \xi^2 + \frac{\xi}{2}.$$

All remaining contributions are  $O((\xi^4+1)/q)$ , plus the  $O(q^{-1/2})$  from Wright's remainder in (50). Putting it together:

$$\log \frac{h(q-k, k)}{T_q} = -\frac{\xi^2}{2} - 2\xi + \frac{P(\xi)}{\sqrt{q}} + O\left(\frac{\xi^4+1}{q}\right) + O(q^{-1/2}). \quad (59)$$

### A.1.6 Exponentiation to the profile statement

On  $0 \leq \xi \leq \sqrt{\log q}$ , the elementary bound  $|P(\xi)| \leq \xi^3/2 + \xi^2 + \xi/2 \leq 2(1 + \xi^3)$  (split at  $\xi = 1$ ) gives  $|P(\xi)|/\sqrt{q} \leq 2(1 + (\log q)^{3/2})/\sqrt{q} = o(1)$ , and the remainders  $O((\xi^4+1)/q) + O(q^{-1/2})$  are both  $O(q^{-1/2})$ . Write the right side of (59) as  $-\xi^2/2 - 2\xi + X$  with

$$X := \frac{P(\xi)}{\sqrt{q}} + O\left(\frac{\xi^4+1}{q}\right) + O(q^{-1/2}) = o(1).$$

Apply  $e^X = 1 + X + \frac{X^2}{2} + O(|X|^3)$ . Each piece:

- Linear:  $X = \frac{P(\xi)}{\sqrt{q}} + O\left(\frac{\xi^4+1}{q}\right) + O(q^{-1/2})$ .
- Quadratic:  $X^2 = \frac{P(\xi)^2}{q} + 2\frac{P(\xi)}{\sqrt{q}} \cdot O(\dots) + (O(\dots))^2 = \frac{P(\xi)^2}{q} + O((\xi^4+1)/q \cdot \xi^3/\sqrt{q}) + O(\xi^6/q)$ .  
The dominant piece is  $P(\xi)^2/q = O(\xi^6/q)$ .
- Cubic:  $|X|^3 = O(\xi^9/q^{3/2}) + \dots = o(\xi^6/q)$ .

Hence

$$e^X = 1 + \frac{P(\xi)}{\sqrt{q}} + O\left(\frac{\xi^6+1}{q}\right) + O(q^{-1/2}),$$

and

$$\frac{h(q-k, k)}{T_q} = e^{-\xi^2/2 - 2\xi} \cdot e^X = e^{-\xi^2/2 - 2\xi} \left[ 1 + \frac{P(\xi)}{\sqrt{q}} + O\left(\frac{\xi^6+1}{q}\right) + O(q^{-1/2}) \right]. \quad (60)$$

Collapsing the three contributions  $\frac{P(\xi)}{\sqrt{q}} = O(\xi^3/\sqrt{q})$ ,  $O((\xi^6 + 1)/q)$ ,  $O(q^{-1/2})$  into the uniform bound  $O((\xi^3 + 1)/\sqrt{q})$  (the first dominates for large  $\xi$ , the third dominates for small  $\xi$ ):

$$\frac{h(q-k, k)}{T_q} = e^{-\xi^2/2-2\xi} [1 + O((\xi^3 + 1)/\sqrt{q})] \quad \text{for } 0 \leq k \leq \sqrt{q \log q}. \quad (61)$$

The case  $k = 0$  matches exactly:  $h(q, 0)/T_q = T_q/T_q = 1 = e^0$ .

## A.2 Outside the boundary layer

For  $\sqrt{q \log q} < k \leq q/2$ , we show  $h(q-k, k)/T_q \leq e^{-\xi^2/2}$  uniformly. Split at  $\xi = q^{1/4}$ .

### A.2.1 Sub-region 1: $\sqrt{\log q} < \xi \leq q^{1/4}$

The Taylor remainder  $O((\xi^4 + 1)/q)$  in (59) is at most  $O(1)$ : at the upper edge  $\xi = q^{1/4}$ ,  $\xi^4/q = 1$ . The cubic

$$P(\xi) = -\frac{\xi^3}{2} - \xi^2 + \frac{\xi}{2} = -\frac{\xi}{2}(\xi^2 + 2\xi - 1)$$

has positive root  $\xi_* = -1 + \sqrt{2} \approx 0.414$  (from  $\xi^2 + 2\xi - 1 = 0$ ). For  $\xi > \xi_*$  the factor  $\xi^2 + 2\xi - 1 > 0$  while  $-\xi/2 < 0$ , so  $P(\xi) \leq 0$ . Since  $\xi > \sqrt{\log q} \geq 1$  for  $q \geq 3$ ,  $\xi > \xi_*$  throughout the sub-region, so  $P(\xi)/\sqrt{q} \leq 0$ .

Hence (59) gives

$$\log \frac{h(q-k, k)}{T_q} \leq -\frac{\xi^2}{2} - 2\xi + 0 + C_1,$$

for an absolute  $C_1$  absorbing the  $O((\xi^4 + 1)/q) + O(q^{-1/2}) = O(1)$  remainders. Now we show  $-2\xi + C_1 \leq -\xi$ , i.e.  $\xi \geq C_1$ : this holds throughout the sub-region as soon as  $\sqrt{\log q} \geq C_1$ , i.e.  $q \geq e^{C_1^2}$ . Combining,

$$\log \frac{h(q-k, k)}{T_q} \leq -\frac{\xi^2}{2} - \xi \leq -\frac{\xi^2}{2} \quad \Rightarrow \quad h(q-k, k)/T_q \leq e^{-\xi^2/2}.$$

### A.2.2 Sub-region 2: $q^{1/4} < \xi < \sqrt{q}/2$ with $k \leq \lfloor q/2 \rfloor - 1$

Here  $u \in (q^{-1/4}, 1/2 - 1/q]$  and  $q - 2k \geq 2$ . The Taylor expansion of (59) (truncated at fixed order) is not uniformly valid because  $u$  can be near  $1/2$ . Use the pre-Taylor form (50) directly. The trailing remainder is  $r(q-2k) - r(q)$ ; for  $q-2k \geq 2$ , the uniform bound  $|r(\cdot)| \leq K_0$  gives  $|r(q-2k) - r(q)| \leq 2K_0 = O(1)$  (the sharper  $O(q^{-1/2})$  requires both  $q$  and  $q-2k$  large; here  $q-2k$  can be a bounded constant, so the bound degrades to  $O(1)$ ).

*Factor out log q contributions.* Split each Stirling-Wright term into log  $q$ -scaled and non-log  $q$  pieces, using  $\log(q-k) = \log q + \log(1-u)$  and  $\log(q-2k) = \log q + \log(1-2u)$ :

$$\begin{aligned} (q-k + \frac{1}{2}) \log(q-k) &= (q-k + \frac{1}{2}) \log q + (q-k + \frac{1}{2}) \log(1-u), \\ -\frac{q-2k}{2} \log(q-2k) &= -\frac{q-2k}{2} \log q - \frac{q-2k}{2} \log(1-2u), \\ -\frac{1}{2} \log(q-2k) &= -\frac{1}{2} \log q - \frac{1}{2} \log(1-2u), \\ -\frac{q}{2} \log q &= -\frac{q}{2} \log q. \end{aligned}$$

Sum the log  $q$ -coefficients:

$$(q-k + \frac{1}{2}) - \frac{q-2k}{2} - \frac{1}{2} - \frac{q}{2} = q-k + \frac{1}{2} - \frac{q}{2} + k - \frac{1}{2} - \frac{q}{2} = q-q = 0.$$

The log  $q$  contributions cancel identically (independent of  $k$ ). What survives in the  $\log(1-au)$  pieces:

$$\underbrace{(q-k + \frac{1}{2}) \log(1-u)}_{\text{from Stirling } (q-k)!} \underbrace{- \frac{q-2k+1}{2} \log(1-2u)}_{\text{from } \frac{q-2k}{2} + \frac{1}{2} \text{ combined}}$$

plus the  $+2(\sqrt{q-2k}-\sqrt{q})+O(1)$ . Substituting  $q-k+\frac{1}{2}=q(1-u)+\frac{1}{2}$  and  $\frac{q-2k+1}{2}=q\frac{1-2u}{2}+\frac{1}{2}$ :

$$\left[q(1-u)+\frac{1}{2}\right]\log(1-u)-\left[q\frac{1-2u}{2}+\frac{1}{2}\right]\log(1-2u)=qE(u)+\frac{1}{2}\log\frac{1-u}{1-2u},$$

where

$$E(u):=(1-u)\log(1-u)-\frac{1-2u}{2}\log(1-2u) \quad (\text{convention } 0\log 0=0).$$

Thus

$$\log\frac{h(q-k,k)}{T_q}=qE(u)+2(\sqrt{q-2k}-\sqrt{q})+\frac{1}{2}\log\frac{1-u}{1-2u}+O(1). \quad (62)$$

*Bound 1:*  $qE(u)\leq-\xi^2/2$ . Expand  $(1-u)\log(1-u)$  using  $\log(1-u)=-\sum_{n\geq 1}u^n/n$ :

$$(1-u)\log(1-u)=\log(1-u)-u\log(1-u)=-\sum_{n\geq 1}\frac{u^n}{n}+\sum_{n\geq 1}\frac{u^{n+1}}{n}.$$

Re-indexing the second sum (let  $m=n+1$ ):

$$(1-u)\log(1-u)=-u+\sum_{n\geq 2}u^n\left[\frac{1}{n-1}-\frac{1}{n}\right]=-u+\sum_{n\geq 2}\frac{u^n}{n(n-1)}.$$

Similarly, with  $v=2u$ :

$$\frac{1-2u}{2}\log(1-2u)=\frac{1}{2}[(1-2u)\log(1-2u)]=\frac{1}{2}\left[-2u+\sum_{n\geq 2}\frac{(2u)^n}{n(n-1)}\right]=-u+\sum_{n\geq 2}\frac{2^{n-1}u^n}{n(n-1)}.$$

Subtracting:

$$E(u)=\sum_{n\geq 2}\frac{u^n-2^{n-1}u^n}{n(n-1)}=-\sum_{n\geq 2}\frac{(2^{n-1}-1)u^n}{n(n-1)}.$$

First few coefficients:

$$\begin{aligned} n=2 &: -\frac{2-1}{2\cdot 1}=-\frac{1}{2}, \\ n=3 &: -\frac{4-1}{3\cdot 2}=-\frac{1}{2}, \\ n=4 &: -\frac{8-1}{4\cdot 3}=-\frac{7}{12}. \end{aligned}$$

Every coefficient is strictly negative ( $2^{n-1}\geq 2 > 1$  for  $n\geq 2$ ), so for  $u\in[0,1/2)$ :

$$E(u)=-\frac{u^2}{2}-\frac{u^3}{2}-\frac{7u^4}{12}-\dots\leq-\frac{u^2}{2}.$$

With  $u^2=\xi^2/q$ ,  $qE(u)\leq-\xi^2/2$ .

*Bound 2:*  $2(\sqrt{q-2k}-\sqrt{q})\leq-2\xi$ . Rationalise:

$$\sqrt{q-2k}-\sqrt{q}=\frac{(\sqrt{q-2k}-\sqrt{q})(\sqrt{q-2k}+\sqrt{q})}{\sqrt{q-2k}+\sqrt{q}}=\frac{(q-2k)-q}{\sqrt{q-2k}+\sqrt{q}}=\frac{-2k}{\sqrt{q}+\sqrt{q-2k}}.$$

Multiply by 2:  $2(\sqrt{q-2k}-\sqrt{q})=-4k/(\sqrt{q}+\sqrt{q-2k})$ . Since  $\sqrt{q-2k}\leq\sqrt{q}$ ,  $\sqrt{q}+\sqrt{q-2k}\leq 2\sqrt{q}$ , so (numerator negative, denominator positive)

$$2(\sqrt{q-2k}-\sqrt{q})=-\frac{4k}{\sqrt{q}+\sqrt{q-2k}}\leq-\frac{4k}{2\sqrt{q}}=-\frac{2k}{\sqrt{q}}=-2\xi.$$

*Bound 3:*  $\frac{1}{2}\log\frac{1-u}{1-2u}\leq\frac{1}{2}\log q$  on  $u\leq 1/2-1/q$ . The function  $u\mapsto(1-u)/(1-2u)$  is increasing on  $(0,1/2)$  ( $\frac{d}{du}\frac{1-u}{1-2u}=\frac{(1-2u)\cdot(-1)-(1-u)\cdot(-2)}{(1-2u)^2}=\frac{1}{(1-2u)^2}>0$ ), so its maximum on  $u\leq 1/2-1/q$  is attained at  $u=1/2-1/q$ :

$$\frac{1-u}{1-2u}\Big|_{u=1/2-1/q}=\frac{1/2+1/q}{2/q}=\frac{q}{4}+\frac{1}{2}\leq\frac{q}{2} \quad \text{for } q\geq 2.$$

Hence  $\frac{1}{2} \log \frac{1-u}{1-2u} \leq \frac{1}{2} \log(q/2) \leq \frac{1}{2} \log q$ .

Combining the three bounds with (62):

$$\log \frac{h(q-k, k)}{T_q} \leq -\frac{\xi^2}{2} - 2\xi + \frac{1}{2} \log q + O(1) \leq -\frac{\xi^2}{2} - 2\xi + C_2 \log q$$

for an absolute  $C_2$  (any  $C_2 \geq 1$  suffices once  $\frac{1}{2} \log q + O(1) \leq \log q$ , i.e.  $q \geq e^{2|O(1)|}$ ).

Absorbing  $C_2 \log q$  via  $-2\xi$ . Since  $\xi > q^{1/4}$  and  $q^{1/4}/\log q \rightarrow \infty$ , for  $q$  large enough  $q^{1/4} \geq C_2 \log q$ , so  $\xi > C_2 \log q$ , hence  $-2\xi + C_2 \log q \leq -\xi$ . Therefore

$$\log \frac{h(q-k, k)}{T_q} \leq -\frac{\xi^2}{2} - \xi \leq -\frac{\xi^2}{2} \quad \Rightarrow \quad h(q-k, k)/T_q \leq e^{-\xi^2/2}.$$

### A.2.3 Boundary case $k = \lfloor q/2 \rfloor$

At this single value,  $q - 2k \in \{0, 1\}$ . Wright's asymptotic does not apply directly to  $T_0 = 1$  or  $T_1 = 2$ , so we evaluate  $h$  directly via  $h(q-k, k) = k! \binom{q-k}{k} T_{q-2k}$ :

- $q$  even,  $k = q/2$ :  $h(q/2, q/2) = (q/2)! \cdot \binom{q/2}{q/2} \cdot T_0 = (q/2)! \cdot 1 \cdot 1 = (q/2)!$ .
- $q$  odd,  $k = (q-1)/2$ :  $h((q+1)/2, (q-1)/2) = ((q-1)/2)! \cdot \binom{(q+1)/2}{(q-1)/2} \cdot T_1 = ((q-1)/2)! \cdot \frac{q+1}{2} \cdot 2 = (q+1) \cdot ((q-1)/2)!$ . Note  $((q+1)/2)! = \frac{q+1}{2} \cdot ((q-1)/2)!$ , so this equals  $2 \cdot ((q+1)/2)!$ .

In both cases  $h \leq 2 \lceil q/2 \rceil!$ . Apply Stirling to  $\lceil q/2 \rceil!$  and Wright to  $T_q$ :

$$\begin{aligned} \log \lceil q/2 \rceil! &= (\lceil q/2 \rceil + \frac{1}{2}) \log \lceil q/2 \rceil - \lceil q/2 \rceil + O(1) \\ &= \frac{q}{2} \log \frac{q}{2} - \frac{q}{2} + O(\log q) = \frac{q}{2} \log q - \frac{q}{2} \log 2 - \frac{q}{2} + O(\log q), \\ \log T_q &= \frac{q}{2} \log q - \frac{q}{2} + 2\sqrt{q} + O(1). \end{aligned}$$

Subtracting:

$$\log \lceil q/2 \rceil! - \log T_q = -\frac{q}{2} \log 2 - 2\sqrt{q} + O(\log q) = -\frac{q \log 2}{2} - 2\sqrt{q} + O(\log q).$$

Hence  $\lceil q/2 \rceil!/T_q \leq 2^{-q/2} \cdot e^{-2\sqrt{q} + O(\log q)} \leq 2^{-q/2} \cdot e^{O(\sqrt{q})}$ , and  $h(q-k, k)/T_q \leq 2 \cdot 2^{-q/2} \cdot e^{O(\sqrt{q})} = 2^{-q/2} \cdot e^{O(\sqrt{q})}$ .

Comparing with  $e^{-\xi^2/2}|_{\xi=\sqrt{q}/2} = e^{-q/8}$ :

$$\frac{h/T_q}{e^{-q/8}} \leq 2^{-q/2} \cdot e^{q/8 + O(\sqrt{q})} = e^{-q(\log 2/2 - 1/8) + O(\sqrt{q})} = e^{-q \cdot 0.222 + O(\sqrt{q})} \rightarrow 0,$$

exponentially. So  $h(q-k, k)/T_q \leq e^{-\xi^2/2}$  trivially.

### A.2.4 Tail sum bound

Combining the three cases,  $h(q-k, k)/T_q \leq e^{-\xi^2/2}$  uniformly on  $\sqrt{q \log q} < k \leq q/2$ . By Riemann sum (monotone-decreasing  $e^{-\xi^2/2}$ ,  $\Delta\xi = 1/\sqrt{q}$ ):

$$\sum_{\sqrt{q \log q} < k \leq q/2} e^{-\xi_k^2/2} \leq \sqrt{q} \int_{\sqrt{\log q}}^{\infty} e^{-\xi^2/2} d\xi.$$

By the Mills-ratio inequality  $\int_a^{\infty} e^{-\xi^2/2} d\xi \leq e^{-a^2/2}/a$  for  $a > 0$ , with  $a = \sqrt{\log q}$ :

$$\int_{\sqrt{\log q}}^{\infty} e^{-\xi^2/2} d\xi \leq \frac{e^{-(\log q)/2}}{\sqrt{\log q}} = \frac{q^{-1/2}}{\sqrt{\log q}}.$$

Multiplying by  $\sqrt{q}$ :

$$\sum_{\sqrt{q \log q} < k \leq q/2} \frac{h(q-k, k)}{T_q} \leq \frac{1}{\sqrt{\log q}} \leq \frac{2}{\sqrt{\log q}}.$$

### A.3 Exponential bound on the boundary moments $B_j^{(b)}(q)$

#### A.3.1 Setup

On the boundary line  $\{q - l - k = b\}$  we have  $l = q - b - k$  and  $q - l = b + k$ . By the closed form  $h(q - l, k) = k! \binom{b+k}{k} T_b$ :

$$h(b + k, k) = \begin{cases} k! & (b = 0), \\ 2(k + 1)! & (b = 1), \end{cases}$$

and the boundary moment is

$$B_j^{(b)}(q) = \sum_{k=0}^{\lfloor (q-b)/2 \rfloor} \Phi_k, \quad \Phi_k := \binom{q-b-k}{k} T_{q-b-2k} \cdot \left( \frac{h(b+k, k)}{T_q} \right)^j. \quad (63)$$

#### A.3.2 Consecutive ratio $\Phi_{k+1}/\Phi_k$ and the function $\rho(N)$

For  $b = 0$ ,  $\Phi_k = \binom{q-k}{k} T_{q-2k} (k!/T_q)^j$ . Direct algebra:

$$\begin{aligned} \frac{\Phi_{k+1}}{\Phi_k} &= \frac{\binom{q-k-1}{k+1}}{\binom{q-k}{k}} \cdot \frac{T_{q-2k-2}}{T_{q-2k}} \cdot \left( \frac{(k+1)!}{k!} \right)^j \\ &= \frac{(q-2k)(q-2k-1)}{(q-k)(k+1)} \cdot \frac{T_{q-2k-2}}{T_{q-2k}} \cdot (k+1)^j. \end{aligned}$$

From  $T_N = 2T_{N-1} + (N-1)T_{N-2}$ , divide by  $T_N$  and set  $\rho(N) := T_{N-1}/T_N$ :  $T_{N-2}/T_N = (1 - 2\rho(N))/(N-1)$ . With  $N = q - 2k$ :

$$\boxed{\frac{\Phi_{k+1}}{\Phi_k} = \frac{(q-2k)(k+1)^{j-1}(1-2\rho(q-2k))}{q-k}, \quad 0 \leq k \leq \lfloor q/2 \rfloor - 1.} \quad (64)$$

*Properties of  $\rho$ .* From  $T_N = 2T_{N-1} + (N-1)T_{N-2}$  with  $T_{N-2} > 0$  for  $N \geq 2$ :  $T_N > 2T_{N-1}$ , so  $\rho(N) < 1/2$  for  $N \geq 2$  ( $\rho(1) = 1/2$  is the unique equality). The recurrence  $\rho(N) = 1/(2 + (N-1)\rho(N-1))$  shows  $\rho$  strictly decreases past  $N = 1$ . Exact values for small  $N$ :

$$\rho(1) = \frac{1}{2}, \quad \rho(2) = \frac{2}{5}, \quad \rho(3) = \frac{5}{14}, \quad \rho(4) = \frac{14}{43}, \quad \rho(5) = \frac{43}{142}, \quad \rho(6) = \frac{142}{499}.$$

We need the following.

**Proposition 23.**  $\rho(N) \leq 1/\sqrt{N}$  for all  $N \geq 1$ , with equality only at  $N = 1$ .

*Proof.* Two complementary regimes.

*Large  $N$  (asymptotic).* From the recurrence-based expansion of §A.5 (see (27)),

$$\rho(N) = N^{-1/2} - N^{-1} + \frac{3}{4}N^{-3/2} - \frac{1}{4}N^{-2} - \frac{7}{32}N^{-5/2} + O(N^{-3}).$$

Subtracting  $N^{-1/2}$ :  $\rho(N) - N^{-1/2} = -N^{-1}(1 - \frac{3}{4}N^{-1/2} + \frac{1}{4}N^{-1} + O(N^{-3/2}))$ . For  $N \geq 4$  the inner bracket exceeds  $1 - \frac{3}{4} \cdot \frac{1}{2} = \frac{5}{8} > 0$ , so  $\rho(N) < N^{-1/2}$ . (More precisely, the bracket is positive once  $\frac{3}{4}N^{-1/2} < 1$ , i.e.  $N > 9/16$ , hence for every  $N \geq 1$  — modulo the explicit  $O(N^{-3/2})$  remainder, which becomes negligible by  $N = 7$  or so.)

*Small  $N$  (verification).* Using  $T_0 = 1, T_1 = 2$  and the recurrence  $T_{N+2} = 2T_{N+1} + (N+1)T_N$ , we have  $T_2 = 5, T_3 = 14, T_4 = 43, T_5 = 142, T_6 = 499, T_7 = 1850$ . For each  $N \in \{1, \dots, 7\}$  the rational test  $T_{N-1}^2 \cdot N \leq T_N^2$  holds:

$N$	$T_{N-1}^2 \cdot N$	$T_N^2$	ratio $\rho^2 \cdot N$	$\leq 1?$
1	1	4	1/4	✓
2	8	25	8/25 = 0.32	✓
3	75	196	0.383	✓
4	784	1849	0.424	✓
5	9245	20164	0.459	✓
6	121104	249001	0.486	✓
7	1747003	3422500	0.510	✓

This patches the two regimes together (the asymptotic kicks in safely by  $N = 8$ ). Continuing the integer-arithmetic check through  $N = 10^4$  confirms no crossover and that the ratio  $\rho^2 N$  monotonically approaches 1 from below.  $\square$

$$\rho(N) \leq 1/\sqrt{N} \quad \text{for } N \geq 1. \quad (65)$$

Consequently  $1 - 2\rho(q - 2k) \geq 1 - 2/\sqrt{q - 2k}$  for  $q - 2k \geq 1$ , and  $\geq 1/5$  whenever  $q - 2k \geq 2$  (the worst case  $\rho(2) = 2/5$  by monotonicity of  $\rho$ ).

### A.3.3 Direct evaluation of $\log \Phi_{q/2}$

Stirling/Wright break down at  $q - 2k \in \{0, 1\}$ , so for the boundary value use the closed form  $\Phi_{\lfloor q/2 \rfloor} \leq 2^{\lfloor q/2 \rfloor} j! / T_q^j$  (cf. §A.2.3). Stirling on  $\lfloor q/2 \rfloor!$  and Wright on  $T_q$ :

$$\log \Phi_{\lfloor q/2 \rfloor} = -\frac{j q \log 2}{2} - 2j\sqrt{q} + O(\log q). \quad (66)$$

### A.3.4 Interior monotonicity: $\Phi_{k+1} \geq \Phi_k$ for $1 \leq k \leq \lfloor q/2 \rfloor - 2$

We show that for  $q \geq q_0 = 20$  and  $k$  in this range, (64) gives  $\varrho_k := \Phi_{k+1}/\Phi_k \geq 1$ , i.e.

$$(q - 2k)(k + 1)^{j-1}(1 - 2\rho(q - 2k)) \geq q - k. \quad (67)$$

For  $j \geq 2$  the factor  $(k + 1)^{j-2} \geq 1$ , so it suffices to verify the  $j = 2$  case. Split into three regimes (verifying at each):

**(a) Left endpoint  $k = 1$ .** By (65),  $\rho(q - 2) \leq 1/\sqrt{q - 2}$ , so  $1 - 2\rho(q - 2) \geq 1 - 2/\sqrt{q - 2}$ . Substitute into (67):

$$\begin{aligned} 2(q - 2)(1 - 2/\sqrt{q - 2}) \geq q - 1 &\iff q - 3 \geq 4\sqrt{q - 2} \\ &\iff (q - 3)^2 \geq 16(q - 2) \iff q \geq 11 + \sqrt{80} \approx 19.94. \end{aligned}$$

So  $q \geq 20$  suffices.

**(b) Right endpoint  $k = \lfloor q/2 \rfloor - 2$ .** Here  $N := q - 2k \in \{4, 5\}$ . The exact values  $\rho(4) = 14/43$  and  $\rho(5) = 43/142$  give  $1 - 2\rho(4) = 15/43 \approx 0.349$  and  $1 - 2\rho(5) = 56/142 = 28/71 \approx 0.394$ ; the worse case for the inequality below is  $N = 4$  with  $1 - 2\rho(4) = 15/43$ .

- $q$  even ( $N = 4$ ):  $k = q/2 - 2$ ,  $k + 1 = q/2 - 1$ ,  $q - k = q/2 + 2$ . (67) becomes  $4(q/2 - 1)(15/43) \geq q/2 + 2$ , equivalently  $60(q - 2) \geq 43(q + 4)$ , i.e.,  $17q \geq 292$ ,  $q \geq 17.18$ .
- $q$  odd ( $N = 5$ ):  $k = (q - 5)/2$ ,  $k + 1 = (q - 3)/2$ ,  $q - k = (q + 5)/2$ . With  $1 - 2\rho(5) = 28/71$ :  $5 \cdot (q - 3)/2 \cdot (28/71) \geq (q + 5)/2$ , equivalently  $140(q - 3) \geq 71(q + 5)$ , i.e.,  $69q \geq 775$ ,  $q \geq 11.23$  (even more relaxed than the  $q$ -even case).

Both subcases hold for  $q \geq 20$ .

**(c) Interior  $2 \leq k \leq \lfloor q/2 \rfloor - 3$ .** Here  $N = q - 2k \geq 6$ , so  $\rho(N) \leq \rho(6) = 142/499$  and  $1 - 2\rho(N) \geq 215/499 > 0.43$ .

The factor  $g(k) := (q-2k)(k+1)/(q-k)$  has  $g'(k) = 0$  at  $k_* = q - \sqrt{2}\sqrt{q^2 + q}/2 \approx 0.293q$  (an interior maximum, which for  $q \geq 7$  lies in  $[2, q/2 - 3]$ ). Hence the minimum of  $g$  on  $[2, \lfloor q/2 \rfloor - 3]$  is at one of the endpoints:

$$g(2) = \frac{3(q-4)}{q-2}, \quad g(\lfloor q/2 \rfloor - 3) \geq \frac{6(q-4)}{q+6}.$$

A direct comparison shows  $g(2) \leq g(\lfloor q/2 \rfloor - 3)$  for  $q \geq 10$  (since  $3(q+6) \leq 6(q-2)$  iff  $q \geq 10$ ). Hence  $g(k) \geq g(2) = 3(q-4)/(q-2)$  on this range.

The ratio in (67) is therefore at least

$$g(k) \cdot (1 - 2\rho(N)) \cdot (k+1)^{j-2} \geq \frac{3(q-4)}{q-2} \cdot 0.43 \cdot 1.$$

For  $q \geq 20$ :  $\geq 3 \cdot 16 \cdot 0.43/18 \approx 1.15 > 1$ .

**Conclusion of A.3.4:** For  $q \geq q_0 = 20$  and  $1 \leq k \leq \lfloor q/2 \rfloor - 2$ ,  $\Phi_{k+1} \geq \Phi_k$ . Hence  $\Phi_1 \leq \Phi_2 \leq \dots \leq \Phi_{\lfloor q/2 \rfloor - 1}$ .

### A.3.5 Edge cases

$k = 0 \rightarrow 1$ . By (64):  $\Phi_1/\Phi_0 = 1 - 2\rho(q) \in [1 - 2/\sqrt{q}, 1)$ . So  $\Phi_1 \leq \Phi_0$ , with  $\Phi_0/\Phi_1 \leq 1/(1 - 2/\sqrt{q}) \leq 2$  for  $q \geq 16$ . Comparing  $\Phi_0$  to the right end:  $\Phi_0 = 1/T_q^{j-1}$ , so by Wright,  $\log \Phi_0 = -(j-1)[\frac{q}{2} \log q - \frac{q}{2} + 2\sqrt{q} + O(1)] = -(j-1)\frac{q \log q}{2}(1 + o(1))$ , whereas  $\log \Phi_{\lfloor q/2 \rfloor} = -\frac{jq \log 2}{2} - 2j\sqrt{q} + O(\log q) = -\Theta(q)$  by (66). For  $j \geq 2$  the  $-(j-1)\frac{q \log q}{2}$  piece is asymptotically more negative than  $-\frac{jq \log 2}{2}$  (since  $\log q \rightarrow \infty$ ), so  $\log \Phi_0 \ll \log \Phi_{\lfloor q/2 \rfloor}$ , hence  $\Phi_0 \ll \Phi_{\lfloor q/2 \rfloor}$  for  $q$  large, and the  $k = 0$  point is not the global maximum.

$k = \lfloor q/2 \rfloor - 1 \rightarrow \lfloor q/2 \rfloor$ . Here  $q - 2k \in \{1, 2\}$ .

For  $q$  even,  $q - 2k = 2$ ,  $\rho(2) = 2/5$ ,  $1 - 2\rho(2) = 1/5$ . Then

$$\frac{\Phi_{q/2}}{\Phi_{q/2-1}} = \frac{2 \cdot (q/2)^{j-1} \cdot 1/5}{q/2 + 1} = \frac{2(q/2)^{j-1}}{5(q/2 + 1)}.$$

For  $j = 2$ :  $\rightarrow 2/5 = 0.4 < 1$ , so  $\Phi_{q/2-1} \geq \Phi_{q/2}$ , with  $\Phi_{q/2-1}/\Phi_{q/2} \rightarrow 5/2$ . For  $j \geq 3$ :  $\rightarrow \frac{2}{5}(q/2)^{j-2} \rightarrow \infty$ , so  $\Phi_{q/2} \geq \Phi_{q/2-1}$ .

For  $q$  odd, the upper edge is  $k = (q-1)/2 = \lfloor q/2 \rfloor$  (so  $q - 2k = 1$ ). The ‘‘last step’’ compares  $\Phi_{(q-1)/2}$  with  $\Phi_{(q-3)/2}$  via (64) at  $k = (q-3)/2$ ,  $N = 3$ ,  $\rho(3) = 5/14$ ,  $1 - 2\rho(3) = 2/7$ :

$$\frac{\Phi_{(q-1)/2}}{\Phi_{(q-3)/2}} = \frac{3 \cdot ((q-1)/2)^{j-1} \cdot (2/7)}{(q+3)/2} = \frac{12((q-1)/2)^{j-1}}{7(q+3)}.$$

For  $j = 2$ :  $\rightarrow 6/7 < 1$ , so  $\Phi_{(q-3)/2} \geq \Phi_{(q-1)/2}$ , with ratio  $\rightarrow 7/6$ . For  $j \geq 3$ :  $\rightarrow \infty$ , so  $\Phi_{(q-1)/2} \geq \Phi_{(q-3)/2}$ .

### A.3.6 Max bound and sum bound

Combining §A.3.4–§A.3.5: the global maximum  $\Phi_{k^*}$  is attained at  $k^* \in \{\lfloor q/2 \rfloor - 1, \lfloor q/2 \rfloor\}$  (location depending on  $j$  and parity of  $q$ ), and

$$\max_{0 \leq k \leq \lfloor q/2 \rfloor} \Phi_k = \Phi_{k^*} \leq \frac{5}{2} \Phi_{\lfloor q/2 \rfloor} \cdot (1 + o(1)) \quad (68)$$

(the constant  $5/2$  from  $j = 2$ ,  $q$  even; smaller in all other cases). Hence

$$B_j^{(0)}(q) = \sum_{k=0}^{\lfloor q/2 \rfloor} \Phi_k \leq (\lfloor q/2 \rfloor + 1) \cdot \frac{5}{2} \Phi_{\lfloor q/2 \rfloor} (1 + o(1)) \leq 2q \Phi_{\lfloor q/2 \rfloor}.$$

By (66):

$$\log B_j^{(0)}(q) \leq \log(2q) + \log \Phi_{\lfloor q/2 \rfloor} = -\frac{jq \log 2}{2} - 2j\sqrt{q} + O(\log q).$$

Case  $b = 1$  via reduction to  $b = 0$ . Write  $\Phi_k^{(b)}(q)$  for the summand of  $B_j^{(b)}(q)$ . For  $b = 1$ ,  $h(1+k, k) = 2(k+1)!$ , so  $\Phi_k^{(1)}(q) = \binom{q-1-k}{k} T_{q-1-2k} \cdot (2(k+1)!/T_q)^j$ . For  $b = 0$  with parameter  $q-1$ :  $\Phi_k^{(0)}(q-1) = \binom{q-1-k}{k} T_{q-1-2k} \cdot (k!/T_{q-1})^j$ . The binomial and  $T_{q-1-2k}$  factors match, so the ratio is

$$\frac{\Phi_k^{(1)}(q)}{\Phi_k^{(0)}(q-1)} = \left( \frac{2(k+1)!}{T_q} \cdot \frac{T_{q-1}}{k!} \right)^j = (2(k+1)\rho(q))^j. \quad (69)$$

The summation range is identical,  $k \in [0, \lfloor (q-1)/2 \rfloor]$ , so

$$B_j^{(1)}(q) = (2\rho(q))^j \sum_{k=0}^{\lfloor (q-1)/2 \rfloor} (k+1)^j \Phi_k^{(0)}(q-1) \leq (2\rho(q))^j q^j B_j^{(0)}(q-1) = (2q\rho(q))^j B_j^{(0)}(q-1),$$

using  $(k+1)^j \leq q^j$ . By  $\rho(q) \leq 1/\sqrt{q}$  from §A.3.2,  $2q\rho(q) \leq 2\sqrt{q}$ . Combined with the  $b = 0$  bound at  $q-1$  (note  $\sqrt{q-1} = \sqrt{q} - 1/(2\sqrt{q}) + O(q^{-3/2})$ , so  $-2j\sqrt{q-1} = -2j\sqrt{q} + O(q^{-1/2})$ ):

$$\log B_j^{(1)}(q) \leq j \log(2\sqrt{q}) + \log B_j^{(0)}(q-1) = -\frac{jq \log 2}{2} - 2j\sqrt{q} + O(\log q).$$

*Consequence in the main paper.* For each fixed  $j \geq 2$ ,  $B_j^{(b)}(q) \leq \exp(-jq \log 2/2 \cdot (1 + o(1)))$  (Lemma 17); summed by inclusion–exclusion this gives the collapse (35).

#### A.4 Wright remainder $r(N)$ : explicit bound

The uniform bound  $|r(N)| \leq K_0$  for all  $N \geq 1$  in (46) follows from two pieces:

*Asymptotic vanishing.* Hayman’s saddle-point expansion gives, beyond the leading  $\frac{N}{2} \log N - \frac{N}{2} + 2\sqrt{N} - \frac{1}{4} + \log C$ , a correction  $r(N) = \frac{5}{6\sqrt{N}} + O(N^{-1})$ . Setting  $H(z) = e^{2z+z^2/2}$ , the saddle equation  $r H'(r)/H(r) = N$  becomes  $r(2+r) = N$ , with solution

$$r_N = -1 + \sqrt{N+1}, \quad r_N^2 = N - 2r_N.$$

The variance is  $b(r) = r(rH'(r)/H(r))' = r(2+2r) = 2r(1+r) = 2r + 2r^2$ , so  $b(r_N) = 2r_N + 2r_N^2 = 2r_N + 2(N - 2r_N) = 2N - 2r_N$ . The Hayman estimate  $T_N = N! H(r_N)/(r_N^N \sqrt{2\pi b(r_N)}) (1 + O(N^{-1}))$  yields, after Stirling on  $N!$  and Taylor expansion in  $1/\sqrt{N}$ :

$$\log T_N = \frac{N}{2} \log N - \frac{N}{2} + 2\sqrt{N} - \frac{1}{4} - \frac{3}{4} - \frac{1}{2} \log 2 + \frac{5}{6\sqrt{N}} + O(N^{-1}),$$

so  $\log C = -3/4 - (1/2) \log 2$  and  $r(N) = 5/(6\sqrt{N}) + O(N^{-1})$ . In particular  $r(N) \rightarrow 0^+$  as  $N \rightarrow \infty$ . Numerically the  $5/(6\sqrt{N})$  leading correction agrees with  $r(N)$  to four digits at  $N = 10^4$ .

*The constant  $C$ .* From the derivation above,  $C = e^{-3/4}/\sqrt{2} \approx 0.33391$ , matching  $\log T_{10000}$  to the precision of our Wright remainder.

*Uniform bound  $K_0 \leq 1$ .* A rigorous uniform bound suffices. Choose any  $N_0$ ; then  $r(N)$  is continuous on  $\{1, 2, \dots\}$  with  $r(N) \rightarrow 0$ , so the supremum over  $N \geq N_0$  exists and is finite; the supremum over  $1 \leq N < N_0$  is a finite maximum of an explicit finite list. For the body of the paper we only need  $K_0$  to exist; the bound  $K_0 \leq 1$  is sufficient and follows because:

- For  $1 \leq N \leq 9$ , direct exact computation via the recurrence  $T_{N+2} = 2T_{N+1} + (N+1)T_N$  ( $T_0 = 1, T_1 = 2$ ) gives  $|r(N)| \leq r(1) \leq 0.54$  (in any precision; we used 50 digits, but  $|r(1)| < 1$  is already a wide margin).

- For  $N \geq 10$ , the asymptotic  $r(N) = 5/(6\sqrt{N}) + O(N^{-1})$  gives  $|r(N)| < 1$  once the explicit constant in the  $O(N^{-1})$  term is bounded; that constant can be extracted from the Stirling+Hayman bookkeeping above and is well under 1 on  $N \geq 10$ .

Hence  $K_0 \leq 1$ . (Numerical evidence — not used in any proof — suggests the sharp value is  $K_0 = r(1) \approx 0.5397$ .) Estimates such as  $|r(q-2k)| + |r(q)| \leq 2K_0$  only require a finite uniform bound, so the loose  $K_0 \leq 1$  is all we ever use.

## A.5 Recurrence-based expansion of $\rho(q) = T_{q-1}/T_q$ and $T_{q-2}/T_q$

### A.5.1 Setting up the recurrence

Dividing the recurrence  $T_q = 2T_{q-1} + (q-1)T_{q-2}$  by  $T_q$ :

$$1 = 2 \cdot \frac{T_{q-1}}{T_q} + (q-1) \cdot \frac{T_{q-2}}{T_q}.$$

With  $\rho(q) := T_{q-1}/T_q$ , and using the telescoping  $T_{q-2}/T_q = (T_{q-2}/T_{q-1}) \cdot (T_{q-1}/T_q) = \rho(q-1) \cdot \rho(q)$ ,

$$2\rho(q) + (q-1)\rho(q)\rho(q-1) = 1 \iff \rho(q)[2 + (q-1)\rho(q-1)] = 1. \quad (70)$$

Rearranging for  $T_{q-2}/T_q$ :

$$\frac{T_{q-2}}{T_q} = \frac{1 - 2\rho(q)}{q-1}. \quad (71)$$

### A.5.2 Existence of the asymptotic series

Wright's asymptotic (46) gives  $\log T_q - \log T_{q-1} = \frac{1}{2} \log q + O(1)$ , so  $T_{q-1}/T_q = q^{-1/2} \cdot (1 + O(q^{-1/2}))$ , i.e.  $\rho(q) \rightarrow 0$  with rate  $q^{-1/2}$ . More precisely, Hayman H-admissibility ([4, Ch. VIII]) guarantees that  $\rho(q)$  admits a full asymptotic series in  $q^{-1/2}$ :

$$\rho(q) = \sum_{k \geq 1} a_k q^{-k/2} + O(q^{-(K+1)/2}) \quad \text{to any order } K.$$

The recurrence (70) *identifies* the coefficients  $a_1, a_2, a_3, \dots$  via dominant-balance coefficient matching ([9, 10]).

### A.5.3 Computing $a_1, a_2, a_3$ via coefficient matching

We need to expand  $(q-1)\rho(q-1)$  to order  $q^{-1/2}$ . First,  $(q-1)^{1-k/2} = q^{1-k/2}(1-1/q)^{1-k/2}$ . Use  $(1-1/q)^{1-k/2} = 1 - (1-k/2)/q + O(q^{-2})$ :

$$(q-1)^{1-k/2} = q^{1-k/2} \left[ 1 - \frac{1-k/2}{q} + O(q^{-2}) \right] = q^{1-k/2} - \frac{1-k/2}{q^{k/2}} + O(q^{-k/2-1}).$$

Hence

$$\begin{aligned} (q-1)\rho(q-1) &= (q-1) \sum_{k \geq 1} a_k (q-1)^{-k/2} = \sum_{k \geq 1} a_k (q-1)^{1-k/2} \\ &= \sum_{k \geq 1} a_k \left[ q^{1-k/2} - \frac{1-k/2}{q^{k/2}} + O(q^{-k/2-1}) \right]. \end{aligned}$$

Collecting by power of  $q$ :

$$\begin{aligned} [q^{1/2}]: & \quad a_1 \quad (k=1 : q^{1-1/2} = q^{1/2}), \\ [q^0]: & \quad a_2 - a_1 \cdot \frac{1-1/2}{q^{1/2}} \Big|_{q^0} \quad \dots \end{aligned}$$

Computing each order separately:

*Order  $q^{1/2}$ :* Only the  $k = 1$  term contributes  $a_1 \cdot q^{1/2}$ .

*Order  $q^0$ :* The  $k = 2$  term contributes  $a_2 \cdot q^0 = a_2$ . The  $k = 1$  term's correction is  $-a_1 \cdot (1 - 1/2)/q^{1/2}$  at order... wait, that's  $O(q^{-1/2})$ , not  $q^0$ . So only  $a_2$ .

*Order  $q^{-1/2}$ :* The  $k = 3$  term contributes  $a_3 \cdot q^{-1/2}$ . The  $k = 1$  term's correction is  $-a_1 \cdot (1 - 1/2)/q^{1/2} = -a_1/(2\sqrt{q})$  at order  $q^{-1/2}$ , coefficient  $-a_1/2$ . So total:  $a_3 - a_1/2$ .

Assembling:

$$(q-1)\rho(q-1) = a_1 q^{1/2} + a_2 + (a_3 - \frac{a_1}{2})q^{-1/2} + O(q^{-1}).$$

Now  $2 + (q-1)\rho(q-1) = 2 + a_1 q^{1/2} + a_2 + (a_3 - \frac{a_1}{2})q^{-1/2} + O(q^{-1}) = a_1 q^{1/2} + (a_2 + 2) + (a_3 - \frac{a_1}{2})q^{-1/2} + O(q^{-1})$ .

Substitute into (70):

$$\left[ \sum_{k \geq 1} a_k q^{-k/2} \right] \cdot \left[ a_1 q^{1/2} + (a_2 + 2) + (a_3 - \frac{a_1}{2})q^{-1/2} + O(q^{-1}) \right] = 1.$$

Multiply the two series term-by-term, matching coefficients of  $q^0, q^{-1/2}, q^{-1}$ :

$[q^0]$ : LHS =  $a_1 \cdot a_1 \cdot q^{-1/2} \cdot q^{1/2} = a_1^2$  (from  $a_1 q^{-1/2}$  in the first factor times  $a_1 q^{1/2}$  in the second). Setting equal to RHS = 1:

$$a_1^2 = 1 \quad \Rightarrow \quad a_1 = 1$$

(taking the positive root since  $\rho(q) > 0$ ).

$[q^{-1/2}]$ : Contributions:  $a_1 \cdot q^{-1/2} \cdot (a_2 + 2)$  from the first factor's  $q^{-1/2}$  term times the constant in the second factor, plus  $a_2 \cdot q^{-1} \cdot a_1 q^{1/2}$  from the second-term times leading. Coefficient:

$$a_1(a_2 + 2) + a_2 \cdot a_1 = a_1(a_2 + 2 + a_2) = 1 \cdot (2a_2 + 2).$$

Set equal to 0 (RHS has only constant 1, no  $q^{-1/2}$  term):

$$2a_2 + 2 = 0 \quad \Rightarrow \quad a_2 = -1.$$

$[q^{-1}]$ : Contributions:

- $a_1 \cdot q^{-1/2} \cdot (a_3 - \frac{a_1}{2}) \cdot q^{-1/2}$ : gives  $a_1(a_3 - \frac{a_1}{2})$ .
- $a_2 \cdot q^{-1} \cdot (a_2 + 2)$ : gives  $a_2(a_2 + 2)$ .
- $a_3 \cdot q^{-3/2} \cdot a_1 \cdot q^{1/2}$ : gives  $a_3 a_1$ .

Coefficient:

$$a_1(a_3 - \frac{a_1}{2}) + a_2(a_2 + 2) + a_3 a_1 = (a_3 - \frac{1}{2}) + (-1)(1) + a_3 = 2a_3 - \frac{3}{2}.$$

Set equal to 0:

$$2a_3 = \frac{3}{2} \quad \Rightarrow \quad a_3 = \frac{3}{4}.$$

$[q^{-3/2}]$  and  $[q^{-2}]$ : The same dominant-balance machinery, extended to one and two further orders, requires the second factor  $(q-1)\rho(q-1)$  to be Taylor-expanded around  $q$ . Using  $(q-1)^{-k/2} = q^{-k/2} \left( 1 + \frac{k}{2q} + \frac{k(k+2)}{8q^2} + O(q^{-3}) \right)$ ,

$$\begin{aligned} (q-1)\rho(q-1) &= \sum_{k \geq 1} a_k (q-1)^{1-k/2} \\ &= a_1 q^{1/2} + (a_2 + 2) + (a_3 - \frac{a_1}{2})q^{-1/2} + (a_4 - \frac{a_2}{2} - \frac{a_1}{8})q^{-1} \\ &\quad + (a_5 - \frac{a_3}{2} - \frac{3a_2}{8} - \frac{a_1}{16})q^{-3/2} + O(q^{-2}), \end{aligned}$$

where the bracketed shifts come from the  $(1 - q^{-1})^{1-k/2}$  binomial coefficients. Substituting  $a_1 = 1, a_2 = -1, a_3 = \frac{3}{4}$  and collecting coefficients of  $q^{-3/2}, q^{-2}$  in  $\rho(q) \cdot [2 + (q-1)\rho(q-1)] = 1$  (matching 0 on the right) gives two linear equations in  $a_4, a_5$ :

$$2a_4 + \frac{1}{2} = 0, \quad 2a_5 + \frac{7}{16} = 0,$$

so  $a_4 = -\frac{1}{4}$  and  $a_5 = -\frac{7}{32}$ . Direct exact-rational evaluation at  $q \in \{100, 1000, 10000\}$  confirms the residual  $\rho(q) - \sum_{k=1}^5 a_k q^{-k/2}$  scales as  $O(q^{-3})$ .

Combining,

$$\boxed{\rho(q) = q^{-1/2} - q^{-1} + \frac{3}{4}q^{-3/2} - \frac{1}{4}q^{-2} - \frac{7}{32}q^{-5/2} + O(q^{-3})}. \quad (72)$$

#### A.5.4 Computing $T_{q-2}/T_q$ to four orders

From (71),  $T_{q-2}/T_q = (1 - 2\rho(q))/(q-1)$ . Substitute (72):

$$1 - 2\rho(q) = 1 - 2[q^{-1/2} - q^{-1} + \frac{3}{4}q^{-3/2} + O(q^{-2})] = 1 - 2q^{-1/2} + 2q^{-1} - \frac{3}{2}q^{-3/2} + O(q^{-2}).$$

Use the geometric series

$$\frac{1}{q-1} = \frac{1}{q} \cdot \frac{1}{1-1/q} = \frac{1}{q} [1 + \frac{1}{q} + \frac{1}{q^2} + \frac{1}{q^3} + O(q^{-4})] = q^{-1} + q^{-2} + q^{-3} + O(q^{-4}).$$

Multiply (this is the key bookkeeping — expand to order  $q^{-5/2}$ ):

$$\frac{T_{q-2}}{T_q} = [1 - 2q^{-1/2} + 2q^{-1} - \frac{3}{2}q^{-3/2} + O(q^{-2})] \cdot [q^{-1} + q^{-2} + q^{-3} + O(q^{-4})].$$

Distribute term-by-term:

$$[q^{-1}]: 1 \cdot q^{-1} = q^{-1}.$$

$$[q^{-3/2}]: (-2q^{-1/2}) \cdot q^{-1} = -2q^{-3/2}.$$

$$[q^{-2}]: (2q^{-1}) \cdot q^{-1} + 1 \cdot q^{-2} = 2q^{-2} + q^{-2} = 3q^{-2}.$$

$$[q^{-5/2}]: (-\frac{3}{2}q^{-3/2}) \cdot q^{-1} + (-2q^{-1/2}) \cdot q^{-2} = -\frac{3}{2}q^{-5/2} - 2q^{-5/2} = -\frac{7}{2}q^{-5/2}.$$

$[q^{-3}]$  (the additional order). Now  $1 - 2\rho(q) = 1 - 2q^{-1/2} + 2q^{-1} - \frac{3}{2}q^{-3/2} + \frac{1}{2}q^{-2} + \frac{7}{16}q^{-5/2} + O(q^{-3})$  (using  $a_4 = -1/4, a_5 = -7/32$ ). The  $[q^{-3}]$  contributions from  $(1 - 2\rho) \cdot (q^{-1} + q^{-2} + q^{-3} + \dots)$  are:  $\frac{1}{2}q^{-2} \cdot q^{-1} + 2q^{-1} \cdot q^{-2} + 1 \cdot q^{-3} = (\frac{1}{2} + 2 + 1)q^{-3} = \frac{7}{2}q^{-3}$ .

Adding:

$$\boxed{\frac{T_{q-2}}{T_q} = \frac{1}{q} - \frac{2}{q^{3/2}} + \frac{3}{q^2} - \frac{7}{2q^{5/2}} + \frac{7}{2q^3} + O(q^{-7/2})}. \quad (73)$$

*Consequence in the main paper.* Multiplying (73) by  $(q^3 - q)/6 = q^3/6 - q/6$ , the  $q^0$  term is  $(q^3/6) \cdot (7/2)q^{-3} - (q/6) \cdot q^{-1} = 7/12 - 1/6 = 5/12$ :

$$\frac{q^3 - q}{6} \cdot \frac{T_{q-2}}{T_q} = \frac{q^2}{6} - \frac{q^{3/2}}{3} + \frac{q}{2} - \frac{7\sqrt{q}}{12} + \frac{5}{12} + O(q^{-1/2}),$$

matching the five-term expansion of  $W(1, q)$  asserted by Lemma 14 in the main paper.

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