Abstract. In this paper we enumerate \(k\)-noncrossing RNA pseudoknot structures with given minimum stack-length. We show that the numbers of \(k\)-noncrossing structures without isolated base pairs are significantly smaller than the number of all \(k\)-noncrossing structures. In particular we prove that the number of 3- and 4-noncrossing RNA structures with stack-length \(\geq 2\) is for large \(n\) given by \(\frac{311^{2}470}{n!}\) and \(1.217 \cdot 10^{7}n \cdot 2.5881^n\) and \(1.217 \cdot 10^{7}n \cdot 3.0382^n\), respectively. We furthermore show that for \(k\)-noncrossing RNA structures the drop in exponential growth rates between the number of all structures and the number of all structures with stack-size \(\geq 2\) increases significantly. Our results are of importance for prediction algorithms for pseudoknot-RNA and provide evidence that there exist neutral networks of RNA pseudoknot structures.

1. Introduction

An RNA structure is the helical configuration of an RNA sequence, described by its primary sequence of nucleotides A, G, U and C together with the Watson-Crick (A-U, G-C) and (U-G) base pairing rules. Subject to these single stranded RNA form helical structures. Since the function of many RNA sequences is oftentimes tantamount to their structures, it is of central importance to understand RNA structure in the context of studying the function of biological RNA, as well as in the design process of artificial RNA. In the following we use a coarse grained notion of structure by concentrating on the pairs of nucleotide positions corresponding to the chemical bonds and ignoring any spatial embedding. There are several ways to represent these RNA structures [21, 31]. We choose the diagram representation [23] which is particularly well suited for displaying the crossings of the Watson-Crick base pairs. A diagram is a labeled graph over the vertex set \([n] = \{1, \ldots, n\}\) with degree \(\leq 1\), represented by drawing its vertices 1, \ldots, \(n\) in a horizontal line and its arcs \((i, j)\),
where $i < j$, in the upper half-plane. The vertices and arcs correspond to nucleotides and Watson-Crick (A-U, G-C) and (U-G) base pairs, respectively. We categorize diagrams according to the 3 parameters ($k, \lambda, \sigma$): the maximum number of mutually crossing arcs, $k - 1$, the minimum arc-length, $\lambda$ and the minimum stack-length, $\sigma$. Here the length of an arc $(i, j)$ is $j - i$ and a stack of length $\sigma$ is a sequence of "parallel" arcs of the form $((i, j), (i + 1, j - 1), \ldots, (i + (\sigma - 1), j - (\sigma - 1)))$, see Figure 1. We call an arc of length $\lambda$ a $\lambda$-arc.

![Figure 1](image1.png)

**Figure 1.** $k$-noncrossing diagrams: in the upper diagram the arcs red/blue/green mutually cross, the arc with minimum length 3 is $(3, 6)$ and the arc $(1, 5)$ is isolated. Hence this is a 4-noncrossing, $\lambda = 3, \sigma = 1$ diagram without isolated vertices. Analogously, below we have a 3-noncrossing (no red/green cross), $\lambda = 4, \sigma = 2$ diagram with isolated vertices 3, 13.

In the following we call a $k$-noncrossing diagram with arc-length $\geq 2$ and stack-length $\geq \sigma$ a $k$-noncrossing RNA structure (of type $(k, \sigma)$). We denote the set (number) of $k$-noncrossing RNA structures of type $(k, \sigma)$ by $T_{k, \sigma}(n)$ ($T_{k, \sigma}(n)$) and refer to $k$-noncrossing RNA structures for $k \geq 3$ as pseudoknot RNA structures. Intuitively, a higher number of pairwise crossing arcs is tantamount to higher structural complexity and crossing bonds are reality [20]. These pseudoknot bonds [32] occur in functional RNA (RNaseP [14]), ribosomal RNA [13] and are conserved in the catalytic core of group I introns, see Figure 2 where we show the diagram representation of the catalytic core region of the group I self-splicing intron [3]. For $k = 2$ we have RNA structures with no 2 crossing arcs, i.e. the well-known RNA secondary structures, whose combinatorics was pioneered by Waterman *et al.* [17 28 29 31 50]. RNA secondary structures are structures of type $(2,1)$. 
There are many reasons why pseudoknot structures are fascinating. First, compared to secondary structures their “mathematical” properties are much more intriguing \cite{10, 11, 12}. Their enumeration employs the nontrivial concepts of vacillating tableaux \cite{11, 12} and singular expansions \cite{11, 12}. Secondly, the recurrence relation for the numbers of 3-noncrossing RNA \cite{10} is, in contrast to that for secondary structures, “enumerative” but not “constructive”. This indicates that prediction of pseudoknot RNA is much more involved compared to the dynamic programming routine used for secondary structures. Nevertheless, there exist several prediction algorithms for RNA pseudoknot structures \cite{19, 26, 1, 15} which are able to express certain “types” of pseudoknots. In this context the notion of the “language of RNA” has been tossed \cite{27}. The combinatorial analysis in \cite{10, 11, 12} shows that 3-noncrossing RNA structures ($T_{3,1}(n)$) exhibit an exponential growth rate of $\frac{1}{2} + \sqrt{\frac{21}{2}} \approx 4.7913$ and even when considering only structures with minimum arc-length 3 the rate is 4.5492. This is bad news, since this rate exceeds already for $k = 3$ the number of sequences over the natural alphabet. Therefore, \textit{a priori}, not all 3-noncrossing structures can be folded by sequences. The situation becomes worse for higher $k$: the results of \cite{11, 12} imply the following exponential growth rates for $k$-noncrossing RNA structures:\footnote{\textit{Here} $\gamma_{k,1}$ denotes the dominant real singularity of the generating function}
Can we identify and analyze those $k$-noncrossing structures that do “occur”? To this end, let us consider this question in the biophysical context: RNA structures are formed by Watson-Crick (A-U, G-C) and (U-G) base pairs and, due to the specific chemistry of the latter, parallel bonds are thermodynamically more stable. This fact is well-known and has led to the notion of “canonical” structures [24], i.e. structures in which there exist no isolated base pair, see Figure 3. The question then is, do canonical $k$-noncrossing structures exhibit significantly smaller growth rates? Why this (to our knowledge) has not been seriously pursued could be explained by a result due to Schuster et.al. [6], who have proved the following: the number of RNA secondary structures, $T_{2,1}(n)$, exhibits an exponential growth rate of $\gamma_{2,1}^{-1} = 2.6180$ while the number of canonical RNA secondary structures $T_{2,2}(n)$ has an exponential growth rate of $\gamma_{2,2}^{-1} = 1.9680$. In other words, the exponential growth rate drops less than 25% when passing from arbitrary to canonical secondary structures. We remark that Schuster’s enumerative result is of central importance, since the growth rate of canonical secondary structures implies the existence of a “many to one” sequence to structure mapping. This has, subsequently, led to the concept of neutral networks [18].

In the following we will develop a novel combinatorial framework which allows to enumerate any RNA structure class of type $(k, \sigma)$, for any $k, \sigma$. We then can report good news: there is indeed a significant drop in the exponential growth rates when passing from $k$-noncrossing RNA structures to their canonical counterparts for $k \geq 3$. Explicitly we can give the following data

| $k$ | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| $\gamma_{k,1}^{-1}$ | 2.6180 | 4.7913 | 6.8540 | 8.8873 | 10.9087 | 12.9232 | 14.9321 | 16.9405 | 18.9466 |
where the case $k = 2$ is due to [6], which is independently confirmed by our approach. In particular, for 3-noncrossing RNA structures, we have a drop in exponential growth rate from 4.7913 to 2.5881, more than 46% and for $k = 10$ there is a drop of more than 74%. As a result, the number of canonical 3-noncrossing RNA structures is very close to that of arbitrary secondary structures. Intuitively this makes perfect sense since canonicity implies parallel arcs which limits severely crossings and it can be expected to have dramatic effect on $k$-noncrossing RNA for large $k$. In other words, the biophysical constraints (thermodynamic stability) counteracts the combinatorial variety, see Figure 4.

\[\begin{array}{cccccccccc}
 k & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
 \gamma_{k,1}^{-1} & 2.6180 & 4.7913 & 6.8540 & 8.8873 & 10.9087 & 12.9232 & 14.9321 & 16.9405 & 18.9466 \\
 \gamma_{k,2}^{-1} & 1.9680 & 2.5881 & 3.0382 & 3.4138 & 3.7439 & 4.0420 & 4.3159 & 4.5714 & 4.8114 \\
\end{array}\]

The main idea in this paper is to consider a new type of $k$-noncrossing structure, that can be considered as being "dual" to canonical structures. We consider $k$-noncrossing structures in which there exists no two arcs of the form $(i, j), (i + 1, j - 1)$. These structures are called $k$-noncrossing core-structures and $C_k(n)$ denotes their number. The key observation with respect to core-structures is the following: any structure has a unique core obtained by identifying all arcs contained in stacks by a single arc and keeping isolated vertices. Furthermore, the number of all structures is a sum of the numbers of the corresponding core structures with positive integer coefficients. In

**Figure 4.** Biophysical constraints inducing parallel arcs: the hammerhead ribozyme [2]. Its two tertiary interactions are shown in green lines. The gap after C25 indicates that some nucleotides are omitted, which are involved in an unrelated structural motif.
Figure 5 we illustrate the idea of how a core-structure is obtained. It is of particular interest to note that Figure 5 shows that deriving the core-structure can reduce the minimum arc-length, but cannot produce arcs of the form \((i, i + 1)\). In Theorem 3 we derive the generating function for core-structures which shows that “most” \(k\)-noncrossing structures are in fact core-structures. Denoting the exponential growth rate of \(k\)-noncrossing core-structures by \(\kappa_k^{-1}\) we have the situation

| \(k\) | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 |
|------|----|----|----|----|----|----|----|----|----|
| \(\gamma_{k,1}^{-1}\) | 2.6180 | 4.7913 | 6.8540 | 8.8873 | 10.9087 | 12.9232 | 14.9321 | 16.9405 | 18.9466 |
| \(\kappa_k^{-1}\) | 2.5152 | 4.7097 | 6.7921 | 8.8378 | 10.8672 | 12.8866 | 14.9031 | 16.9119 | 18.9215 |

In Theorem 4 we derive a functional identity for the generating function for \(k\)-noncrossing RNA structures with stack-length \(\geq \sigma\), which allows to obtain exact and asymptotic results on \(T_{k,\sigma}(n)\), i.e. all \(k\)-noncrossing RNA structures with stack-length \(\geq \sigma\). In its proof the number of \(k\)-noncrossing core-structures plays a central role. As for the quality of the asymptotic expressions we compare in the table below subexponential factors for 3- and 4-noncrossing RNA structures with stack-length \(\geq 2\), \(t_{3,2}(n) = \frac{311\cdot 2470\cdot 4!}{n(n-1)(n-2)(n-3)(n-4)}\) and \(t_{4,2}(n) = 1.217 \cdot 10^7 n^{-\frac{5}{2}}\) with \(T_{3,2}(n) \gamma_{3,2}^n\) and \(T_{4,2}(n) \gamma_{4,2}^n\), respectively. Here \(\gamma_{k,\sigma}^{-1}\) denotes the respective exponential growth rate:
The subexponential factor

| $n$  | $\frac{T_{3,2}(n)}{\gamma_{3,2}^n}$ | $t_{3,2}(n)$ | $\frac{T_{4,2}(n)}{\gamma_{4,2}^n}$ | $t_{4,2}(n)$ |
|------|--------------------------------|-------------|--------------------------------|-------------|
| 50   | $1.214 \times 10^{-5}$          | $2.938 \times 10^{-5}$ | $3.115 \times 10^{-8}$          | $1.763 \times 10^{-7}$ |
| 60   | $5.498 \times 10^{-6}$          | $1.140 \times 10^{-5}$ | $6.884 \times 10^{-9}$          | $2.599 \times 10^{-8}$ |
| 70   | $2.776 \times 10^{-6}$          | $5.143 \times 10^{-6}$ | $1.841 \times 10^{-9}$          | $5.151 \times 10^{-9}$ |
| 80   | $1.522 \times 10^{-6}$          | $2.589 \times 10^{-6}$ | $5.708 \times 10^{-10}$         | $1.268 \times 10^{-9}$ |
| 90   | $8.905 \times 10^{-7}$          | $1.416 \times 10^{-6}$ | $1.991 \times 10^{-10}$         | $3.680 \times 10^{-9}$ |
| 100  | $5.487 \times 10^{-7}$          | $8.268 \times 10^{-7}$ | $7.650 \times 10^{-11}$         | $1.217 \times 10^{-10}$ |

2. SOME BASIC FACTS

In this Section we provide the basic facts needed for proving Theorems 3 in Section 3 and Theorem 4 in Section 4. For background on crossings and nestings in diagrams and partitions we recommend the paper of Chen et al. [4] and for the analytic combinatorics and asymptotic analysis the book of Flajolet [7]. Our results are based on the generating function of $k$-noncrossing RNA structures [10], and asymptotic analysis of $k$-noncrossing RNA structures [11, 12], summarized in Theorem 1 below.

Let us first recall our basic terminology, by $T_{k,\sigma}(n)$ we denote the set of $k$-noncrossing RNA structures with minimum stack length $\sigma$ and let $T_{k,\sigma}(n)$ denote their number. That is $T_{k,\sigma}(n)$ can be identified with the set of diagrams with degree $\leq 1$, represented by drawing the vertices 1, \ldots, $n$ in a horizontal line and its arcs $(i, j)$, where $i < j$, in the upper half plane with arc-length $\geq 2$ and stack-length $\geq \sigma$, in which the maximum number of mutually crossing arcs is $k-1$. Furthermore let $T_{k,\sigma}(n, h)$ denote the set of $k$-noncrossing RNA structures stack-length $\geq \sigma$ having $h$ arcs and let $T_{k,\sigma}(n, h)$ denote their number. We denote by $f_k(n, \ell)$ the number of $k$-noncrossing diagrams with arbitrary arc-length and $\ell$ isolated points. In Figure 6 we display the various types of diagrams involved.
The following identities are due to Grabiner et. al. [9]

\begin{align}
\sum_{n \geq 0} f_k(n, 0) \cdot \frac{x^n}{n!} &= \text{det}[I_{i-j}(2x) - I_{i+j}(2x)] |_{i,j=1}^{k-1} \\
\sum_{n \geq 0} \left\{ \sum_{\ell=0}^{n} f_k(n, \ell) \right\} \cdot \frac{x^n}{n!} &= e^x \text{det}[I_{i-j}(2x) - I_{i+j}(2x)] |_{i,j=1}^{k-1}
\end{align}

where \( I_r(2x) = \sum_{j \geq 0} \frac{2^{j+r}}{j!(r+j)!} \) denotes the hyperbolic Bessel function of the first kind of order \( r \). Eq. (2.1) and (2.2) allow "in principle" for explicit computation of the numbers \( f_k(n, \ell) \). In particular for \( k = 2 \) and \( k = 3 \) we have the formulas

\begin{align}
f_2(n, \ell) &= \binom{n}{\ell} C_{(n-\ell)/2} \\
f_3(n, \ell) &= \binom{n}{\ell} \left[ C_{\frac{n-\ell}{2}} C_{\frac{n-\ell}{2}} - C_{\frac{n-\ell}{2}+\frac{1}{2}} \right],
\end{align}

where \( C_m \) denotes the \( m \)-th Catalan number. The second formula results from a determinant formula enumerating pairs of nonintersecting Dyck-paths. In view of

\[ f_k(n, \ell) = \binom{n}{\ell} f_k(n - \ell, 0) \]

everything can be reduced to perfect matchings, where we have the following situation: there exists an asymptotic approximation of the hyperbolic Bessel function due to [16] and employing the subtraction of singularities-principle [16] one can prove

\begin{align}
\forall k \in \mathbb{N}; \quad f_k(2n, 0) \sim \varphi_k(n) \left( \frac{1}{\rho_k} \right)^n,
\end{align}
where \( \rho_k \) is the dominant real singularity of \( \sum_{n \geq 0} f_k(2n, 0) z^n \) and \( \varphi_k(n) \) is a polynomial over \( n \).

Via Hadamard’s formula, \( \rho_k \) can be expressed as
\[
(2.5) \quad \rho_k = \lim_{n \to \infty} (f_k(2n, 0))^{-\frac{1}{n}}.
\]

Eq. (2.4) allows for any \( k \) to obtain \( \varphi_k(n) \), explicitly.

As for the generating function and asymptotics of \( k \)-noncrossing RNA structures we have the following result

**Theorem 1.** \([10, 11]\) Let \( k \in \mathbb{N}, k \geq 2 \). Then the number of \( k \)-noncrossing RNA structures with \( \frac{n-\ell}{2} \) arcs, \( T_{k,1}(n, \frac{n-\ell}{2}) \) and the number of \( k \)-noncrossing RNA structures, \( T_{k,1}(n) \) are given by
\[
T_{k,1}(n, \frac{n-\ell}{2}) = \sum_{b=0}^{[n/2]} (-1)^b \binom{n-b}{b} f_k(n-2b, \ell)
\]
(2.6)
\[
T_{k,1}(n) = \sum_{b=0}^{[n/2]} (-1)^b \binom{n-b}{b} \left\{ \sum_{\ell=0}^{n-2b} f_k(n-2b, \ell) \right\},
\]
(2.7)
where \( \{ \sum_{\ell=0}^{n-2b} f_k(n-2b, \ell) \} \) is given via eq. (2.2) and furthermore
\[
T_{3,1}(n) \sim \frac{10.4724 \cdot 4!}{n(n-1) \ldots (n-4)} \left( \frac{5 + \sqrt{21}}{2} \right)^n.
\]

The following functional identity is due to \([11]\) and relates the bivariate generating function for \( T_{k,1}(n, h) \), the number of RNA pseudoknot structures with \( h \) arcs to the generating function of \( k \)-noncrossing perfect matchings.

**Lemma 1.** Let \( k \in \mathbb{N}, k \geq 2 \) and \( z, u \) be indeterminants over \( \mathbb{C} \). Then we have
\[
(2.8) \quad \sum_{n \geq 0} \sum_{h \leq n/2} T_{k,1}(n, h) \ u^{2h} z^n = \frac{1}{u^2 z^2 - z + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{uz}{u^2 z^2 - z + 1} \right)^{2n}.
\]

In particular we have for \( u = 1 \),
\[
(2.9) \quad \sum_{n \geq 0} T_{k,1}(n) \ z^n = \frac{1}{z^2 - z + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{z}{z^2 - z + 1} \right)^{2n}.
\]
In view of Lemma 1 it is of interest to deduce relations between the coefficients from the equality of generating functions. The class of theorems that deal with this deduction are called transfer-theorems \[7\]. One key ingredient in this framework is a specific domain in which the functions in question are analytic, which is “slightly” bigger than their respective radius of convergence. It is tailored for extracting the coefficients via Cauchy’s integral formula. Details on the method can be found in \[7\] and its application to 3-noncrossing RNA in \[11\]. To be precise the domain in question is

**Definition 1.** Given two numbers \(\phi, R\), where \(R > 1\) and \(0 < \phi < \frac{\pi}{2}\) and \(\rho \in \mathbb{R}\) the open domain \(\Delta_{\rho}(\phi, R)\) is defined as

\[
\Delta_{\rho}(\phi, R) = \{z \mid |z| < R, z \neq \rho, |\text{Arg}(z - \rho)| > \phi\}
\]

A domain is a \(\Delta_{\rho}\)-domain if it is of the form \(\Delta_{\rho}(\phi, R)\) for some \(R\) and \(\phi\). A function is \(\Delta_{\rho}\)-analytic if it is analytic in some \(\Delta_{\rho}\)-domain.

We use the notation

\[
(f(z) = O(g(z)) \text{ as } z \to \rho) \iff (f(z)/g(z) \text{ is bounded as } z \to \rho)
\]

and if we write \(f(z) = O(g(z))\) it is implicitly assumed that \(z\) tends to a (unique) singularity. \([z^n] f(z)\) denotes the coefficient of \(z^n\) in the power series expansion of \(f(z)\) around 0.

**Theorem 2.** \([8]\) Let \(f(z), g(z)\) be a \(\Delta_{\rho}\)-analytic functions given by power series \(f(z) = \sum_{n \geq 0} a_n z^n\) and \(g(z) = \sum_{n \geq 0} b_n z^n\). Suppose \(f(z) = O(g(z))\) for all \(z \in \Delta_{\rho}\) and \(b_n \sim \varphi(n)(\rho^{-1})^n\), where \(\varphi(n)\) is a polynomial over \(n\). Then

\[
a_n = [z^n] f(z) \sim K [z^n] g(z) = K b_n \sim K \varphi(n)(\rho^{-1})^n
\]

for some constant \(K\).

Transfer theorems are accordingly a translation of error terms from functions to coefficients and guaranteed when the functions in question are analytic in some \(\Delta_{\rho}\)-domain.

### 3. Core-structures

As discussed in the Introduction, a core-structure is a \(k\)-noncrossing structure with no stacked base pairs. We denote the set and number of core-structures over \([n]\) by \(C_k(n)\) and \(c_k(n)\), respectively.
Analogously $C_k(n,h)$ and $\mathcal{C}_k(n,h)$ denote the set and the number of core-structures having $h$ arcs. In Lemma 2 below we establish that the number of all $k$-noncrossing structures with stack-length $\geq \sigma$ is a sum of the numbers of $k$-noncrossing cores with positive integer coefficients.

**Lemma 2. (Core-lemma)** For $k, h, \sigma \in \mathbb{N}$, $k \geq 2$, $1 \leq h \leq n/2$ we have

\[
T_{k,\sigma}(n,h) = \sum_{b=\sigma-1}^{h-1} \binom{b + (2 - \sigma)(h - b) - 1}{h - b - 1} C_k(n - 2b, h - b).
\]

**Remark 1.** Lemma 2 cannot be used in order to enumerate diagrams with arc-length $\geq \lambda$, where $\lambda > 2$ and stack-length $\sigma$. Basically, $k$-noncrossing structures with arc-length $\geq \lambda$ have core-structures with arc-length 2, see Figure 7. The enumeration of $k$-noncrossing RNA structures with arc-length $\geq 3$ and stack-length $\geq 2$ is work in progress.

\[
\text{Figure 7.}\text{ Core-structures will in general have 2-arcs: the structure } \delta \in T_{3,2} (19) \text{ (lhs) is mapped into its core } c(\delta) \text{ (rhs). Clearly } \delta \text{ has arc-length } \geq 5 \text{ and as a consequence of the collapse of the stack } ((i+1,j+3),\ldots,(i+j)) \text{ (the blue arcs are being removed) into the arc } (i+4,j), \text{ c(}\delta\text{) contains the 2-arc } (i,i+5).\]

**Proof.** First, there exists a mapping from $k$-noncrossing structures with $h$ arcs and minimum stack size $\sigma$ over $[n]$ into core-structures:

\[
c: T_{k,\sigma}(n,h) \rightarrow \bigcup_{0 \leq b \leq h-1} C_k(n - 2b, h - b), \quad \delta \mapsto c(\delta)
\]

where the core-structure $c(\delta)$ is obtained in two steps: first we map arcs and isolated vertices as follows

\[
\forall \ell \geq \sigma - 1; \quad ((i-\ell,j+\ell),\ldots,(i,j)) \mapsto (i,j) \quad \text{and} \quad j \mapsto j \quad \text{if } j \text{ is isolated.}
\]

and second we relabel the vertices of the resulting diagram from left to right in increasing order. That is we replace each stack by a single arc and keep isolated points and then relabel, see Figure 8.
We have to prove that \( c: T_{k,\sigma}(n,h) \rightarrow \bigcup_{0 \leq b \leq h-1} \mathcal{C}_k(n-2b, h-b) \) is well-defined, i.e., that \( c \) cannot produce 1-arcs. Indeed, since \( \delta \in T_{k,\sigma}(n,h) \), \( \delta \) does not contain 1-arcs we can conclude that \( c(\delta) \) has by construction arcs of length \( \geq 2 \). \( c \) is by construction surjective. Keeping track of multiplicities gives rise to the map

\[
(3.4) \quad f_{k,\sigma}: T_{k,\sigma}(n,h) \rightarrow \bigcup_{0 \leq b \leq h-1} \left[ \mathcal{C}_k(n-2b, h-b) \times \left\{ (a_j)_{1 \leq j \leq h-b} \mid \sum_{j=1}^{h-b} a_j = b, \ a_j \geq \sigma - 1 \right\} \right],
\]

given by \( f_{k,\sigma}(\delta) = (c(\delta), (a_j)_{1 \leq j \leq h-b}) \). We can conclude that \( f_{k,\sigma} \) is well-defined and a bijection.

We proceed computing the multiplicities of the resulting core-structures:

**Claim.**

\[
|\{ (a_j)_{1 \leq j \leq h-b} \mid \sum_{j=1}^{h-b} a_j = b; \ a_j \geq \sigma - 1 \}| = \left( \frac{b + (2 - \sigma)(h-b) - 1}{h-b-1} \right).
\]

Clearly, \( a_j \geq \sigma - 1 \) is equivalent to \( \mu_j = a_j - \sigma + 2 \geq 1 \) and we have

\[
\sum_{j=1}^{h-b} \mu_j = \sum_{j=1}^{h-b} (a_j - \sigma + 2) = b + (2 - \sigma)(h-b).
\]

We next show that

\[
|\{ (\mu_j)_{1 \leq j \leq h-b} \mid \sum_{j=1}^{h-b} \mu_j = b + (2 - \sigma)(h-b); \ \mu_j \geq 1 \}|
\]

is equal the number of \( (h-b - 1) \)-subset in \( \{1, 2, \ldots, b + (2 - \sigma)(h-b) - 1\} \). Consider the set

\[
\{ \mu_1, \mu_1 + \mu_2, \ldots, \mu_1 + \mu_2 + \cdots + \mu_{h-b-1} \}
\]

consisting of \( h-b-1 \) distinct elements of \( [b + (2 - \sigma)(h-b) - 1] = \{1, 2, \ldots, b + (2 - \sigma)(h-b) - 1\} \).

Therefore \( \{ \mu_1, \mu_1 + \mu_2, \ldots, \mu_1 + \mu_2 + \cdots + \mu_{h-b-1} \} \) is a \( (h-b-1) \)-subset of \( [b + (2 - \sigma)(h-b) - 1] \).

Given any \( (h-b-1) \)-subset of \( [b + (2 - \sigma)(h-b) - 1] \), we can arrange its elements in linear order and retrieve the sequence \( \{ \mu_i \mid 1 \leq i \leq h-b \} \) of positive integers with sum \( b + (2 - \sigma)(h-b) \). Therefore

**Figure 8.** The mapping \( c: T_{k,\sigma}(n,h) \rightarrow \bigcup_{0 \leq b \leq h-1} \mathcal{C}_k(n-2b, h-b) \) is obtained in two steps: first contraction of the stacks and secondly relabeling of the resulting diagram.
the above assignment is a bijection. Since the number of \((h - b - 1)\)-subsets of \([b + (2 - \sigma)(h - b) - 1]\)

is given by \(\binom{b + (2 - \sigma)(h - b) - 1}{h - b - 1}\) the Claim follows.

We can conclude from the Claim and eq. (3.4) that

\[ T_{k,\sigma}(n, h) = \sum_{b=\sigma-1}^{h-1} \binom{b + (2 - \sigma)(h - b) - 1}{h - b - 1} C_k(n - 2b, h - b) \]

holds and the lemma follows. \(\square\)

Next, we prove a functional identity between the bivariate generating functions of \(T_{k,\sigma}(n, h)\) and \(C_k(n, h)\). This identity plays a central role in proving Theorem 3 and Theorem 4 in Section 4.

**Lemma 3.** Let \(k, \sigma \in \mathbb{N}, k \geq 2\) and let \(u, x\) be indeterminants. Then we have the functional relation

\[ \sum_{n \geq 0}^{h \leq \Phi} T_{k,\sigma}(n, h) u^h x^n = \sum_{n \geq 0}^{h \leq \Phi} C_k(n, h) \left( \frac{u \cdot (ux)^{\sigma-1}}{1 - ux^2} \right)^h x^n + \frac{x}{1 - x} \]

and in particular, for \(u = 1\)

\[ \sum_{n \geq 0}^{h \leq \Phi} T_{k,\sigma}(n) x^n = \sum_{n \geq 0}^{h \leq \Phi} C_k(n, h) \left( \frac{1}{1 - x^2} \right)^h x^n + \frac{x}{1 - x} \]

**Proof.** We set \(\sum_{n \geq 0}^{h \leq \Phi} C_k(n, h) u^h x^n = \sum_{n \geq 0} \phi_h(x) u^h\)

and compute

\[ \sum_{n \geq 0}^{h \leq \Phi} T_{k,\sigma}(n, h) u^h x^n = \sum_{n \geq 0} \sum_{h \leq \Phi} \sum_{b \leq h-1} C_k(n - 2b, h - b) \binom{b + (2 - \sigma)(h - b) - 1}{h - b - 1} u^h x^n + \sum_{i \geq 1} x^i \]

where the term \(\sum_{i \geq 1} x^i = \frac{x}{1 - x}\) comes from the fact that for \(h = 0\) the binomial

\[ \binom{b + (2 - \sigma)(h - b) - 1}{h - b - 1} \]

is zero, while the lhs counts for any \(i \geq 1\) the unique structure having only isolated vertices. We proceed to compute

\[ = \sum_{h \geq 0} \sum_{b \leq h-1} \sum_{n \geq 2h} C_k(n - 2b, h - b) x^{n-2b} \binom{b + (2 - \sigma)(h - b) - 1}{h - b - 1} u^h x^{2b} + \frac{x}{1 - x} \]

\[ = \sum_{b \geq 0} \phi_{h-b}(x) \binom{b + (2 - \sigma)(h - b) - 1}{h - b - 1} u^h x^{2b} + \frac{x}{1 - x} . \]
Setting \( m = h - b \) and subsequently interchanging the summation indices we arrive at

\[
\sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} T_{k,\sigma}(n, h) u^h x^n = \sum_{b \geq 0} \sum_{1 \leq m} \varphi_m(x) \left( \binom{b + (2 - \sigma)m - 1}{m - 1} \right) u^m (ux^2)^b + \frac{x}{1 - x}
\]

\[
= \sum_{m \geq 0} \varphi_m(x) \left( \frac{u \cdot (ux^2)^{\sigma - 1}}{1 - ux^2} \right)^m + \frac{x}{1 - x}
\]

\[
= \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} C_{k}(n, h) \left( \frac{u \cdot (ux^2)^{\sigma - 1}}{1 - ux^2} \right)^h x^n + \frac{x}{1 - x},
\]

whence Lemma \( \spadesuit \) \( \square \)

We next enumerate core-structures. The Theorem has two main parts, the first is the “inversion” of Lemma \( \spadesuit \). It allows to express core-structures via all structures and follows by Möbius inversion. The second part deals with the asymptotics of core-structures. The asymptotic formula follows then from transfer Theorems (the super-critical case) \( \spadesuit \) applied to some version of the functional identity of Lemma \( \spadesuit \).

**Theorem 3. (Core-structures)** Suppose \( k \in \mathbb{N}, \ k \geq 2 \), let \( x \) be an indeterminant, \( \rho_k \) the dominant, positive real singularity of \( \sum_{n \geq 0} f_k(2n, 0) x^n \) (eq. \( 2.13 \)) and \( u_1(x) = \frac{1}{1 + x^2} \). Then for \( h \geq 1 \), the numbers of \( k \)-noncrossing core-structures, \( C_k(n) \) are given by

\[
C_k(n, h) = \sum_{b=0}^{h-1} (-1)^{h-b-1} \binom{h-1}{b} T_{k,1}(n - 2h + 2b + 2, b + 1).
\]

Furthermore we have the functional equation

\[
\sum_{n \geq 0} C_k(n) x^n = \frac{1}{u_1 x^2 - x + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{u_1 x}}{u_1 x^2 - x + 1} \right)^{2n} - \frac{x}{1 - x}
\]

and the asymptotic expression

\[
C_k(n) \sim \varphi_k(n) \left( \frac{1}{\kappa_k} \right)^n,
\]

where \( \kappa_k \) is the dominant positive real singularity of \( \sum_{n \geq 0} C_k(n) x^n \) and the minimal positive real solution of the equation \( \frac{\sqrt{u_1 x}}{u_1 x^2 - x + 1} = \rho_k \) and \( \varphi_k(n) \) is a polynomial over \( n \) derived from the asymptotic expression of \( f_k(2n, 0) \sim \varphi_k(n) \left( \frac{1}{\rho_k} \right)^n \) of eq. \( 2.14 \).
Proof. We set

$$\forall 0 \leq i \leq h - 1; \quad a(i) = C_k(n - 2(h - 1 - i), i + 1)$$

$$\forall 0 \leq i \leq h - 1; \quad b(i) = T_{k,1}(n - 2(h - 1 - i), i + 1).$$

We first employ Lemma 2 for $\sigma = 1$:

$$T_k(n, h) = \sum_{b=0}^{h-1} \binom{h-1}{b} C_k(n - 2b, h - b) \iff b(h - 1) = \sum_{i=0}^{h-1} \binom{h-1}{i} a(i).$$

Via Möbius-inversion we arrive at

$$a(h - 1) = \sum_{i=0}^{h-1} (-1)^{h-1-i} \binom{h-1}{i} b(i),$$

which is equivalent to

$$C_k(n, h) = \sum_{b=0}^{h-1} (-1)^{h-b-1} \binom{h-1}{b} T_{k,1}(n - 2h + 2b + 2, b + 1),$$

whence eq. (3.15). We proceed by proving eq. (3.13). First Lemma 3 implies:

$$\sum_{n \geq 0} \sum_{h \leq n/2} T_{k,1}(n, h) u^h x^n = \sum_{n \geq 0} \sum_{h \leq n/2} C_k(n, h) \left( \frac{u}{1 - u x^2} \right)^h x^n + \frac{x}{1 - x}$$

and we inspect that $u_1(x) = \frac{1}{1+x^2}$ is the unique solution for $\frac{u}{1 - u x^2} = 1$. Accordingly we obtain

$$\sum_{n \geq 0} \sum_{h \leq n/2} T_{k,1}(n, h) u_1^h x^n = \sum_{n \geq 0} C_k(n) x^n + \frac{x}{1 - x}.$$
whence eq (3.13). As for eq. (3.14) we consider the functional equation
\[
\sum_{n \geq 0} C_k(n) x^n = \frac{1}{u_1 x^2 - x + 1} \sum_{n \geq 0} f_k(2n, 0) \left(\frac{\sqrt{u_1} x}{u_1 x^2 - x + 1}\right)^n - \frac{x}{1-x}.
\]
Let us denote \(W(x) = \sum_{n \geq 0} f_k(2n, 0) \left(\frac{\sqrt{u_1} x}{u_1 x^2 - x + 1}\right)^n\).

**Claim.** All dominant singularities of \(\sum_{n \geq 0} C_k(n) x^n\) are dominant singularities of \(W(z)\) and \(\kappa_k\) is a dominant singularity.

To prove the Claim we observe that a dominant singularity of \(\sum_{n \geq 0} C_k(n) x^n\) is either a singularity of \(W(z)\) or \(\frac{1}{u_1 z^2 - z + 1}\). Suppose there exists some singularity \(\zeta \in \mathbb{C}\) which is a root of \(u_1 z^2 - z + 1\). By construction \(|\zeta| \leq \kappa_k\), then we arrive at the contradiction \(|W(\zeta)| > W(\kappa_k)|\). Therefore all dominant singularities of \(\sum_{n \geq 0} C_k(n) z^n\) are dominant singularities of \(W(z)\). By Pringsheim’s Theorem [25], \(\sum_{n \geq 0} C_k(n) z^n\) has a dominant positive real singularity which by construction equals \(\rho_k\) and the Claim follows.

The Claim immediately implies that the exponential growth rate is the inverse of the minimal positive real solution of the equation \(\frac{\sqrt{u_1} x}{u_1 x^2 - x + 1}\) = 0. According to [27], the power series \(\sum_{n \geq 0} f_k(2n, 0) z^n\) has an analytic continuation in a \(\Delta_{\rho_k}\)-domain and we have \([z^n]W(z) \sim K \varphi_k(n) (\rho^{-1})^n\), where \(\varphi_k(n)\) is given by eq. (2.4). We can therefore employ Theorem 2, which via eq. (3.13) allows us to transfer the subexponential factors from the asymptotic expressions for \(f_k(2n, 0)\) to \(C_k(n)\). From this eq. (3.14) follows and the proof of Theorem 3 is complete. \(\square\)

### 4. Pseudoknot RNA with stack-length \(\geq \sigma\)

In this Section we combine Lemma 1 and Lemma 3 in order to derive the generating function of \(k\)-noncrossing RNA pseudoknot structures with minimum stack-size \(\sigma\). It is worth mentioning that core-structures are only implicit (via Lemma 3) in its proof: all expressions and relations are based on \(T_{k,1}(n', h')\) and \(T_{k,1}(n)\), respectively. The latter are given by Theorem 1. Our main result reads
Theorem 4. Let \( k, \sigma \in \mathbb{N}, k \geq 2 \), let \( x \) be an indeterminant and \( \rho_k \) the dominant, positive real singularity of \( \sum_{n \geq 0} f_k(2n, 0) z^n \) (eq. 2.5). Then

\[
T_{k,\sigma}(n, h) = \sum_{b=\sigma-1}^{h-1} \sum_{j=0}^{(h-b)-1} \binom{b+(2-\sigma)(h-b)-1}{h-b-1} (-1)^{(h-b)-j-1} \left( \frac{h-b-1}{j} \right) T_{k,1}(n-2h+2j+2, j+1).
\]

Furthermore, \( T_{k,\sigma}(n) \), satisfies the following identity

\[
\sum_{n \geq 0} T_{k,\sigma}(n) x^n = \frac{1}{u_0 x^2 - x + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{u_0 x}}{u_0 x^2 - x + 1} \right)^{2n},
\]

where \( u_0 = \left( \frac{x^2}{x^2-x^2+1} \right)^{\sigma-1} \). Furthermore

\[
T_{k,\sigma}(n) \sim \varphi_k(n) \left( \frac{1}{\gamma_{k,\sigma}} \right)^n
\]

holds, where \( \gamma_{k,\sigma} \) is a dominant singularity of \( \sum_{n \geq 0} T_{k,\sigma}(n) x^n \) and the minimal positive real solution of the equation

\[
\sqrt{\frac{(x^2)^{\sigma-1}}{(x^2)^{\sigma-1}-x^2+1} x} = \rho_k
\]

and \( \varphi_k(n) \) is a polynomial over \( n \) derived from the asymptotic expression of \( f_k(2n, 0) \sim \varphi_k(n) \left( \frac{1}{\rho_k} \right)^n \) of eq. (2.4).

In the following we present the first 18 numbers of \( T_{3,2}(n) \), \( T_{3,3}(n) \), \( T_{4,2}(n) \) and \( T_{4,3}(n) \):

| \( n \) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|
| \( T_{3,2}(n) \) | 1 | 1 | 1 | 1 | 2 | 4 | 8 | 15 | 28 | 55 | 110 | 222 | 448 | 913 | 1890 | 3964 | 8385 | 17846 |
| \( T_{3,3}(n) \) | 1 | 1 | 1 | 1 | 1 | 2 | 4 | 8 | 15 | 28 | 55 | 110 | 222 | 455 | 944 | 1995 | 4274 | 9244 |

| \( n \) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|
| \( T_{4,2}(n) \) | 1 | 1 | 1 | 1 | 2 | 4 | 8 | 15 | 28 | 55 | 110 | 223 | 455 | 944 | 1995 | 4274 | 9244 | 20182 |
| \( T_{4,3}(n) \) | 1 | 1 | 1 | 1 | 1 | 2 | 4 | 8 | 14 | 23 | 36 | 56 | 91 | 155 | 275 | 491 | 869 |
Proof. The first assertion follows from Lemma 2 and eq. (3.15), which allows to express the terms $C_k(n - 2b, h - b)$ via $T_{k,1}(n', h')$. In order to prove eq. (4.2) we apply Lemma 3 twice. First, Lemma 3 implies for arbitrary $\sigma$ and $u = 1$

\[
\sum_{n \geq 0} T_{k,\sigma}(n) x^n = \sum_{n \geq 0} C_k(n, h) \left( \frac{(x^2)^{\sigma-1}}{1 - x^2} \right)^h x^n + \frac{x}{1-x}
\]

and secondly, it guarantees for arbitrary $u \in \mathbb{C}$ and $\sigma = 1$

\[
\sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} T_{k,1}(n, h) u^h x^n = \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} C_k(n, h) \left( \frac{u}{1-ux^2} \right)^h x^n + \frac{x}{1-x}.
\]

The key observation (the “bridge”) is here the relation between $\sigma$ and $u$ via the terms $(x^2)^{\sigma-1}$ and $\frac{u}{1-ux^2}$. It is clear that for any $\sigma \in \mathbb{N}$ there exists an unique solution $u_0$ for

\[
\frac{(x^2)^{\sigma-1}}{1 - x^2} = \frac{u}{1 - ux^2}
\]

given by $u_0 = \frac{(x^2)^{\sigma-1}}{(x^2)^{\sigma-1} - x^2 + 1}$. This allows to express

\[
\sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} C_k(n, h) \left( \frac{(x^2)^{\sigma-1}}{1 - x^2} \right)^h x^n + \frac{x}{1-x}
\]

for any $\sigma$ via the bivariate generating function $\sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} T_{k,1}(n, h) u^h x^n$. Now we employ Lemma 1 which provides an interpretation of the latter as follows:

\[
\sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} T_{k,1}(n, h) u^h x^n = \frac{1}{ux^2 - x + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{ux}}{ux^2 - x + 1} \right)^{2n}.
\]

We accordingly obtain

\[
\sum_{n \geq 0} T_{k,\sigma}(n) x^n = \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} C_k(n, h) \left( \frac{(x^2)^{\sigma-1}}{1 - x^2} \right)^h x^n + \frac{x}{1-x}
\]

\[
= \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} C_k(n, h) \left( \frac{u_0}{1-u_0x^2} \right)^h x^n + \frac{x}{1-x}
\]

\[
= \frac{1}{u_0x^2 - x + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{u_0x}}{u_0x^2 - x + 1} \right)^{2n}.
\]

and eq. (4.3) follows. We set $V(z) = \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{u_0z}}{u_0z^2 - z + 1} \right)^{2n}$.

Claim. All dominant singularities of $\sum_{n \geq 0} T_{k,\sigma}(n) z^n$ are singularities of $V(z)$ and in particular
$\gamma_{k,\sigma}$ is a dominant singularity.

To prove the Claim we observe that a dominant singularity of

$$\frac{1}{u_0 x^2 - x + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{u_0 x}}{u_0 x^2 - x + 1} \right)^{2n}$$

is either a singularity of $V(z)$ or $\frac{1}{u_0 z^2 - z + 1}$. Suppose there exists some singularity $\zeta \in \mathbb{C}$ which is a root of $\frac{1}{u_0 z^2 - z + 1}$. By construction $\zeta \neq 0$ and $\zeta$ is necessarily a singularity of $V(z)$. Suppose $|\zeta| \leq \kappa_k$, then we arrive at the contradiction $|V(\zeta)| > |V(\kappa_k)|$ since $V(\zeta)$ is not finite and

$$V(\kappa_k) = \sum_{n \geq 0} f_k(2n, 0) \rho_k^{2n} < \infty.$$ 

Therefore all dominant singularities of $\sum_{n \geq 0} T_{k,\sigma}(n) z^n$ are singularities of $V(z)$. By Pringsheim’s Theorem [25], $\sum_{n \geq 0} T_{k,\sigma}(n) z^n$ has a dominant positive real singularity which by construction equals $\gamma_{k,\sigma}$ and the Claim follows.

The equation

$$(4.8) \quad \frac{\sqrt{(x^2)^{\sigma - 1} x}}{(x^2)^{\sigma - 1} x^2 - x^2 + 1} = \rho_k$$

has a minimal positive real solution and the Claim implies that its inverse equals the exponential growth-rate. According to [27] the power series $\sum_{n \geq 0} f_k(2n, 0) z^n$ has an analytic continuation in a $\Delta_{\rho_k}$-domain and we have $[z^n]V(z) \sim K \varphi_k(n) (\rho^{-1})^n$, where $\varphi_k(n)$ is given by eq. (2.4). In view of eq. (4.1) we can therefore employ Theorem 2, which allows us to transfer the subexponential factors from the asymptotic expressions for $f_k(2n, 0)$ to $T_{k,\sigma}(n)$, whence eq. (4.2). This completes the proof of Theorem 4.

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