2

Basic concepts

Not so many words—just the reason *a simple mathematician*
Los Alamos 1996

In this chapter we provide the mathematical foundation for the following results. One main objective here is the self-contained derivation of the generating function of k-noncrossing matchings, which will play a central role for RNA pseudoknot structures.

We begin with the combinatorial framework needed for the reflection principle, facilitating the enumeration of nonrecursive combinatorial objects. The reflection principle [49] requires some understanding of group actions and familiarity with formal power series. This combinatorial section concludes with the discussion of D-finite generating functions [125–127].

Next we discuss the basic ideas behind the singularity analysis which are due to [42]. The proofs of the main theorems there can be found in [42]. We then discuss the implications of singularity analysis for k-noncrossing matchings in the context of Theorems 2.7 and 2.8 [80]. Finally we provide a case study for secondary structures in order to familiarize the reader with the new concepts.

We then conclude this chapter by introducing random-induced subgraphs of n-cubes [102, 105, 106]. Aside from providing the basic terminology we present the key tool needed in Chapter 7: vertex boundaries, branching processes, and Janson's inequality.

2.1 *k*-Noncrossing partial matchings

A diagram is a labeled graph over the vertex set $[n] = \{1, 2, \ldots, n\}$ with degree smaller or equal than 1. A diagram is represented by drawing the vertices $1, 2, \ldots, n$ in a horizontal line and the arcs (i, j), where $i < j$, in the upper half plane. The length of an arc (i, j) is $s = j - i$ and an arc of length s is called

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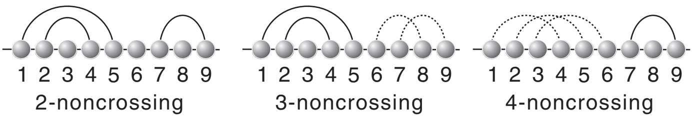

Fig. 2.1. k-Noncrossing diagrams: a 2-noncrossing (*left*), 3-noncrossing (*middle*), and 4-noncrossing diagram (*right*). The *dashed arcs* represent the maximal mutually crossing arcs.

an s-arc. A k-crossing is a set of k distinct arcs $(i_1, j_1), (i_2, j_2), \dots (i_k, j_k)$ such that

$$i_1 < i_2 < \cdots < i_k < j_1 < j_2 < \cdots < j_k.$$

A diagram without any k-crossings is called k-noncrossing diagram or k-noncrossing partial matching (Fig. 2.1). A k-noncrossing diagram without any isolated points is called a k-noncrossing matching. A k-nesting is a set of k distinct arcs such that

$$i_1 < i_2 < \cdots < i_k < j_k < \cdots j_2 < j_1.$$

A diagram without any k-nestings is called a k-nonnesting diagram. Note that partial matchings can have arcs of *any* length, while the diagram representation of RNA structures assumes a minimum arc length of 2 or 4, respectively.

2.1.1 Young tableaux, RSK algorithm, and Weyl chambers

A Young diagram (shape) is a collection of squares arranged in left-justified rows with weakly decreasing number of boxes in each row. A Young tableau, or tableau, is a filling of the squares by numbers which is weakly increasing in each row and strictly decreasing in each column. A tableau is called standard if each entry occurs exactly once; see Fig. 2.2.

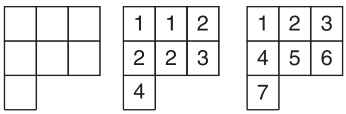

Fig. 2.2. Shape (*left*), Young tableau (*middle*), and standard Young tableau (*right*).

An oscillating tableau is a sequence

$$\varnothing = \mu^0, \mu^1, \dots, \mu^n = \varnothing$$

of standard Young diagrams, such that for $1 \leq i \leq n$, μ^i is obtained from μ^{i-1} by either adding one square or removing one square. For instance, the sequence is an oscillating tableaux; see Fig. 2.3. In the following we consider a specific generalization by allowing for hesitation steps, i.e., we consider $*$-tableaux

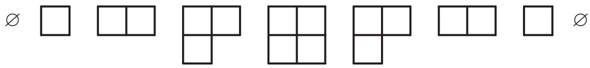

Fig. 2.3. Oscillating tableaux: two subsequent shapes, μ^{i-1} and μ^i, differ by exactly one square.

being sequences $\varnothing = \mu^0, \mu^1, \ldots, \mu^n = \varnothing$ such that for $1 \leq i \leq n$, μ^i is obtained from μ^{i-1} by either adding/removing one square or doing nothing; see Fig. 2.4. Let μ^{i-1} and μ^i be two shapes. If μ^i contains the shape μ^{i-1} we write $\mu^{i-1} \subseteq \mu^i$ and if, in particular, the shape μ^i is obtained by adding a square to the shape μ^{i-1} we write $\mu^i \setminus \mu^{i-1} = \square$.

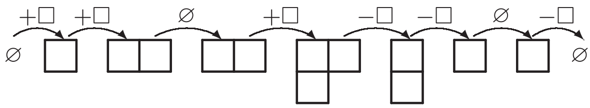

Fig. 2.4. $*$-tableaux: μ^{i-1} and μ^i either differ by one square or are equal.

We next come to a procedure via which elements can be row-inserted into Young tableaux, called RSK algorithm. Suppose we want to insert k into a standard Young tableau λ. Let $\lambda_{i,j}$ denote the element in the ith row and jth column of the Young tableau. Let j be the largest integer such that $\lambda_{1,j-1} \leq k$. (If $\lambda_{1,1} > k$, then $j = 1$.) If $\lambda_{1,j}$ does not exist, then simply add k at the end of the first row. Otherwise, if $\lambda_{1,j}$ exists, then replace $\lambda_{1,j}$ by k. Next insert $\lambda_{1,j}$ into the second row following the above procedure and continue until an element is inserted at the end of a row. As a result we obtain a new standard Young tableau with k included. For instance, inserting the sequence of integers $(5, 2, 4, 1, 6, 3)$, see Fig. 2.5, starting with an empty shape yields the following sequence of standard Young tableaux:

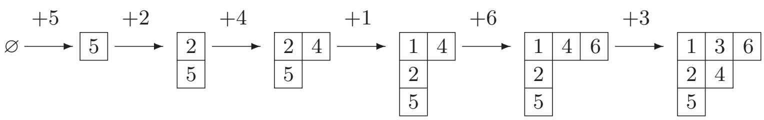

Fig. 2.5. RSK insertion: the sequence of integers $(5, 2, 4, 1, 6, 3)$ is RSK inserted, starting with an empty shape. The labeling of the *arrows* by "$+x$" indicates the RSK insertion of the integer x.

One key observation with respect to the RSK algorithm is that it can be, in some sense, "inverted" [27]. To be precise, we have

Lemma 2.1. *Suppose we are given two shapes μ^{i-1}, μ^i such that $\mu^{i-1} \backslash \mu^i = \square$ and a standard Young tableaux T_{i-1} of shape μ^{i-1}. Then there exists a unique j contained in T_{i-1} and a standard Young tableaux T_i of shape μ^i such that T_{i-1} is obtained from T_i by inserting j via the RSK algorithm.*

Proof. Indeed, suppose μ^{i-1} differs from μ^i in the first row. Then j is the element at the end of the first row in T_{i-1}. Otherwise suppose ℓ is the row of the square being removed from T_{i-1}. Remove the square and insert its element x into the $(\ell-1)$th row at precisely the position, where the removed element y would push it down via the RSK algorithm. That is, y is maximal subject to $y < x$. Since each column is strictly increasing y always exists. Iterating this process results in exactly one element j being removed from T_i and a new filling of the shape μ^{i-1}, i.e., a unique tableau T_{i-1}. By construction, inserting j with the RSK algorithm produces T_{i-1}.

In Fig. 2.6 we give an illustration of Lemma 2.1. We shall furthermore see that $*$-tableaux can be interpreted as lattice walks. This interpretation allows for the application of powerful principles tailored for their enumeration. For this purpose we provide next some basic background on lattice walks.

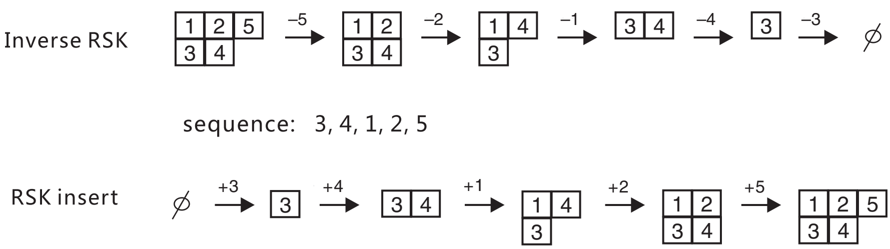

Fig. 2.6. The RSK algorithm and its inverse. First we extract via the inverse RSK and then reinsert using RSK, recovering the original Young tableau. The *arrows* are labeled by "$+x$" and $-x$" in case of RSK insertion and extraction, respectively.

Let $\mathbb{Z}^{k-1}$ denote the $(k-1)$-dimensional lattice. We consider walks in $\mathbb{Z}^{k-1}$ having the steps s contained in $\{\pm e_i, 0 \mid 1 \le i \le k-1\}$, where e_i denotes the ith unit vector and 0 corresponds to a hesitation step. That is for $a, b \in \mathbb{Z}^{k-1}$ a walk from a to b, $\gamma_{a,b}$, of length n is an n tuple $(s_1, \dots, s_n)$ where $s_h \in \{\pm e_i, 0 \mid 1 \le i \le k-1\}$ such that $b = a + \sum_{h=1}^n s_h$; see Fig. 2.7. We set $\gamma_{a,b}(s_r) = a + \sum_{h=1}^r s_h \in \mathbb{Z}^{k-1}$, i.e., the element at which the walk resides at step r.

2.1.2 The Weyl group

We next introduce the Weyl group B_{k-1}. For this purpose we consider the abelian group

$$E_{k-1} \cong \langle -1 \rangle^{k-1},$$

whose elements are $(k-1)$-tuples with coordinates being ± 1. E_{k-1} is generated by the elements ϵ_i, having coordinates "1" everywhere except of the ith coordinate which is "-1." We note that the symmetric group S_{k-1} and E_{k-1} act on $\mathbb{Z}^{k-1}$ via

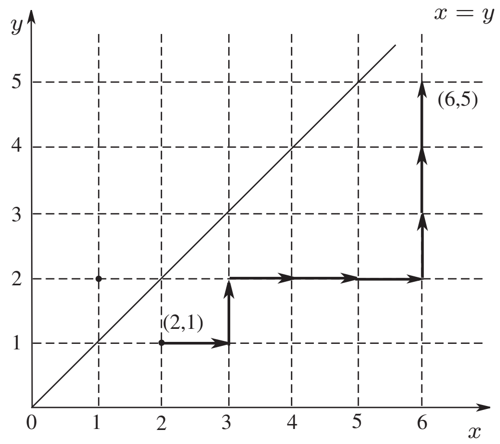

Fig. 2.7. Lattice walks: a walk from $(2,1)$ to $(6,5)$ of length 8 inside the fundamental Weyl chamber $C_0 = \{(x_1,x_2) \in \mathbb{Z}^2 \mid 0 \le x_2 \le x_1\}$. See the text for the definition of C_0.

$$\sigma(x_i)_{1\le i\le k-1} = (x_{\sigma^{-1}(i)})_{1\le i\le k-1},$$
$$\epsilon_i(x_1,\dots,x_i,\dots,x_{k-1}) = (x_1,\dots,-x_i,\dots,x_{k-1}).$$

It is straightforward to verify that $\{(\epsilon,\sigma) \mid \sigma \in S_{k-1},\, \epsilon \in E_{k-1}\}$ carries a natural group structure via

$$(\epsilon_i,\sigma)\cdot(\epsilon_j,\sigma') = (\epsilon_i\cdot(\sigma\epsilon_j\sigma^{-1}),\sigma\sigma') = (\epsilon_i\epsilon_{\sigma(j)},\sigma\sigma').$$

This is the Weyl group B_{k-1}, i.e., the semidirect product $E_{k-1} \rtimes S_{k-1}$, and generated by the set $M_{k-1} = \{\epsilon_{k-1}\} \cup \{\rho_j \mid 2 \le j \le k-1\}$, where $\rho_j = (j-1,\;\; j)$ denotes the canonical transposition, i.e., ρ_j transposes the coordinates x_{j-1} and x_j. Since $\mathsf{B}_{\mathsf{k-1}}$ acts on a basis vector $e_1,\dots,e_n$ as a permutation, followed by some sign changes, the root system of $\mathsf{B}_{\mathsf{k-1}}$ [54] is given by

$$\varDelta_{k-1} = \{\pm e_i \mid 1 \le i \le k-1\} \cup \{e_i \pm e_j \mid 1 \le i,j \le k-1\}.$$

We observe that there exists a bijection between

$$\varDelta'_{k-1} = \{e_{k-1}, e_{j-1}-e_j \mid 2 \le j \le k-1\}$$

and the set of generators M_{k-1} which maps each $\alpha \in \varDelta'_{k-1}$ into a reflection as follows (in particular, B_{k-1} is generated by reflections):

$$\begin{aligned}\{e_{k-1}\} \cup \{e_{j-1}-e_j \mid 2 \le j \le k-1\} &\longrightarrow \{\epsilon_{k-1}\} \cup \{\rho_j \mid 2 \le j \le k-1\},\\ \alpha &\mapsto \left(\beta_\alpha \colon x \mapsto x - 2\frac{\langle \alpha, x\rangle}{\langle \alpha,\alpha\rangle}\alpha\right)\end{aligned} \tag{2.1}$$

where $\langle x, x'\rangle$ denotes the standard scalar product in $\mathbb{R}^{k-1}$. It is clear that $\varDelta'_{k-1}$ is a basis of $\mathbb{R}^{k-1}$. We refer to the subspaces $\langle e_i\rangle$ for $1 \le i \le k-1$ and

$\langle e_{j-1} - e_j \rangle$ for $2 \leq j \leq k-1$ as walls. A Weyl chamber is defined as the set of $x \in \mathbb{Z}^{k-1}$ with the property that $\langle \alpha, x \rangle \geq 0$ for all $\alpha \in \Delta'_{k-1}$. We denote Weyl chambers by "C" and refer to the particular Weyl chamber

$$\{x \in \mathbb{Z}^{k-1} \mid 0 \leq x_{k-1} \leq x_{k-2} \leq \cdots \leq x_1\} \tag{2.2}$$

as the fundamental Weyl chamber, C_0. Any element β of B_{k-1} can be expressed in several ways as a product of reflections and the minimal number of M_{k-1}-reflections needed to represent $\beta \in \mathsf{B}_{k-1}$ is called the length of β, denoted by $\ell(\beta)$. According to a theorem of Iwahori [74], multiplication of β by a M_{k-1}-reflection, β_α, changes $\ell(\beta)$ by either $+1$ or -1, respectively. Therefore we have

$$(-1)^{\ell(\beta_\alpha \beta)} = (-1)^{1+\ell(\beta)}. \tag{2.3}$$

We next show how to compute the length of an element of $\beta \in \mathsf{B}_{k-1}$. Such a β can be written as $\beta = \eta\sigma$, where $\sigma \in S_{k-1}$, $\eta = (\eta_1, \ldots, \eta_{k-1})$, $\eta_i \in \{+1, -1\}$. Let furthermore

$$B = \{i \mid \eta_i = -1, \beta = (\eta_i)_{1 \leq i \leq k-1}\sigma\}.$$

Let us make the action of β on an element of $\mathbb{Z}^{k-1}$ explicit

$$\beta(x_i)_{1 \leq i \leq k-1} = \eta\sigma(x_i)_{1 \leq i \leq k-1} = \left(\prod_{i \in B} \epsilon_i\right)(x_{\sigma^{-1}(i)})_{1 \leq i \leq k-1}.$$

Here $\epsilon_i(x_1, \ldots, x_i, \ldots, x_{k-1}) = (x_1, \ldots, -x_i, \ldots, x_{k-1})$ and the product is taken in B_{k-1}. Accordingly we have

$$\ell(\beta) = \ell(\eta\sigma) = \ell\left(\prod_{i \in B} \epsilon_i \circ \sigma\right), \tag{2.4}$$

where $\epsilon_j = \tau_j \epsilon_{k-1} \tau_j$ and $\tau_j = (k-1, k-2) \cdot \cdots \cdot (j+1, \quad j)$. Since the ϵ_{k-1} and the τ_j are M_{k-1}-reflections we can conclude from eq. (2.3)

$$(-1)^{\ell(\beta)} = (-1)^{\ell\left(\prod_{i \in B}(\tau_i \epsilon_{k-1} \tau_i)\sigma\right)} = (-1)^{|B| + \ell(\sigma)}$$

and consequently

$$(-1)^{\ell(\beta)} = \operatorname{sgn}(\sigma) \prod_{i \in B} \eta_i = \operatorname{sgn}(\sigma) \prod_{i=1}^{k-1} \eta_i. \tag{2.5}$$

2.1.3 From tableaux to paths and back

In this section we connect the concepts of $*$-tableaux and specific lattice walks contained in Weyl chambers. Our main result is instrumental for the enumeration of RNA structures. It will allow us to interpret k-noncrossing partial matchings as walks in $\mathbb{Z}^{k-1}$ which remain in the interior of the Weyl chamber C_0. The result is due to Chen et al. [25]. The original bijection between oscillating tableaux and matchings is due to Stanley and was generalized by Sundaram [129]. In Chapter 3 we generalize these ideas in the context of tangled diagrams and prove a generalization of Theorem 2.2. This enables us to develop a framework for RNA tertiary structures.

Theorem 2.2. *(Chen et al. [25]) There exists a bijection between k-noncrossing partial matchings and walks of length n in $\mathbb{Z}^{k-1}$ which start and end at $a = (k-1, k-2, \ldots, 1)$, denoted by $\gamma_{a,a}$, having steps $0, \pm e_i$, $1 \leq i \leq k-1$ such that $0 < x_{k-1} < \cdots < x_1$ at any step, i.e., we have a bijection*

$$M_k(n) \longrightarrow \{\gamma_{a,a} \mid \gamma_{a,a} \text{ remains inside the Weyl chamber } C_0\},$$

where $M_k(n)$ denotes the set of k-noncrossing partial matchings over $[n]$.

Proof. *Claim* 1. There exists a bijection between the set of $*$-tableaux of length n and partial matchings over $[n]$.

Given a tableau $(\mu^i)_{i=0}^n$, where μ^i differs from μ^{i-1} by at most one square, we define a sequence $(G_n^0, T_0), (G_n^1, T_1), \ldots, (G_n^n, T_n)$, recursively, where G_n^i is a diagram and T_i is a standard Young tableau. We define G_n^0 to be the diagram with empty arc set and T_0 to be the empty standard Young tableau. The tableau T_i is obtained from T_{i-1} and the diagram G_n^i is obtained from G_n^{i-1} by the following procedure:

1. (Insert origins) For $\mu^i \supsetneq \mu^{i-1}$, then T_i is obtained from T_{i-1} by adding the entry i in the square $\mu^i \backslash \mu^{i-1}$.
2. (Isolated vertices) For $\mu^i = \mu^{i-1}$ then set $T_i = T_{i-1}$
3. (Remove origins) For $\mu^i \subsetneq \mu^{i-1}$, then let T_i be the unique standard Young tableau of shape μ^i and j be the unique number such that T_{i-1} is obtained from T_i by row-inserting j with the RSK algorithm. Then set $E_{G_n^i} = E_{G_n^{i-1}} \cup \{(j,i)\}$, where $E_{G_n^i}$ is the arc set of the diagram G_n^i.

For instance, given the sequence of tableau $(\mu^i)_{i=0}^7$

$$\varnothing \longrightarrow \boxed{} \longrightarrow \begin{array}{|c|c|}\hline & \\ \hline \end{array} \longrightarrow \boxed{} \longrightarrow \begin{array}{|c|}\hline \\ \hline \\ \hline \end{array} \longrightarrow \boxed{} \longrightarrow \boxed{} \longrightarrow \varnothing. \qquad (*)$$

The previous procedure gives rise to the fillings of μ_i and the diagram G_n^i:

$$\varnothing \longrightarrow \boxed{1} \longrightarrow \begin{array}{|c|c|}\hline 1 & 2 \\ \hline \end{array} \longrightarrow \boxed{1} \longrightarrow \begin{array}{|c|}\hline 1 \\ \hline 4 \\ \hline \end{array} \longrightarrow \boxed{4} \longrightarrow \boxed{4} \longrightarrow \varnothing$$

$$\begin{aligned} E_{G_n^0} &= \varnothing, & E_{G_n^4} &= \{(2,3)\}, \\ E_{G_n^1} &= \varnothing, & E_{G_n^5} &= \{(2,3),(1,5)\}, \\ E_{G_n^2} &= \varnothing, & E_{G_n^6} &= \{(2,3),(1,5)\}, \\ E_{G_n^3} &= \{(2,3)\}, & E_{G_n^7} &= \{(2,3),(1,5),(4,7)\}. \end{aligned}$$

The resulting partial matching G_n^7 is given by

Let $G_n = G_n^n$. Obviously, G_n is a diagram, and the set of i where $\mu^i = \mu^{i-1}$ equals the set of isolated vertices of G_n. By construction each entry j is removed exactly once whence no edges of the form (j,i) and (j,i') can be obtained. Therefore G_n has degree ≤ 1 and we have a well-defined mapping

$$\psi\colon \{(\mu^i)_{i=0}^n \mid (\mu^i)_{i=0}^n \text{ is a } *\text{-tableaux}\} \longrightarrow \\ \{G_n|G_n \text{ is a partial matching over } [n]\}.$$

It is clear from the above procedure that G_n is a partial matching and then ψ is injective. To prove subjectivity we observe that each diagram G_n induces an $*$-tableaux as follows. We set $\mu_{G_n}^n = \varnothing$ and $T_n = \varnothing$. Starting from vertex $i = n, n-1, \ldots, 1, 0$ we derive a sequence of Young tableaux $(T_n, T_{n-1}, \ldots, T_0)$ as follows:

I. If i is a terminus of a G_n-arc (j,i) add j via the RSK algorithm to T_i set $\mu_{G_n}^{i-1} \supsetneq \mu_{G_n}^i$ to be the shape of T_{i-1} (corresponds to (3)).
II. If i is an isolated G_n-vertex set $\mu_{G_n}^{i-1} = \mu_{G_n}^i$ (corresponds to (2)).
III. If i is the origin of a G_n-arc (i,k) let $\mu_{G_n}^{i-1} \subsetneq \mu_{G_n}^i$ be the shape of T_{i-1}, the standard Young tableau obtained by removing the square containing i (corresponds to (1)).

Then we have *by construction* $\psi((\mu_{G_n}^i)_{i=0}^n) = G_n$, whence ψ is bijective.

Claim 2. G_n is k-noncrossing if and only if all shapes μ^i in the $*$-tableaux have less than k rows.

From Claim 1 we know $\psi^{-1}(G_n) = (\varnothing = \mu^0, \mu^1, \ldots, \mu^n = \varnothing)$, so it suffices to prove that the maximal number of rows in the shape set $\psi^{-1}(G_n)$ is less than k. First we observe that the arcs $(i_1, j_1), \ldots (i_\ell, j_\ell)$ form a ℓ-crossing of G_n if and only if there exists a tableau T_i such that elements $i_1, i_2, \ldots i_\ell$ are in the ℓ squares of T_i and being deleted in increasing order $i_1 < i_2 < \ldots < i_\ell$ afterwards. Next, we will obtain a permutation π_i from the entries in each tableau T_i recursively as follows:

1. If T_{i-1} is obtained from T_i by row-inserting j with the RSK algorithm, then $\pi_{i-1} = \pi_i j$.
2. If $T_{i-1} = T_i$, then $\pi_i = \pi_{i-1}$.
3. If T_{i-1} is obtained from T_i by deleting the entry i, then π_{i-1} is obtained from π_i by deleting i.

If $\pi = r_1 r_2 \ldots r_t$, then the entries being deleted afterward are in the order $r_t, \ldots, r_2, r_1$.

Using the RSK algorithm w.r.t. the permutation π_i, the resulting row-inserting Young tableau is exactly T_i. We prove this by induction in reverse order of the $*$-tableaux. It is trivial for the case $i = n$. Suppose it holds for j, $1 \le j \le n$. Consider the above three cases: inserting an element, doing nothing, and deleting an element. In the first case, the assertion is implied by the RSK algorithm in the construction of the $*$-tableaux. In the second case, it holds by the induction hypothesis on step j.

It remains to consider the third case, that is, removing the entry from T_j to get T_{j-1}. We show that also in this case the insertion Young tableau of π_i equals the labeled tableau T_i. Write $\pi_j = x_1x_2\dots x_p j y_1 y_2 \dots y_q$ and $\pi_{j-1} = x_1x_2\dots x_p y_1 y_2 \dots y_q$. In view of step 3 j is larger than elements $x_1, x_2, \dots, x_p, y_1, \dots y_q$. We need to prove that the insertion tableau S_{j-1} of π_{j-1} by the RSK algorithm is exactly the same as deleting the entry j in T_j. We proceed by induction on q. In the case $q = 0$, T_j is obtained from T_{j-1} by adding j at the end of the first row. Suppose the assertion holds for $q-1$, that is $S_{j-1}(x_1x_2\dots x_p y_1 y_2 \dots y_{q-1}) = S_j(x_1x_2\dots x_p j y_1 y_2 \dots y_{q-1}) \setminus \boxed{j}$. Consider inserting y_q into S_{j-1}, via the RSK algorithm. If the insertion track path never touches the position of j, then $S_{j-1}(x_1x_2\dots x_p y_1 y_2 \dots y_{q-1}y_q) = S_j(x_1x_2\dots x_p j y_1 y_2 \dots y_{q-1}y_q) \setminus \boxed{j}$. Otherwise, if the insertion path touched j and pushed j into the next row, then since j is greater than any other entry, j must be moved to the end of next row and the push process stops. Accordingly, the insertion path in $S_{j-1}(x_1x_2\dots x_p y_1 y_2 \dots y_{q-1})$ is the same path as in $S_j(x_1x_2\dots x_p j y_1 y_2 \dots y_{q-1})$ except the last step moving j to a new position j, so deleting j will get $S_{j-1}(x_1x_2\dots x_p y_1 y_2 \dots y_{q-1}y_q) = S_j(x_1x_2\dots x_p j y_1 y_2 \dots y_{q-1}y_q) \setminus \boxed{j}$. According to Schensted's theorem [115], for any permutation π, assume A is the corresponding insertion Young tableau by using the RSK algorithm on π. Then the length of the longest decreasing subsequences of π is the number of rows in A, whence the assertion.

Now we can prove Claim 2. A diagram contains an ℓ-crossing if and only if there exists a π_i which has decreasing subsequence of length ℓ. And the insertion Young tableau of π_i equals the labeled tableau T_i. According to Schensted's theorem, π has a decreasing sequence of length ℓ if and only if rows of T_i is ℓ.

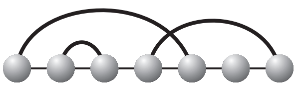

Fig. 2.8. The diagram corresponding to the sequence of tableaux in eq. $(*)$.

For instance, consider the partial matching of Fig. 2.8. We then obtain the sequence $\pi = (\varnothing \leftarrow 1 \leftarrow 12 \leftarrow 1 \leftarrow 1 \leftarrow 41 \leftarrow 4 \leftarrow 4 \leftarrow \varnothing)$. For the segment $\pi_1 = 1 \leftarrow \pi_2 = 12$ we have $j = 2$ and $q = 0$. Since the insertion track path never touches the position of $\boxed{2}$

$$S(1) = \boxed{1} = \boxed{1\,|\,2} \setminus \boxed{2} = \boxed{1} = S(12) \setminus \boxed{2}.$$

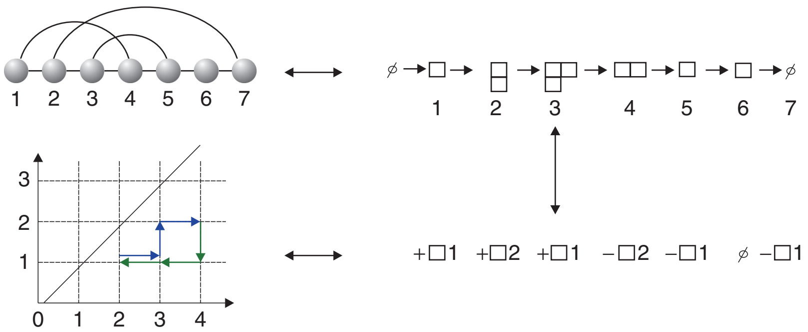

Fig. 2.9. The basic correspondences between partial matchings, $*$-tableaux, and walks inside the Weyl chamber C_0. Here "$\pm\square_i$" denotes the addition and removal of a square in the ith row, respectively.

For the segment $\pi_4 = 1 \leftarrow \pi_5 = 41$ we have $j = 4$ and $q = 1$:

$$S(1) = \boxed{1} = \begin{array}{|c|}\hline 1 \\ \hline 4 \\ \hline \end{array} \diagdown \boxed{4} = \boxed{1} = S(41) \diagdown \boxed{4}.$$

Here the insertion path touches $\boxed{4}$ and 4 moves to the end of the next row, where the push process stops.

Claim 3. There is a bijection between $*$-tableaux with at most $k-1$ rows of length n and walks with steps $\pm e_i, 0$ which stay in the interior of C_0 starting and ending at $(k-1, k-2, \dots, 1)$ see Fig. 2.9.

This bijection is obtained by setting for $1 \leq \ell \leq k-1$, x_ℓ to be the length of the ℓ-th row. By definition of standard Young tableaux, we have $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, i.e., the length of each row is weakly decreasing. This property also characterizes walks that stay within the Weyl chamber C_0, i.e., where we have $x_1 > x_2 > \cdots > x_{k-1} > 0$ since a walk from $(k-1, \dots, 2, 1)$ to itself in the interior of C_0 corresponds to a walk from the origin to itself in the region $x_1 \geq x_2 > \cdots \geq x_{k-1} \geq 0$. In an $*$-tableau μ^i differs from μ^{i-1} by at most one square and adding or deleting a square in the ℓth row or doing nothing corresponds to steps $\pm e_\ell$ and 0, respectively. Since the $*$-tableau is of empty shape, we have walks from the origin to itself, whence Claim 3 follows and the proof of the theorem is complete.

To summarize, given an $*$-tableaux of empty shape, $(\varnothing, \lambda^1, \dots, \lambda^{n-1}, \varnothing)$, reading $\lambda^i \setminus \lambda^{i-1}$ from left to right, at step i, we do the following:

- For a $+\square$-step we insert i into the new square
- For a $\varnothing$-step we do nothing
- For a $-\square$-step we extract the unique entry, $j(i)$, of the tableaux T^{i-1}, which via RSK insertion into T^i recovers it (Fig. 2.6)

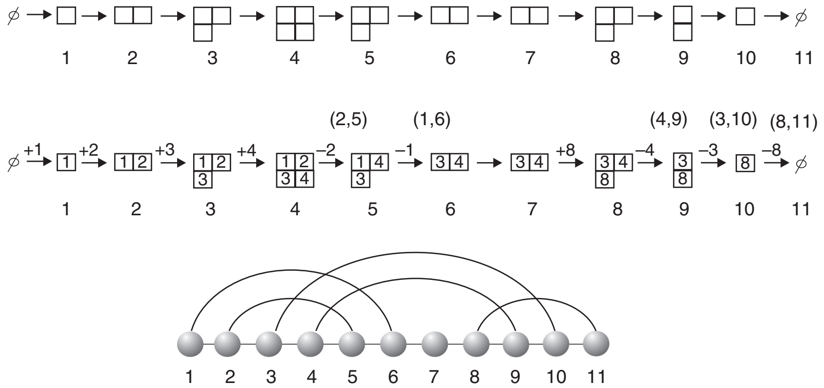

Fig. 2.10. From $*$-tableaux to partial matchings. If $\lambda^i \setminus \lambda^{i-1} = -\Box$, then the unique number is extracted, which, if RSK inserted into λ^i, recovers λ^{i-1}. This yields the arc set of a k-noncrossing, partial matching.

The latter extractions generate the arc set $\{(i, j(i)) \mid i \text{ is a } -\Box\text{-step}\}$ of a k-noncrossing diagram; see Fig. 2.10. Given a k-noncrossing diagram, starting with the empty shape, consider the sequence $(n, n-1, \ldots, 1)$ and do the following:

- If j is the endpoint of an arc (i, j), then RSK insert i.
- If j is the startpoint of an arc (j, s), then remove the square containing j.
- If j is an isolated point, then do nothing; see Fig. 2.11.

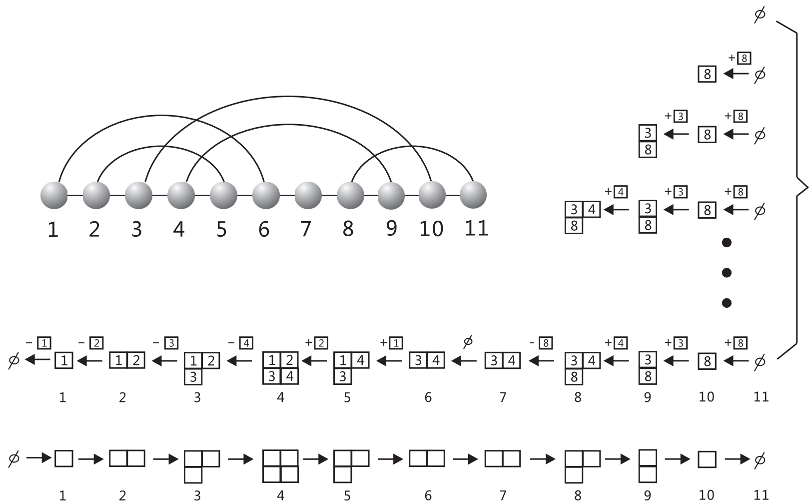

Fig. 2.11. From k-noncrosssing diagrams to $*$-tableaux using RSK insertion of the origins of arcs and removal of squares at the termini.

2.1.4 The generating function via the reflection principle

In this section we compute the enumerative generating function of k-noncrossing partial matchings. Our computation is based on the reflection principle. The key idea behind the reflection principle goes back to André [5, 49] and is to count walks that remain in the interior of a Weyl chamber by observing that all "bad" walks, i.e., those which touch a wall, cancel themselves. The particular method for deriving this pairing is via reflecting the walk choosing a point where it touches a wall. The following observation is essential for the reflection principle, formulated in Theorem 2.4.

Lemma 2.3. *Let $\Delta'_{k-1} = \{e_{k-1}, e_{j-1} - e_j \mid 2 \le j \le k-1\}$. Then every walk starting at some lattice point in the interior of a Weyl chamber, C, having steps $\pm e_i, 0$ that crosses from inside C into outside C touches a subspace $\langle e_{j-1} - e_j \mid 2 \le j \le k-1\rangle$ or $\langle e_j \mid 1 \le j \le k-1\rangle$.*

Proof. To prove the lemma we can, without loss of generality, assume

$$C = C_0 = \{(x_1, \dots, x_{k-1}) \mid x_1 \ge x_2 \ge \cdots \ge x_{k-1} \ge 0\}.$$

Then the assertion is that every walk having steps $\pm e_i, 0$ that crosses from the inside C_0 into outside C_0 intersects either $\langle e_{k-1}\rangle$ or $\langle e_{j-1} - e_j\rangle$ for $2 \le j \le k-1$. This is correct since to leave C_0 is tantamount to the existence of some i such that $x_i < x_{i+1}$. Let s_j be minimal w.r.t. $a + \sum_h^{j+1} s_h \notin C_0$. Since we have steps $\pm e_i, 0$ we conclude $x_{k-1} = 0$ or $x_j = x_{j-1}$ for some $2 \le j \le k-1$, whence the lemma.

Let $\Gamma_n(a, b)$ be the number of walks $\gamma_{a,b}$. For $a, b \in C_0$ (eq. (2.2)) let $\Gamma_n^+(a, b)$ denote the number of walks $\gamma_{a,b}$ that never touches a wall, i.e., remain in the interior of C_0. Finally for $a, b \in \mathbb{Z}^{k-1}$, let $\Gamma_n^-(a, b)$ denote the number of walks $\gamma_{a,b} = (s_1, \dots, s_n)$ that hit a wall at some step s_r. $\ell(\beta)$ denotes the length of $\beta \in \mathsf{B}_{k-1}$. For $a = b = (k-1, \dots, 1)$ we have according to Theorem 2.2

$$\Gamma_n^+(a, a) = \mathsf{M}_k(n),$$

where $\mathsf{M}_k(n) = |M_k(n)|$, i.e., the number of all k-noncrossing partial matchings over $[n]$.

Theorem 2.4. (Reflection Principle) *(Gessel and Viennot [49]) Suppose $a, b \in C_0$, then we have*

$$\Gamma_n^+(a, b) = \sum_{\beta \in \mathsf{B}_{k-1}} (-1)^{\ell(\beta)}\, \Gamma_n(\beta(a), b).$$

Theorem 2.4 allows us to compute the exponential generating function for $\Gamma_n^+(a, b)$, which is the number of walks from a to b that remain in the interior of C_0 [53]. Fig. 2.12 gives a simple application of reflection principles in lattice walk.

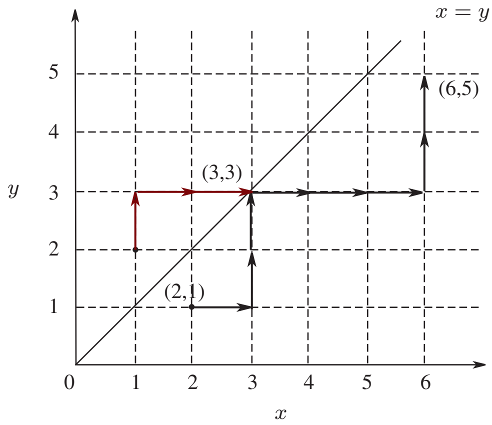

Fig. 2.12. Illustration of the reflection principle: "bad" walks cancel each other. Each lattice walk (here we consider only walks with steps $(1,0)$ or $(0,1)$) from $(2,1)$ to $(6,5)$ that hits the wall $y = x$ can uniquely be reflected into the walk from $(1,2)$ to $(6,5)$. Setting $a = (2,1)$, $b = (n+2, n+1)$, and $\tilde{a} = (1,2)$, the largest root corresponds to the subspace $\langle e_2 - e_1 \rangle$. We display a walk that hits this wall after three steps. Its initial segment (*red*) is then reflected leading to a walk from $(2,1)$ to $(6,5)$. Reflection implies $\Gamma_n^+(a,b) = \Gamma_n(a,b) - \Gamma_n(\tilde{a},b) = C_n$, where C_n is Catalan number.

Proof. Totally order the roots of Δ. Let $\Gamma_n^-(a,b)$ be the number of walks γ from a to b, $a, b \in \mathbb{Z}^{k-1}$ of length n using the steps s, $s \in \{\pm e_i, 0\}$ such that $\langle \gamma(s_r), \alpha \rangle = 0$ for some $\alpha \in \Delta$ (i.e., the walk intersects with the subspace $\langle \alpha \rangle$). According to Lemma 2.3 every walk that crosses from inside C into outside C touches a wall from which we can draw two conclusions:

$$\Gamma_n(a,b) = \Gamma_n^+(a,b) + \Gamma_n^-(a,b),$$
$$\beta \neq \mathsf{id} \quad \Longrightarrow \quad \Gamma_n(\beta(a),b) = \Gamma_n^-(\beta(a),b).$$

Claim. $\sum_{\beta \in \mathsf{B}_{k-1}} (-1)^{\ell(\beta)} \, \Gamma_n^-(\beta(a),b) = 0.$
Let $(s_1, \dots, s_n)$ be a walk from $\beta(a)$ to b. By assumption there exists some step s_r at which we have $\langle \gamma_{\beta(a),b}(s_r), \alpha \rangle = 0$, for $\alpha \in \Delta$, where $\langle \ , \ \rangle$ denotes the standard scalar product in $\mathbb{R}^{k-1}$. Let α^* be the largest root for which we have $\langle \gamma_{\beta(a),b}(s_r), \alpha^* \rangle = 0$ and $\beta_{\alpha^*}(x) = x - \frac{2\langle \alpha^*, x \rangle}{\langle \alpha^*, \alpha^* \rangle} \alpha^*$ its associated reflection (eq. (2.1)). We consider the walk

$$(\beta_{\alpha^*}(s_1), \dots, \beta_{\alpha^*}(s_r), s_{r+1}, \dots, s_n).$$

Now by definition $(\beta_{\alpha^*}(s_1), \dots, \beta_{\alpha^*}(s_r), s_{r+1}, \dots, s_n)$ starts at $(\beta_{\alpha^*} \circ \beta)(a)$ and we have according to eq. (2.3)

$$(-1)^{\ell(\beta_{\alpha^*} \circ \beta)} = (-1)^{\ell(\beta)+1}.$$

Therefore to each element $\gamma_{\beta(a),b}$ of $\Gamma_n^-(\beta(a),b)$ having sign $(-1)^{\ell(\beta)}$ there exists a $\gamma_{\beta_{\alpha^*}\beta(a),b} \in \Gamma_n^-(\beta_{\alpha^*}\beta(a),b)$ with sign $(-1)^{\ell(\beta)+1}$ and the claim follows. We immediately derive

$$\begin{aligned}
&\sum_{\beta\in \mathsf{B}_{k-1}} (-1)^{\ell(\beta)}\, \Gamma_n(\beta(a),b) \\
&= \Gamma_n(a,b) + \sum_{\beta\in \mathsf{B}_{k-1},\beta\neq \mathsf{id}} (-1)^{\ell(\beta)}\, \underbrace{\Gamma_n(\beta(a),b)}_{=\Gamma_n^-(\beta(a),b)} \\
&= \Gamma_n^+(a,b) + \underbrace{\Gamma_n^-(a,b) + \sum_{\beta\in \mathsf{B}_{k-1},\beta\neq \mathsf{id}} (-1)^{\ell(\beta)}\, \Gamma_n^-(\beta(a),b)}_{\sum_{\beta\in \mathsf{B}_{k-1}} (-1)^{\ell(\beta)}\, \Gamma_n^-(\beta(a),b)=0},
\end{aligned}$$

whence the theorem.

We can now achieve our main objective and specify the generating functions of the walks $\Gamma_n^+(a,b)$ having steps $0, \pm e_i$ and ${\Gamma'}_n^+(a,b)$ having steps $\pm e_i$ as a determinant of Bessel functions [53].

Theorem 2.5. (Grabiner and Magyar [53]) *Let* $I_r(2x) = \sum_{j\geq 0} \frac{x^{2j+r}}{j!(r+j)!}$ *be the hyperbolic Bessel function of the first kind of order* r. *Then the exponential generating functions for* $\Gamma_n^+(a,b)$ *and* ${\Gamma'}_n^+(a,b)$ *are given by*

$$\begin{aligned}
\sum_{n\geq 0} \Gamma_n^+(a,b)\frac{x^n}{n!} &= e^x \mathsf{det}[I_{b_j-a_i}(2x) - I_{a_i+b_j}(2x)]|_{i,j=1}^{k-1}, \\
\sum_{n\geq 0} {\Gamma'}_n^+(a,b)\frac{x^n}{n!} &= \mathsf{det}[I_{b_j-a_i}(2x) - I_{a_i+b_j}(2x)]|_{i,j=1}^{k-1}.
\end{aligned}$$

Proof. Let u_i, $1 \leq i \leq k-1$, be indeterminants and $u = (u_i)_1^{k-1}$. We define $u^{b-a} = \prod_{i=1}^{k-1} u_i^{b_i-a_i}$. Let $F(x,u)$ be a generating function, then $F(x,u)|_{u^{b-a}}$ equals the family of coefficients $a_i(u)$ at u^{b-a} of $\sum_{i\geq 0} a_i(u)x^i = F(x,u)$. We first consider unrestricted walks from a to b whose cardinality is given by

$$\Gamma_n(a,b) = \left[1 + \sum_{i=1}^{k-1}(u_i + u_i^{-1})\right]^n \Bigg|_{u^{b-a}}.$$

The exponential generating function of $\Gamma_n(a,b)$ is

$$\sum_{n\geq 0} \Gamma_n(a,b)\frac{x^n}{n!} = \sum_{n\geq 0} \left[1 + \sum_{i=1}^{k-1}(u_i + u_i^{-1})\right]^n \Bigg|_{u^{b-a}} \frac{x^n}{n!}$$

$$
\begin{aligned}
&= \sum_{n\geq 0} \frac{[1+\sum_{i=1}^{k-1}(u_i+u_i^{-1})]^n}{n!} x^n \Big|_{u^{b-a}} \\
&= e^x \cdot \mathsf{exp}[x\sum_{i=1}^{k-1}(u_i+u_i^{-1})]\Big|_{u^{b-a}} \\
&= e^x \cdot \prod_{i=1}^{k-1} \left(\mathsf{exp}(x(u_i+u_i^{-1}))\Big|_{{u_i}^{b_i-a_i}} \right).
\end{aligned}
$$

According to Theorem 2.4 we have

$$
\begin{aligned}
\sum_{n\geq 0} \Gamma_n^+(a,b)\frac{x^n}{n!} &= \sum_{n\geq 0}\sum_{\beta\in B_{k-1}} (-1)^{\ell(\beta)}\, \Gamma_n(\beta(a),b)\frac{x^n}{n!} \\
&= \sum_{\beta\in B_{k-1}} (-1)^{\ell(\beta)} \sum_{n\geq 0} \Gamma_n(\beta(a),b)\frac{x^n}{n!} \\
&= e^x \sum_{\beta\in B_{k-1}} (-1)^{\ell(\beta)} \prod_{i=1}^{k-1} \mathsf{exp}(x(u_i+u_i^{-1}))\Big|_{u^{b-\beta(a)}},
\end{aligned}
$$

whereas in case of ${\Gamma'_n}^+(a,b)$

$$
\sum_{n\geq 0} {\Gamma'_n}^+(a,b)\frac{x^n}{n!} = \sum_{\beta\in B_{k-1}} (-1)^{\ell(\beta)} \prod_{i=1}^{k-1} \mathsf{exp}(x(u_i+u_i^{-1}))\Big|_{u^{b-\beta(a)}}
$$

holds. We continue by analyzing $\sum_{n\geq 0} \Gamma_n^+(a,b)\frac{x^n}{n!}$. Equation (2.5) provides an interpretation of the term $(-1)^{\ell(\beta)}$:

$$
(-1)^{\ell(\beta)} = \mathrm{sgn}(\sigma)\prod_{i\in B}\eta_i = \mathrm{sgn}(\sigma)\prod_{i=1}^{k-1}\eta_i,
$$

where $\eta_i = \pm 1$. Based on this interpretation we compute

$$
\begin{aligned}
&\sum_{n\geq 0} \Gamma_n^+(a,b)\frac{x^n}{n!} = \\
&e^x \sum_{\sigma\in S_{k-1}} \sum_{\eta_i=-1,+1} \mathrm{sgn}(\sigma)\prod_{i=1}^{k-1}\eta_i \left(\mathsf{exp}(x(u_i+u_i^{-1}))\Big|_{u_i^{b_i-\eta_i a_{\sigma_i}}} \right) = \\
&e^x \sum_{\sigma\in S_{k-1}} \mathrm{sgn}(\sigma)\prod_{i=1}^{k-1} \left(\mathsf{exp}(x(u_i+u_i^{-1}))\Big|_{u_i^{b_i-a_{\sigma_i}}} - \mathsf{exp}(x(u_i+u_i^{-1}))\Big|_{u_i^{b_i+a_{\sigma_i}}} \right).
\end{aligned}
$$

We proceed by analyzing the terms $\mathsf{exp}(x(u_i + u_i^{-1}))$:

$$\begin{aligned}
\mathsf{exp}(x(u_i + u_i^{-1})) &= \sum_{n\geq 0} \frac{x^n}{n!}(u_i + u_i^{-1})^n \\
&= \sum_{n\geq 0} \frac{x^n}{n!} \sum_{j=0}^{n} \binom{n}{j} u_i^{n-2j} \\
&= \sum_{n\geq 0} x^n \sum_{j=0}^{n} \frac{u_i^{n-2j}}{j!(n-j)!} \\
&= \sum_{r=-\infty}^{\infty} u_i^r \sum_{j=0}^{\infty} \frac{x^{2j+r}}{j!(j+r)!} \\
&= \sum_{r=-\infty}^{\infty} u_i^r I_r(2x).
\end{aligned}$$

Therefore, for any $r \in \mathbb{Z}$, we have

$$\mathsf{exp}(x(u_i + u_i^{-1}))\Big|_{u_i^r} = \sum_{j\geq 0} \frac{x^{2j+r}}{j!(j+r)!} = I_r(2x).$$

As a result we arrive at

$$\sum_{n\geq 0} \Gamma_n^+(a,b)\frac{x^n}{n!} = e^x \sum_{\sigma\in S_{k-1}} \mathrm{sgn}(\sigma) \prod_{i=1}^{k-1} \left(I_{b_i - a_{\sigma_i}}(2x) - I_{b_i + a_{\sigma_i}}(2x)\right), \quad (2.6)$$

that is

$$\sum_{n\geq 0} \Gamma_n^+(a,b)\frac{x^n}{n!} = e^x \mathsf{det}[I_{b_j - a_i}(2x) - I_{a_i + b_j}(2x)]|_{i,j=1}^{k-1},$$

completing the proof of the theorem.

Let $f_k(n,0)$ denote the number of k-noncrossing matchings without isolated vertices over $[n]$. By abuse of notation we will in later chapters simply write $f_k(n)$ instead of $f_k(n,0)$. When n is odd, by the definition, $f_k(n,0) = 0$. Since $\Gamma_n^+(a,a) = \mathsf{M}_k(n)$ and $\Gamma_n'^+(a,a) = f_k(n,0)$ we obtain according to Theorem 2.5 for the generating functions of matchings and partial matchings as follows:

Corollary 2.6. *Let $I_r(2x) = \sum_{j\geq 0} \frac{x^{2j+r}}{j!(r+j)!}$ be the hyperbolic Bessel function of the first kind of order r. Then the generating functions for matchings and partial matchings are given by*

$$\sum_{n\geq 0} f_k(2n,0)\cdot \frac{x^{2n}}{(2n)!} = \mathsf{det}[I_{i-j}(2x) - I_{i+j}(2x)]|_{i,j=1}^{k-1}, \quad (2.7)$$

$$\sum_{n\geq 0} \mathsf{M}_k(n)\cdot \frac{x^{n}}{n!} = e^x\mathsf{det}[I_{i-j}(2x) - I_{i+j}(2x)]|_{i,j=1}^{k-1}. \quad (2.8)$$

Let

$$\mathbf{H}_k(z) = \sum_{n\geq 0} f_k(2n,0)\cdot \frac{z^{2n}}{(2n)!}.$$

The main importance of Corollary 2.6 lies in the fact that it implies that $\mathbf{H}_k(z)$ is D-finite; see Corollary 2.14. It does not allow to derive "simple" expressions for $\mathbf{H}_k(z)$ for $k \geq 3$.

By taking the approximation of the Bessel function[1], for $-\frac{\pi}{2} < \arg(z) < \frac{\pi}{2}$, and

$$I_r(z) = \frac{e^x}{\sqrt{2\pi z}}\left(\sum_{h=0}^{H} \frac{(-1)^h}{h!8^h}\prod_{t=1}^{h}(4r^2-(2t-1)^2)z^{-h} + \mathrm{O}(|z|^{-H-1})\right)$$

into the determinant given in eq. (2.7), we derive the following asymptotic formula.

Theorem 2.7. (Jin et al. [80]) *For arbitrary $k \in \mathbb{N}$, $k \geq 2$,* $\arg(z) \neq \pm\frac{\pi}{2}$ *holds*

$$\mathbf{H}_k(z) = \left[\prod_{i=1}^{k-1}\Gamma\left(i+1-\frac{1}{2}\right)\prod_{r=1}^{k-2} r!\right]\left(\frac{e^{2z}}{\pi}\right)^{k-1} z^{-(k-1)^2-\frac{k-1}{2}}\ (1+O(|z|^{-1})),$$

where $\Gamma(z)$ denotes the gamma function.

Employing the subtraction of singularities principle [98], in combination with Theorem 2.7, we obtain the following result, which is of central importance for all asymptotic formulas involving k-noncrossing matchings:

Theorem 2.8. (Jin et al. [80]) *For arbitrary $k \in \mathbb{N}$, $k \geq 2$ we have*

$$f_k(2n,0) \sim c_k\, n^{-((k-1)^2+(k-1)/2)}\,(2(k-1))^{2n}, \quad \textit{where } c_k > 0. \tag{2.9}$$

The proofs of Theorems 2.7 and 2.8 are elementary but involved and beyond the scope of this book. We refer the interested reader to [80]. Note that Theorem 2.8 implies that $\rho_k^2 = (2(k-1))^{-2}$ is a singularity of $\mathbf{F}_k(z)$; see Section 2.3.

Instead, we shall proceed by analyzing the relation between k-noncrossing matchings and k-noncrossing partial matchings. For this purpose we recruit the powerful concept of integral representations [36] in which combinatorial quantities like, for instance, binomial coefficients are replaced by contour integrals.

Lemma 2.9. *Let z be an indeterminate over $\mathbb{C}$. Then we have the identity of power series*

$$\forall |z| < \mu_k; \qquad \sum_{n\geq 0}\mathsf{M}_k(n)\,z^n = \left(\frac{1}{1-z}\right)\sum_{n\geq 0} f_k(2n,0)\left(\frac{z}{1-z}\right)^{2n}. \tag{2.10}$$

Proof. We have

$$\mathsf{M}_k(n) = \sum_{m=0}^{\lfloor \frac{n}{2} \rfloor} \binom{n}{2m} f_k(2m, 0),$$

where $\lfloor a \rfloor$ is the largest integer not larger than a. Expressing the combinatorial terms by contour integrals [36] we obtain

$$\begin{aligned}
\binom{n}{2m} &= \frac{1}{2\pi i} \oint_{|u|=\alpha} (1+u)^n u^{-2m-1} du, \\
f_k(2m, 0) &= \frac{1}{2\pi i} \oint_{|v|=\beta} \mathbf{F}_k(v^2) v^{-2m-1} dv,
\end{aligned}$$

where α, β are arbitrary small positive numbers and $\mathbf{F}_k(z) = \sum_{n \geq 0} f_k(2n, 0) z^n$. We derive

$$\begin{aligned}
\mathsf{M}_k(n) &= \frac{1}{(2\pi i)^2} \sum_m \oint_{|u|=\alpha, |v|=\beta} (1+u)^n u^{-2m-1} \mathbf{F}_k(v^2) v^{-2m-1} du dv \\
&= \frac{1}{(2\pi i)^2} \oint_{|u|=\alpha, |v|=\beta} (1+u)^n \frac{uv}{(uv)^2 - 1} \mathbf{F}_k(v^2) du dv \\
&= \frac{1}{(2\pi i)^2} \oint_{|v|=\beta} \mathbf{F}_k(v^2) v^{-1} \left[\oint_{|u|=\alpha} \frac{(1+u)^n u}{(u + \frac{1}{v})(u - \frac{1}{v})} du \right] dv.
\end{aligned}$$

Since $u = \frac{1}{v}$ and $u = -\frac{1}{v}$ are the only singularities (poles) enclosed by the particular contour, eq. (2.10) implies

$$\begin{aligned}
\oint_{|u|=\alpha} \frac{(1+u)^n u}{(u + \frac{1}{v})(u - \frac{1}{v})} du &= 2\pi i \left[\frac{(1+u)^n u}{u - \frac{1}{v}} \Big|_{u=-\frac{1}{v}} + \frac{(1+u)^n u}{u + \frac{1}{v}} \Big|_{u=\frac{1}{v}} \right] \\
&= \pi i \left(\left[1 - \frac{1}{v} \right]^n + \left[1 + \frac{1}{v} \right]^n \right).
\end{aligned}$$

Therefore, for $|z| < \mu_k$

$$\begin{aligned}
&\sum_{n \geq 0} \mathsf{M}_k(n) z^n \\
&= \frac{1}{4\pi i} \sum_{n \geq 0} \oint_{|v|=\beta} \mathbf{F}_k(v^2) v^{-1} \left(\left[1 - \frac{1}{v} \right]^n + \left[1 + \frac{1}{v} \right]^n \right) z^n dv \\
&= \frac{1}{4\pi i} \oint_{|v|=\beta} \mathbf{F}_k(v^2) \frac{1}{v - (v-1)z} dv + \frac{1}{4\pi i} \oint_{|v|=\beta} \mathbf{F}_k(v^2) \frac{1}{v - (v+1)z} dv.
\end{aligned}$$

The first integrand has its unique pole at $v = -\frac{z}{1-z}$ and the second at $v = \frac{z}{1-z}$, respectively:

$$\frac{1}{v - (v-1)z} = \frac{1}{v + \frac{z}{1-z}} \frac{1}{1-z} \quad \text{and} \quad \frac{1}{v - (v+1)z} = \frac{1}{v - \frac{z}{1-z}} \frac{1}{1-z}.$$

We derive

$$\sum_{n\geq 0}\mathsf{M}_k(n)z^n = \frac{1}{1-z}\left[\frac{1}{2}\mathbf{F}_k\left(\left(\frac{z}{1-z}\right)^2\right)+\frac{1}{2}\mathbf{F}_k\left(\left(\frac{z}{1-z}\right)^2\right)\right]$$
$$= \frac{1}{1-z}\mathbf{F}_k\left(\left(\frac{z}{1-z}\right)^2\right),$$

whence Lemma 2.1.

2.1.5 *D*-finiteness

The power series, $\mathbf{F}_k(x)=\sum_{n\geq 0} f_k(2n,0)x^n$, [125] is of central importance in Section 2.3 in the context of singularity analysis [42]. It is a D-finite power series and allows for analytic continuation in any simply connected domain containing zero.

Definition 2.10. *(a) A sequence $f(n)$ of complex number is said to be P-recursive, if there are polynomials $p_0(n),\ldots,p_m(n)\in\mathbb{C}[n]$ with $p_m(n)\neq 0$, such that for all $n\in\mathbb{N}$*

$$p_m(n)f(n+m)+p_{m-1}(n)f(n+m-1)+\cdots+p_0(n)f(n)=0. \qquad (2.11)$$

(b) A formal power series $F(x)=\sum_{n\geq 0} f(n)x^n$ is rational, if there are polynomials $A(x)$ and $B(x)$ in $\mathbb{C}[x]$ with $B(x)\neq 0$, such that

$$F(x)=\frac{A(x)}{B(x)}.$$

(c) $F(x)$ is algebraic, if there exist polynomials $q_0(x),\ldots,q_m(x)\in\mathbb{C}[x]$ with $q_m(x)\neq 0$, such that

$$q_m(x)F^m(x)+q_{m-1}(x)F^{m-1}(x)+\cdots+q_1(x)F(x)+q_0(x)=0.$$

(d) $F(x)$ is D-finite, if there are polynomials $q_0(x),\ldots,q_m(x)\in\mathbb{C}[x]$ with $q_m(x)\neq 0$, such that

$$q_m(x)F^{(m)}(x)+q_{m-1}(x)F^{(m-1)}(x)+\cdots+q_1(x)F'(x)+q_0(x)F(x)=0, \quad (2.12)$$

where $F^{(i)}(x)=d^iF(x)/dx^i$, and $\mathbb{C}[x]$ is the ring of polynomials in x with complex coefficients.

Let $\mathbb{C}(x)$ denote the rational function field, i.e., the field generated by taking equivalence classes of fractions of polynomials. Let $\mathbb{C}_{\rm alg}[[x]]$ and $\mathcal{D}$ denote the sets of algebraic power series over $\mathbb{C}$ and D-finite power series, respectively. Clearly, a rational formal power series is in particular algebraic. Furthermore, if $u\in\mathbb{C}_{\rm alg}[[x]]$, then u is also D-finite[127].

It is well known that a sequence is P-recursive if and only if its generating function is D-finite[125].

Lemma 2.11. *Suppose $F(z) = \sum_{n\geq 0} f(n)z^n$. Then $F(z)$ is D-finite if only if $f(n)$ is P-recursive.*

Proof. Since

$$z^j F^{(i)}(z) = \sum_{n\geq 0} (n+i-j)_i f(n+i-j) z^n, \tag{2.13}$$

where $(n-j+i)_i = (n-j+i)(n-j+i-1)\cdots(n-j+1)$ denotes the falling factorials, combining eqs. (2.13) and (2.12) implies the recurrence of eq. (2.11) for $f(n)$ by equating the coefficients of z^n. Accordingly, we conclude that the coefficients $f(n)$ of the power series $F(z)$ are P-recursive and we can derive the unique recurrence from the differential equation (2.12) of $F(z)$. If a sequence $f(n)$ is P-recursive, then eq. (2.11) holds. Since each $p_i(n) \in \mathbb{C}[n]$ can be represented as $\mathbb{C}$-linear combination of $(n+i)_j$, $j \geq 0$, the term $\sum_{n\geq 0} p_i(n) f(n+i) z^n$ can also be represented as a $\mathbb{C}$-linear combination of series of the form $\sum_{n\geq 0}(n+i)_j f(n+i)z^n$. In view of

$$\sum_{n\geq 0} (n+i)_j\, f(n+i) z^n = R_i(z) + z^{j-i} F^{(j)}(z),$$

where $R_i(z) \in z^{-1}\mathbb{C}[z^{-1}]$, we can recover eq. (2.12) by multiplying eq. (2.11) with z^n and summing over $n \geq 0$. Thus for a given recurrence of $f(n)$, we can derive a unique differential equation of $F(z)$ in the form (2.12).

Lemma 2.12. *Each P-recursion of $f_k(2n,0)$, $\mathcal{R}$, having polynomial coefficients with greatest common divisor (gcd) one corresponds to a P-recursion of $e_k(n) = f_k(2n,0)/(2n)!$, $\epsilon(\mathcal{R})$. Each P-recursion of $e_k(2n,0)$, $\mathcal{Q}$, corresponds uniquely to a P-recursion of $f_k(2n,0)$, $\omega(\mathcal{Q})$, having polynomial coefficients with gcd one. Furthermore, we have $\omega(\epsilon(\mathcal{R})) = \mathcal{R}$.*

Proof. Suppose we have a P-recurrence $\sum_{i=0}^{r_k} a_i(n) f_k(2(n+i),0) = 0$, where $a_i(n)$ are polynomials in n with integer coefficients, having gcd one and $a_0(n) \neq 0$. Then

$$\sum_{i=0}^{r_k} a_i(n)(2(n+i))_{2i}\, e_k(n+i) = 0,$$

i.e., a P-recurrence for $e_k(n)$. Suppose now we have a P-recurrence for $e_k(n)$, $\sum_{i=0}^{r_k} b_i(n) e_k(n+i) = 0$, where the $b_i(n)$ are all polynomials of n with integer coefficients, and $b_0(n) \neq 0$. We then immediately derive

$$\sum_{i=0}^{r_k} c_i(n) f_k(2(n+i),0) = 0,$$

where $c_i(n) = b_i(n)\frac{(2n)!}{(2(n+i))!}$. $c_i(n)$ are *rational* functions in n. Suppose $d(n)$ is the lcm of the denominators of the $c_i(n)$. Then

$$\sum_{i=0}^{r_k} c_i'(n) f_k(2(n+i), 0) = 0,$$

where the $c_i'(n) = d(n)b_i(n)\frac{(2n)!}{(2(n+i))!}$ are by construction polynomials, having gcd one and $c_0'(n) \neq 0$, whence the lemma.

We proceed by studying closure properties of D-finite power series which are of key importance in the following chapters.

Theorem 2.13. (Stanley [127]) *P-recursive sequences, D-finite, and algebraic power series have the following properties:*

(a) If f, g are P-recursive, then $f \cdot g$ is P-recursive.
(b) If $F, G \in \mathcal{D}$, and $\alpha, \beta \in \mathbb{C}$, then $\alpha F + \beta G \in \mathcal{D}$ and $FG \in \mathcal{D}$.
(c) If $F \in \mathcal{D}$ and $G \in \mathbb{C}_{alg}[[x]]$ with $G(0) = 0$, then $F(G(x)) \in \mathcal{D}$.

Here we omit the proof of (a) and (b) which can be found in [127]. We present, however, a direct proof of (c).

Proof. (c) We assume that $G(0) = 0$ so that the composition $F(G(x))$ is well defined. Let $K = F(G(x))$. Then $K^{(i)}$ is a linear combination of $F(G(x))$, $F'(G(x))$, ..., over $\mathbb{C}[G, G', \ldots]$, i.e., the ring of polynomials in G, $G', \ldots$ with complex coefficients.

Claim. $G^{(i)} \in \mathbb{C}(x, G)$, $i \geq 0$, and therefore $\mathbb{C}[G, G', \ldots] \subset \mathbb{C}(x, G)$, where $\mathbb{C}(x, G)$ denotes the field generated by x and G.
Since G is algebraic, it satisfies

$$q_d(x)G^d(x) + q_{d-1}(x)G^{d-1}(x) + \cdots + q_1(x)G(x) + q_0(x) = 0, \qquad (2.14)$$

where $q_0(x), \ldots, q_d(x) \in \mathbb{C}[x]$, $q_d(x) \neq 0$ and d is minimal, i.e., $(G^i(x))_{i=0}^{d-1}$ is linear independent over $\mathbb{C}[x]$. In other words, for all $(\widetilde{q}_i(x))_{i=1}^{d-1} \neq 0$ we have

$$\widetilde{q}_{d-1}(x)G^{d-1}(x) + \cdots + \widetilde{q}_1(x)G(x) + \widetilde{q}_0(x) \neq 0.$$

We consider

$$P(x, G) = q_d(x)G^d(x) + q_{d-1}(x)G^{d-1}(x) + \cdots + q_1(x)G(x) + q_0(x).$$

Differentiating eq. (2.14) once, we derive

$$0 = \frac{d}{dx}P(x, G) = \frac{\partial P(x, y)}{\partial x}\Big|_{y=G} + G'\frac{\partial P(x, y)}{\partial y}\Big|_{y=G}.$$

The degree of $\frac{\partial P(x,y)}{\partial y}\Big|_{y=G}$ in G is smaller than $d-1$ and $q_d(x) \neq 0$, whence

$\frac{\partial P(x,y)}{\partial y}\Big|_{y=G} \neq 0$. We therefore arrive at

$$G' = - \frac{\left.\frac{\partial P(x,y)}{\partial x}\right|_{y=G}}{\left.\frac{\partial P(x,y)}{\partial y}\right|_{y=G}} \in \mathbb{C}(x, G).$$

Iterating the above argument, we obtain $G^{(i)} \in \mathbb{C}(x, G),\ i \geq 0$, and therefore $\mathbb{C}[G, G', \ldots] \subset \mathbb{C}(x, G)$, whence the claim.

Let $\widetilde{V}$ be the $\mathbb{C}(x, G)$ vector space spanned by $F(G(x))$, $F'(G(x))$, ... Since $F \in \mathcal{D}$, we have $\dim_{\mathbb{C}(x)}\langle F, F', \cdots\rangle < \infty$, immediately implying the finiteness of $\dim_{\mathbb{C}(G)}\langle F(G), F'(G), \cdots\rangle$. Thus, since $\mathbb{C}(G)$ is a subfield of $\mathbb{C}(x, G)$, we derive

$$\dim_{\mathbb{C}(x,G)}\langle F, F', \cdots\rangle < \infty$$

and consequently $\dim_{\mathbb{C}(x,G)} \widetilde{V} < \infty$ and $\dim_{\mathbb{C}(x)} \mathbb{C}(x, G) < \infty$. As a result

$$\dim_{\mathbb{C}(x)} \widetilde{V} = \dim_{\mathbb{C}(x,G)} \widetilde{V} \cdot \dim_{\mathbb{C}(x)} \mathbb{C}(x, G) < \infty$$

follows and since each $K^{(i)} \in \widetilde{V}$, we conclude that $F(G(x))$ is D-finite.

Corollary 2.14. *The generating function of k-noncrossing matchings over $2n$ vertices, $\mathbf{F}_k(z) = \sum_{n\geq 0} f_k(2n, 0)\, z^n$, is D-finite.*

Proof. Corollary 2.6 gives the exponential generating function of $f_k(2n, 0)$

$$\sum_{n\geq 1} f_k(2n, 0)\frac{x^{2n}}{(2n)!} = \mathsf{det}[I_{i-j}(2x) - I_{i+j}(2x)]_{i,j=1}^{k-1}, \tag{2.15}$$

where $I_m(x)$ is Bessel function of the first order. Recall that the Bessel function of the first kind satisfies $I_n(x) = i^{-n}J_n(ix)$ and $J_n(x)$ is the solution of the Bessel differential equation

$$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} + (x^2 - n^2)y = 0.$$

For every fixed $n \in \mathbb{N}$, $J_n(x)$ is D-finite. Let $G(x) = ix$. Clearly, $G(x) \in \mathbb{C}_{\text{alg}}[[x]]$ and $G(0) = 0$, $J_n(ix)$ and $I_n(x)$ are accordingly D-finite in view of the assertion (c) of Theorem 2.13. Analogously we show that $I_n(2x)$ is D-finite for every fixed $n \in \mathbb{N}$. Using eq. (2.15) and assertion (b) of Theorem 2.13, we conclude that

$$\mathbf{H}_k(x) = \sum_{n\geq 0} \frac{f_k(2n, 0)}{(2n)!}\, x^{2n}$$

is D-finite. In other words the sequence $f(n) = \frac{f_k(2n,0)}{(2n)!}$ is P-recursive and furthermore $g(n) = (2n)!$ is, in view of $(2n + 1)(2n + 2)g(n) - g(n + 1) = 0$, P-recursive. Therefore, $f_k(2n, 0) = f(n)g(n)$ is P-recursive. This proves that $\mathbf{F}_k(z) = \sum_{n\geq 0} f_k(2n, 0)z^n$ is D-finite.

2.2 Symbolic enumeration

In the following we will compute various generating functions via the symbolic enumeration method [42].

Definition 2.15. *A combinatorial class is a set $\mathcal{C}$ together with a size function, $w_{\mathcal{C}}\colon \mathcal{C} \longrightarrow \mathbb{Z}^+$, $(\mathcal{C}, w_{\mathcal{C}})$ such that $w_{\mathcal{C}}^{-1}(n)$ is finite for any $n \in \mathbb{Z}^+$.*

Suppose $(\mathcal{C}, w_{\mathcal{C}})$ is a combinatorial class and $c \in \mathcal{C}$. We call $w_{\mathcal{C}}(c)$ the size of c and write simply $w(c)$. There are two special combinatorial classes: $\mathcal{E}$ and $\mathcal{Z}$ which contain only one element of sizes 0 and 1, respectively. The subset of $\mathcal{C}$ which contains all the elements of size n, $w_{\mathcal{C}}^{-1}(n)$, is denoted by $\mathcal{C}_n$, and let $C_n = |\mathcal{C}_n|$. The generating function of a combinatorial class $(\mathcal{C}, w_{\mathcal{C}})$ is given by

$$\mathbf{C}(z) = \sum_{c \in \mathcal{C}} z^{w_{\mathcal{C}}(c)} = \sum_{n \geq 0} C_n\, z^n,$$

where $\mathcal{C}_n \subset \mathcal{C}$. In particular, the generating functions of the classes $\mathcal{E}$ and $\mathcal{Z}$ are

$$\mathbf{E}(z) = 1 \quad \text{and} \quad \mathbf{Z}(z) = z. \tag{2.16}$$

Definition 2.16. *Suppose $\mathcal{C}, \mathcal{D}$ are combinatorial classes. Then $\mathcal{C}$ is isomorphic to $\mathcal{D}$, $\mathcal{C} \cong \mathcal{D}$, if and only if*

$$\forall\, n \geq 0, \quad |\mathcal{C}_n| = |\mathcal{D}_n|.$$

In the following we shall identify isomorphic combinatorial classes and write $\mathcal{C} = \mathcal{D}$ if $\mathcal{C} \cong \mathcal{D}$. We set

- $\mathcal{C} + \mathcal{D} := \mathcal{C} \cup \mathcal{D}$, if $\mathcal{C} \cap \mathcal{D} = \varnothing$ and for $a \in \mathcal{C} + \mathcal{D}$,

$$w_{\mathcal{C}+\mathcal{D}}(a) = \begin{cases} w_{\mathcal{C}}(a) & \text{if } a \in \mathcal{C} \\ w_{\mathcal{D}}(a) & \text{if } a \in \mathcal{D}. \end{cases}$$

- $\mathcal{C} \times \mathcal{D} := \{a = (c, d) \mid c \in \mathcal{C}, d \in \mathcal{D}\}$ and for $a \in \mathcal{C} \times \mathcal{D}$,

$$w_{\mathcal{C}\times\mathcal{D}}(a) = w_{\mathcal{C}}(c) + w_{\mathcal{D}}(d).$$

We furthermore set

- $\mathcal{C}^m := \prod_{h=1}^{m} \mathcal{C}$ and
- $\textsc{Seq}(\mathcal{C}) := \mathcal{E} + \mathcal{C} + \mathcal{C}^2 + \cdots$.

In view of eq. (2.16), $\textsc{Seq}(\mathcal{C})$ is a combinatorial class if and only if there is no element in $\mathcal{C}$ of size 0.

Theorem 2.17. *Suppose $\mathcal{A}$, $\mathcal{C}$, and $\mathcal{D}$ are combinatorial classes with generating functions $\mathbf{A}(z)$, $\mathbf{C}(z)$, and $\mathbf{D}(z)$. Then*

(a) $\mathcal{A}=\mathcal{C}+\mathcal{D} \Longrightarrow \mathbf{A}(z)=\mathbf{C}(z)+\mathbf{D}(z)$,
(b) $\mathcal{A}=\mathcal{C}\times\mathcal{D} \Longrightarrow \mathbf{A}(z)=\mathbf{C}(z)\cdot\mathbf{D}(z)$,
(c) $\mathcal{A}=\textsc{Seq}(\mathcal{C}) \Longrightarrow \mathbf{A}(z)=\frac{1}{1-\mathbf{C}(z)}$.

Proof. Suppose $\mathcal{A}=\mathcal{C}+\mathcal{D}$, then

$$\mathbf{A}(z)=\sum_{a\in\mathcal{A}} z^{w_{\mathcal{A}}(a)}=\sum_{a\in\mathcal{C}} z^{w_{\mathcal{C}}(a)}+\sum_{a\in\mathcal{D}} z^{w_{\mathcal{D}}(a)}=\mathbf{C}(z)+\mathbf{D}(z).$$

In case of $\mathcal{A}=\mathcal{C}\times\mathcal{D}$, we compute

$$\begin{aligned}\mathbf{A}(z)&=\sum_{a\in\mathcal{A}} z^{w_{\mathcal{A}}(a)}\\ &=\sum_{(c,d)\in\mathcal{C}\times\mathcal{D}} z^{w_{\mathcal{C}}(c)+w_{\mathcal{D}}(d)}\\ &=\left(\sum_{c\in\mathcal{C}} z^{w_{\mathcal{C}}(c)}\right)\cdot\left(\sum_{d\in\mathcal{D}} z^{w_{\mathcal{D}}(d)}\right)\\ &=\mathbf{C}(z)\cdot\mathbf{D}(z).\end{aligned}$$

Consequently, in case of $\mathcal{A}=\textsc{Seq}(\mathcal{C})$,

$$\mathbf{A}(z)=1+\mathbf{C}(z)+\mathbf{C}(z)^2+\cdots=\frac{1}{1-\mathbf{C}(z)}.$$

In order to keep track of some specific combinatorial class in order to express multivariate generating functions, we introduce the concept of combinatorial markers. A combinatorial marker is a combinatorial class with only one element of size 0 or one element of size 1.

For instance, suppose $\mathcal{F}_{k,h}$ is the combinatorial class of all k-noncrossing matchings with h arcs and its size function is the length of a matching in $\mathcal{F}_{k,h}$, i.e., the number of vertices. Let $\mathcal{P}_{k,h}$ denote the combinatorial class of all the k-noncrossing partial matchings with h arcs and its size function counting the total number of vertices. Let $\mathcal{Z}$ represent the combinatorial class consisting of a single vertex. Then, plainly

$$\mathcal{P}_{k,h}=\mathcal{F}_{k,h}\times\left(\textsc{Seq}\left(\mathcal{Z}\right)\right)^{2h+1}.$$

Suppose now we want to keep track of the number of isolated vertices in a k-noncrossing partial matching having h arcs. Then we introduce the combinatorial marker μ in order to keep track of the isolated vertices as follows:

$$\mathcal{P}_{k,h}=\mathcal{F}_{k,h}\times\left(\textsc{Seq}\left(\mu\times\mathcal{Z}\right)\right)^{2h+1},$$

whence

$$\mathbf{P}_{k,h}(z,u) = \mathbf{F}_{k,h}(z) \cdot \left(\frac{1}{1-uz}\right)^{2h+1},$$

where $\mathbf{P}_{k,h}(z,u)$ and $\mathbf{F}_{k,h}(z)$ are the generating functions of the combinatorial classes $\mathcal{P}_{k,h}$ and $\mathcal{F}_{k,h}$ and u is an indeterminant.

2.3 Singularity analysis

Let $f(z) = \sum_n a_n z^n$ be a generating function with radius of convergence, R. In light of the fact that explicit formulas for the coefficients a_n can be very complicated or even impossible to obtain, we shall investigate the generating function $f(z)$ by deriving information about a_n for large n.

In the following we are primarily concerned with the estimation of a_n in terms of the exponential factor γ and the subexponential factor $P(n)$, that is, we have the following situation

$$a_n \sim P(n) \cdot \gamma^n, \tag{2.17}$$

where γ is a fixed number and $P(n)$ is a polynomial in n. While this is, of course, a vast simplification of the original problem (explicit computation of the coefficients a_n), eq. (2.17) extracts key information about the coefficients.

2.3.1 Transfer theorems

The derivation of exponential growth rate and subexponential factors of eq. (2.17) mainly rely on singular expansions and transfer theorems. Transfer theorems realize the translation of error terms from functions to coefficients. The underlying basic tool here is, of course, Cauchy's integral formula

$$a_n = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z^{n+1}} dz,$$

where C is any simple closed curve in the region $0 < |x| < R$, containing 0.

In the following we shall employ a particular integration path; see Fig. 2.13. The contour is a path, slightly "outside" the disc of radius R. This contour is comprised of an inner arc segment 3 and an outer arc segment 1 and two connecting linear part segments 2 and 4. The major contribution to the contour integral stems from segments 2, 3, and 4.

The behavior of $f(z)$ close to the dominant singularity is the determining factor for the asymptotic behavior of its coefficients. Let us get started by specifying a suitable domain for our contours.

Definition 2.18. *Given two numbers ϕ, r, where $r > |\rho|$ and $0 < \phi < \frac{\pi}{2}$, the open domain $\Delta_\rho(\phi, r)$ is defined as*

$$\Delta_\rho(\phi, r) = \{z \mid |z| < r, z \neq \rho,\, |\mathrm{Arg}(z-\rho)| > \phi\}.$$

A domain is a Δ_ρ-domain at ρ if it is of the form $\Delta_\rho(\phi, r)$ for some r and ϕ. A function is Δ_ρ-analytic if it is analytic in some Δ_ρ-domain.

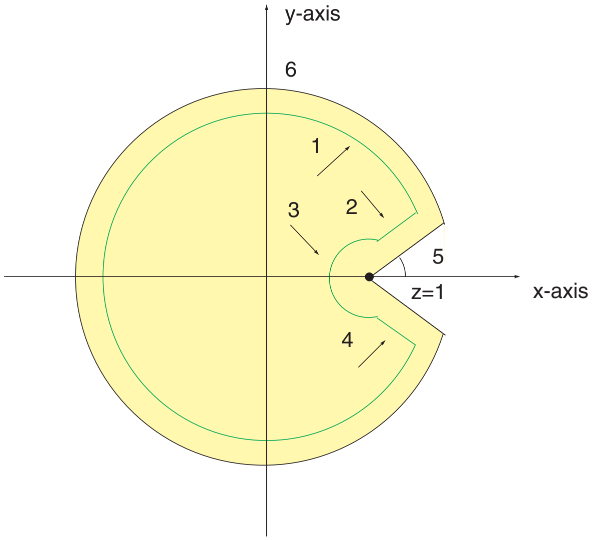

Fig. 2.13. Δ_1-domain enclosing a contour. We assume $z = 1$ to be the unique dominant singularity. The coefficients are obtained via Cauchy's integral formula and the integral path is decomposed into four segments. Segment 1 becomes asymptotically irrelevant since by construction the function involved is bounded on this segment. Relevant are the rectilinear segments 2 and 4 and the inner circle 3. The only contributions to the contour integral are being made here.

Let $[z^n]\,f(z)$ denote the coefficient of z^n of the power series expansion of $f(z)$ at 0. Since the Taylor coefficients have the property

$$\forall\, \gamma \in \mathbb{C} \setminus 0; \quad [z^n]f(z) = \gamma^n [z^n] f\left(\frac{z}{\gamma}\right),$$

we can, without loss of generality, reduce our analysis to the case where $z = 1$ is the unique dominant singularity. We use $U(a, r) = \{z \in \mathbb{C} | |z - a| < r\}$ in order to denote the open neighborhood of a in $\mathbb{C}$. Furthermore, we use the notations

$$\begin{aligned}
(f(z) = O\,(g(z)) \text{ as } z \to \rho) &\iff (f(z)/g(z) \text{ is bounded as } z \to \rho)\,,\\
(f(z) = o\,(g(z)) \text{ as } z \to \rho) &\iff (f(z)/g(z) \to 0 \text{ as } z \to \rho)\,,\\
(f(z) = \Theta\,(g(z)) \text{ as } z \to \rho) &\iff (f(z)/g(z) \to c \text{ as } z \to \rho)\,,\\
(f(z) \sim g(z) \text{ as } z \to \rho) &\iff (f(z)/g(z) \to 1 \text{ as } z \to \rho)\,,
\end{aligned}$$

where c is some constant. If we write $f(z) = O(g(z))$, $f(z) = o(g(z))$, $f(z) = \Theta(g(z))$, or $f(z) \sim g(z)$, it is implicitly assumed that z tends to a (unique) singularity.

Theorem 2.19. (Waterman [41]) *(a) Suppose $f(z) = (1-z)^{-\alpha}$, $\alpha \in \mathbb{C}\backslash\mathbb{Z}_{\leq 0}$, then*

$$[z^n]\, f(z) \sim \frac{n^{\alpha-1}}{\Gamma(\alpha)}\left[1 + \frac{\alpha(\alpha-1)}{2n} + \frac{\alpha(\alpha-1)(\alpha-2)(3\alpha-1)}{24n^2} + \frac{\alpha^2(\alpha-1)^2(\alpha-2)(\alpha-3)}{48n^3} + O\left(\frac{1}{n^4}\right)\right].$$

(b) Suppose $f(z) = (1-z)^r \log(\frac{1}{1-z})$, $r \in \mathbb{Z}_{\geq 0}$, then we have

$$[z^n]f(z) \sim (-1)^r \frac{r!}{n(n-1)\dots(n-r)}.$$

Theorems 2.19 and 2.20 are the key tools for the singularity analysis of the generating function of RNA pseudoknot structures.

Theorem 2.20. (Flajolet and Sedgewick [42]) *Let $f(z)$ be a Δ_1-analytic function at its unique singularity $z = 1$. Let $g(z)$ be a linear combination of functions in the set B, where*

$$B = \{(1-z)^\alpha \log^\beta\left(\frac{1}{1-z}\right) | \alpha, \beta \in \mathbb{R}\},$$

that is, we have in the intersection of a neighborhood of 1 *with the Δ_1-domain*

$$f(z) = \mathrm{o}(g(z)) \quad \textit{for } z \to 1.$$

Then we have

$$[z^n]f(z) = \mathrm{o}\left([z^n]g(z)\right),$$

where $\mathrm{o} \in \{O, o, \Theta, \sim\}$.

Let $S(\rho, n)$ denote the subexponential factor of $[z^n]\, f(z)$ at the dominant singularity ρ. In general [42], if $f(z)$ has multiple dominant singularities, $[z^n]\, f(z)$ is asymptotically determined by the sum over *all* dominant singularities, i.e.,

$$[z^n]\, f(z) \sim \sum_i S(\rho_i, n)\rho_i^n.$$

2.3.2 The supercritical paradigm

In this section we discuss an implication of Theorem 2.20. The supercritical paradigm refers to a composition of two functions where the “inner” function is regular at the singularity of the outer function. In this case the singularity type is that of the “outer” function. What happens is that the inner function only “shifts” the singularity of the outer function.

The scenario considered here is tailored for Chapters 4 and 5.

Theorem 2.21. *Let $\psi(z,s)$ be an algebraic, analytic function in a domain $\mathcal{D} = \{(z,s) \mid |z| \leq r, |s| < \epsilon\}$ such that $\psi(0,s) = 0$. In addition suppose $\gamma(s)$ is the unique dominant singularity of $\mathbf{F}_k(\psi(z,s))$ and unique analytic solution of $\psi(\gamma(s),s) = \rho_k^2$, $|\gamma(s)| \leq r$, $\partial_z \psi(\gamma(s),s) \neq 0$ for $|s| < \epsilon$. Then $\mathbf{F}_k(\psi(z,s))$ has a singular expansion and*

$$[z^n]\mathbf{F}_k(\psi(z,s)) \sim A(s)\, n^{-((k-1)^2+(k-1)/2)} \left(\frac{1}{\gamma(s)}\right)^n, \tag{2.18}$$

uniformly in s contained in a small neighborhood of 0 and $A(s)$ is continuous.

We postpone the proof of Theorem 2.21 to Section 2.4.2. The key property of the singular expansion of Theorem 2.21 is the uniformity of eq. (2.18) in the parameter s.

In the following chapters, we will be working with compositions $\mathbf{F}_k(\vartheta(z))$, where $\vartheta(z)$ is algebraic and satisfies $\vartheta(0) = 0$, that is, we apply Theorem 2.21 for fixed parameter s. According to Theorem 2.13, $\mathbf{F}_k(\vartheta(z))$ is D-finite and Theorem 2.21 implies that if ϑ satisfies certain conditions the subexponential factors of $\mathbf{F}_k(\vartheta(z))$ coincide with those of $\mathbf{F}_k(z)$.

2.4 The generating function $\mathbf{F}_k(z)$

While Theorems 2.7 and 2.8 shed light of the generating function $\mathbf{F}_k(z)$, Theorem 2.21 motivates a closer look in particular at its singular expansion. The key to this is to find the ODE that $\mathbf{F}_k(z)$ satisfies. This is not "just" a matter of computation, in Proposition 2.22 we have to prove that the latter are correct.

2.4.1 Some ODEs

In Section 2.1.5, we have shown that $\mathbf{F}_k(z)$ is D-finite, that is, there exists some $e \in \mathbb{N}$ for which $\mathbf{F}_k(z)$ satisfies an ODE of the form

$$q_{0,k}(z)\frac{d^e}{dz^e}\mathbf{F}_k(z) + q_{1,k}(z)\frac{d^{e-1}}{dz^{e-1}}\mathbf{F}_k(z) + \cdots + q_{e,k}(z)\mathbf{F}_k(z) = 0, \tag{2.19}$$

where $q_{j,k}(z)$ are polynomials. The fact that $\mathbf{F}_k(z)$ is the solution of an ODE implies the existence of an analytic continuation into any simply connected domain [125], i.e., $\Delta_{\rho_k^2}$-analyticity.

Explicit knowledge of the above ODE is of key importance for two reasons:

- Any dominant singularity of a solution is contained in the set of roots of $q_{0,k}(z)$ [125]. In other words the ODE "controls" the dominant singularities that are crucial for asymptotic enumeration.
- Under certain regularity conditions (discussed below) the singular expansion of $\mathbf{F}_k(z)$ follows from the ODE; see Proposition 2.24.

Accordingly, let us first compute for $2 \leq k \leq 9$ the ODEs for $\mathbf{F}_k(z)$.

Proposition 2.22. *For $2 \leq k \leq 9$, $\mathbf{F}_k(z)$ satisfies the ODEs listed in Table 2.1 and we have in particular*

$$q_{0,2}(z) = (4z - 1)\, z, \tag{2.20}$$
$$q_{0,3}(z) = (16z - 1)\, z^2, \tag{2.21}$$
$$q_{0,4}(z) = (144\, z^2 - 40\, z + 1)\, z^3, \tag{2.22}$$
$$q_{0,5}(z) = (1024\, z^2 - 80\, z + 1)\, z^4, \tag{2.23}$$
$$q_{0,6}(z) = (14,400\, z^3 - 4144\, z^2 + 140\, z - 1)\, z^5, \tag{2.24}$$
$$q_{0,7}(z) = (147,456\, z^3 - 12,544\, z^2 + 224\, z - 1)\, z^6, \tag{2.25}$$
$$q_{0,8}(z) = (2,822,400 z^4 - 826,624 z^3 + 31,584 z^2 - 336 z + 1) z^7, \tag{2.26}$$
$$q_{0,9}(z) = (37,748,736 z^4 - 3,358,720 z^3 + 69,888 z^2 - 480 z + 1) z^8, \tag{2.27}$$

Proposition 2.22 immediately implies the following sets of roots:

$$\nabla_2 = \left\{\frac{1}{4}\right\};\ \nabla_4 = \nabla_2 \cup \left\{\frac{1}{36}\right\};\ \nabla_6 = \nabla_4 \cup \left\{\frac{1}{100}\right\};\ \nabla_8 = \nabla_6 \cup \left\{\frac{1}{196}\right\};$$
$$\nabla_3 = \left\{\frac{1}{16}\right\};\ \nabla_5 = \nabla_3 \cup \left\{\frac{1}{64}\right\};\ \nabla_7 = \nabla_5 \cup \left\{\frac{1}{144}\right\};\ \nabla_9 = \nabla_7 \cup \left\{\frac{1}{256}\right\}.$$

Equations (2.20), (2.21), (2.22), (2.23), (2.24), (2.25), (2.26), and (2.27) and Theorem 2.8 show that for $2 \leq k \leq 9$ the unique dominant singularity of $\mathbf{F}_k(z)$ is given by ρ_k^2, where $\rho_k = 1/2(k-1)$.

Proof. The ODEs for $\mathbf{F}_k(z)$, $2 \leq k \leq 9$, listed in Table 2.1, induce according to Lemma 2.11 uniquely respective P-recurrences $\mathcal{R}_k$. For $2 \leq k \leq 9$ the polynomial coefficients of any $\mathcal{R}_k$ have a greatest common divisor (gcd) of 1 and, in addition, the coefficient of the $f_k(2n,0)$-term in $\mathcal{R}_k$ is nonzero. According to Lemma 2.12, each $\mathcal{R}_k$ corresponds to a unique P-recurrence $\epsilon(\mathcal{R}_k)$ for $f_k(2n,0)/(2n)!$, which in turn corresponds uniquely to an ODE for the exponential generating function $\mathbf{H}_k(z) = \sum_{n\geq 0} f_k(2n,0) \cdot \frac{z^{2n}}{(2n)!}$; see Corollary 2.14. We furthermore have according to eq. (2.15)

$$\sum_{n\geq 1} f_k(2n,0)\frac{x^{2n}}{(2n)!} = \mathsf{det}[I_{i-j}(2x) - I_{i+j}(2x)]_{i,j=1}^{k-1}.$$

According to Lemma 2.11 the P-recurrences $\epsilon(\mathcal{R}_k)$ induce respective ODEs for $\mathbf{H}_k(z)$. The key point is now that for $\mathbf{H}_k(z)$, eq. (2.15) provides an interpretation of $\mathbf{H}_k(z)$ as a determinant of Bessel functions. We proceed by verifying for $2 \leq k \leq 9$ that $\mathsf{det}[I_{i-j}(2x) - I_{i+j}(2x)]_{i,j=1}^{k-1}$ satisfies the $\mathbf{H}_k(z)$-ODEs derived from Table 2.1 via Lemmas 2.11 and 2.12. Consequently we have now established the correctness of the derived $\mathbf{H}_k(z)$-ODEs. These allow us via Lemmas 2.12 and 2.11 to recover the ODEs listed in Table 2.1 and the proposition follows.

2.4.2 The singular expansion of $\mathbf{F}_k(z)$

Let us begin by introducing some concepts: a meromorphic ODE is an ODE of the form

$$f^{(r)}(z) + d_1(z) f^{(r-1)}(z) + \cdots + d_r(z) f(z) = 0, \tag{2.28}$$

where $f^{(m)}(z) = \frac{d^m}{dz^m} f(z)$, $0 \leq m \leq r$ and the $d_j(z)$, are meromorphic in some domain Ω. Assuming that ζ is a pole of a meromorphic function $d(z)$, $\omega_\zeta(d)$ denotes the order of the pole ζ. In case $d(z)$ is analytic at ζ we write $\omega_\zeta(d) = 0$.

Meromorphic differential equations have a singularity at ζ if at least one of the $\omega_\zeta(d_j)$ is positive. Such a ζ is said to be a regular singularity if

$$\forall\, 1 \leq j \leq r; \quad \omega_\zeta(d_j) \leq j$$

and an irregular singularity otherwise. The indicial equation $I(\alpha) = 0$ of a differential equation of the form (2.28) at its regular singularity ζ is given by

$$I(\alpha) = (\alpha)_r + \delta_1 (\alpha)_{r-1} + \cdots + \delta_r, \qquad (\alpha)_\ell := \alpha(\alpha-1)\cdots(\alpha-\ell+1),$$

where $\delta_j := \lim_{z\to\alpha} (z-\alpha)^j d_j(z)$.

Theorem 2.23. (Henrici; Wasow [66, 140]) *Suppose we are given a meromorphic differential equation (2.28) with regular singularity ζ. Then, in a slit neighborhood of ζ, any solution of eq. (2.28) is a linear combination of functions of the form*

$$(z-\zeta)^{\alpha_i} \left(\log(z-\zeta)\right)^{\ell_{ij}} H_{ij}(z-\zeta), \quad \textit{for } 1 \leq i \leq r,\ 1 \leq j \leq i,$$

where $\alpha_1, \ldots, \alpha_r$ are the roots of the indicial equation at ζ, ℓ_{ij} are non-negative integer, and each H_{ij} is analytic at 0.

According to Proposition 2.22, the ODEs for $\mathbf{F}_k(z)$ for $2 \leq k \leq 9$ are known. We next proceed by deriving from these ODEs the singular expansion of $\mathbf{F}_k(z)$.

Proposition 2.24. *For $2 \leq k \leq 9$, the singular expansion of $\mathbf{F}_k(z)$ for $z \to \rho_k^2$ is given by*

$$\mathbf{F}_k(z) = \begin{cases} P_k(z-\rho_k^2) + c_k'(z-\rho_k^2)^{((k-1)^2+(k-1)/2)-1} \log(z-\rho_k^2)\,(1+o(1)) \\ P_k(z-\rho_k^2) + c_k'(z-\rho_k^2)^{((k-1)^2+(k-1)/2)-1}\,(1+o(1)) \end{cases}$$

depending on k being odd or even. Furthermore, the terms $P_k(z)$ are polynomials of degree not larger than $(k-1)^2 + (k-1)/2 - 1$, c_k' is some constant, and $\rho_k = 1/2(k-1)$.

Note the appearance of the logarithmic term for odd k in the singular expansion of $\mathbf{F}_k(z)$.

Proof. Claim 1. The dominant singularity ρ_k^2 of the ordinary differential equation of $\mathbf{F}_k(z)$ is regular.
We express eq. (2.19) as

$$\mathbf{F}_k^{(r_k)}(z) + \frac{q_{1,k}(z)}{q_{0,k}(z)}\mathbf{F}_k^{(r_k-1)}(z) + \frac{q_{2,k}(z)}{q_{0,k}(z)}\mathbf{F}_k^{(r_k-2)}(z) + \cdots + \frac{q_{r_k,k}(z)}{q_{0,k}(z)}\mathbf{F}_k(z) = 0,$$

writing $\mathbf{F}_k^{(m)}(z) = \frac{d^m}{dz^m}\mathbf{F}_k(z)$ for $0 \le m \le r_k$. For $2 \le k \le 9$, see Table 2.1, $q_{0,k}(z)$ has simple nonzero roots. Since all singularities of $\mathbf{F}_k(z)$

- are contained in the roots of $q_{0,k}(z)$ and
- according to Theorem 2.8 we have

$$f_k(2n,0) \sim c_k\, n^{-((k-1)^2+(k-1)/2)}\,(2(k-1))^{2n}, \quad \text{where } c_k > 0$$

and accordingly derive

$$q_{0,k}(z) = (z-\rho_k^2)q'_{0,k}(z),$$

where $q'_{0,k}(z)$ has also simple nonzero roots. Let

$$d_{j,k}(z) = q_{j,k}(z)/q_{0,k}(z), \qquad 1 \le j \le k.$$

Then

$$(z-\rho_k^2)^j\, d_{j,k}(z) = (z-\rho_k^2)^j\,\frac{q_{j,k}(z)}{q_{0,k}(z)} = (z-\rho_k^2)^{j-1}\,\frac{q_{j,k}(z)}{q'_{0,k}(z)}. \tag{2.29}$$

We set $\delta_{j,k} = \lim_{z\to\rho_k^2}(z-\rho_k^2)^j\, d_{j,k}(z)$. Equation (2.29) shows that $\delta_{1,k}$ exists and $\delta_{j,k} = 0$ for $j \ge 2$. Furthermore, the order of the pole of $d_{j,k}(z)$, for $j \ge 1$, at ρ_k^2 is at most 1. Therefore, for $2 \le k \le 9$, the dominant singularity, ρ_k^2, is unique and regular.
According to Claim 1 the singularity ρ_k^2 is regular and Theorem 2.23 implies

$$\mathbf{F}_k(z) = \sum_{i=1}^{k}\sum_{j=1}^{i}\lambda_{ij}(z-\rho_k^2)^{\alpha_i}\log^{\ell_{ij}}(z-\rho_k^2)H_{ij}(z-\rho_k^2), \tag{2.30}$$

where ℓ_{ij} is a non-negative integer, H_{ij} is analytic at 0, and $\alpha_1, \alpha_2, \ldots, \alpha_k$ are the roots of the indicial equation, $\lambda_{ij} \in \mathbb{C}$. For $2 \le k \le 9$ we derive from the indicial equations

$$\alpha_i = \begin{cases} i-1 & \text{for } i \le k-1, \\ (k-1)^2 + \frac{k-1}{2} - 1 & \text{for } i = k. \end{cases}$$

Since H_{ij} is analytic at 0, its Taylor expansion at 0 exists

$$(z-\rho_k^2)^{\alpha_i}\log^{\ell_{ij}}(z-\rho_k^2)H_{i,j}(z-\rho_k^2) = \sum_{t=0}^{\infty} a_{ijt}(z-\rho_k^2)^{\alpha_i+t}\log^{\ell_{ij}}(z-\rho_k^2).$$

Substituting the Taylor expansion into (2.30), we obtain

$$\mathbf{F}_k(z) = \sum_{i=1}^{k}\sum_{j=1}^{i}\sum_{t=0}^{\infty} a_{ijt}(z-\rho_k^2)^{\alpha_i+t}\log^{\ell_{ij}}(z-\rho_k^2). \tag{2.31}$$

We set

$$\begin{aligned} M_1 &= \{(i,j,t) \mid 1 \le i \le k, 1 \le j \le i, 0 \le t,\, a_{ijt} \ne 0, \ell_{i,j} > 0\}, \\ M_2 &= \{(i,j,t) \mid 1 \le i \le k, 1 \le j \le i, 0 \le t,\, a_{ijt} \ne 0, \alpha_i + t \notin \mathbb{N}\}, \end{aligned}$$

and $M = M_1 \cup M_2$. Clearly, M is not empty since $\mathbf{F}_k(z)$ would be analytic at $z = \rho_k^2$, otherwise. Let

$$\begin{aligned} m_k &= \min\{\alpha_i + t \mid (i,j,t) \in M,\, a_{ijt} \ne 0\} \\ l_k &= \max\{\ell_{ij} \mid \alpha_i + t = m_k, (i,j,t) \in M,\, a_{ijt} \ne 0\} \end{aligned}$$

and let c_k' denotes the coefficient of $(z-\rho_k^2)^{m_k}\log^{l_k}(z-\rho_k^2)$ in eq. (2.31). By construction we then arrive at

$$\mathbf{F}_k(z) = P_k(z-\rho_k^2) + c_k'(z-\rho_k^2)^{m_k}\log^{l_k}(z-\rho_k^2)(1+o(1)), \tag{2.32}$$

where $P_k(z)$ is a polynomial of degree $\le m_k$ and Theorem 2.20 implies

$$[z^n]\mathbf{F}_k(z) \sim [z^n]c_k'(z-\rho_k^2)^{m_k}\log^{l_k}(z-\rho_k^2). \tag{2.33}$$

We distinguish the cases of k being odd and even. In case of k being odd, the terms α_i are, for $1 \le i \le k$, all positive integers and the same holds for m_k. This implies $l_k \ne 0$, since $\mathbf{F}_k(z)$ would be analytic at ρ_k^2, otherwise. According to [42], we have

$$[z^n]c_k'(z-\rho_k^2)^{m_k}\log^{l_k}(z-\rho_k^2) \sim c_k''\,\left(\rho_k^2\right)^{-n} n^{-m_k-1}\sum_{j\ge 0}\frac{F_{j,k}(\log n)}{n^j},$$

where the $F_{j,k}(z)$ are polynomials whose degree is $l_k - 1$. In view of eq. (2.9)

$$[z^n]\mathbf{F}_k(z) \;\sim\; c_k\,\left(\rho_k^2\right)^{-n} n^{-(k-1)^2-\frac{k-1}{2}}, \tag{2.34}$$

where c_k is some positive constant, whence

$$m_k = (k-1)^2 + \frac{k-1}{2} - 1 \quad \text{and} \quad l_k = 1.$$

In case of k being even, $\alpha_k = (k-1)^2 + \frac{k-1}{2} - 1 \notin \mathbb{Z}$ while $\alpha_i \in \mathbb{Z}$ for $1 \le i < k$. Equation (2.34) implies that m_k is not an integer and according to [42] we have

$$[z^n]c_k'(z-\rho_k^2)^{m_k}\log^{l_k}(z-\rho_k^2) \sim c_k''\,\left(\rho_k^2\right)^{-n}\frac{n^{-m_k-1}}{\Gamma(-m_k)}\sum_{j\ge 0}\frac{E_{j,k}(\log n)}{n^j},$$

where $E_{j,k}(z)$ is a polynomial whose degree is l_k. In view of eq. (2.34) we conclude that

$$m_k = (k-1)^2 + \frac{k-1}{2} - 1 \quad \text{and} \quad l_k = 0.$$

Thus we have proved that for $z \to \rho_k^2$,

$$\mathbf{F}_k(z) = \begin{cases} P_k(z-\rho_k^2) + c_k'(z-\rho_k^2)^{(k-1)^2+\frac{k-1}{2}-1}\log(z-\rho_k^2)\,(1+o(1)) \\ P_k(z-\rho_k^2) + c_k'(z-\rho_k^2)^{(k-1)^2+\frac{k-1}{2}-1}\,(1+o(1))\,, \end{cases}$$

depending on k being odd or even and where $P_k(z)$ is a polynomial of degree $\leq (k-1)^2 + \frac{k-1}{2} - 1$ and c_k' is some constant.

Proposition 2.24 provides for $2 \leq k \leq 9$ the singular expansion of $\mathbf{F}_k(z)$. These particular expansions and a simple scaling property of the Taylor expansion are the key tools for proving Theorem 2.21.

Proof of Theorem 2.21. We consider the composite function $\mathbf{F}_k(\psi(z,s))$. In view of $[z^n]f(z,s) = \gamma^n[z^n]f(\frac{z}{\gamma},s)$ it suffices to analyze the function $\mathbf{F}_k(\psi(\gamma(s)z,s))$ and to subsequently rescale in order to obtain the correct exponential factor. For this purpose we set

$$\widetilde{\psi}(z,s) = \psi(\gamma(s)z,s),$$

where $\psi(z,s)$ is analytic in a domain $\mathcal{D} = \{(z,s) \,||z| \leq r, |s| < \epsilon\}$. Consequently $\widetilde{\psi}(z,s)$ is analytic in $|z| < \widetilde{r}$ and $|s| < \widetilde{\epsilon}$, for some $1 < \widetilde{r}$, $0 < \widetilde{\epsilon} < \epsilon$, since it is a composition of two analytic functions in $\mathcal{D}$. Taking its Taylor expansion at $z=1$,

$$\widetilde{\psi}(z,s) = \sum_{n\geq 0} \widetilde{\psi}_n(s)(1-z)^n, \tag{2.35}$$

where $\widetilde{\psi}_n(s)$ is analytic in $|s| < \widetilde{\epsilon}$. According to Proposition 2.24, the singular expansion of $\mathbf{F}_k(z)$, for $z \to \rho_k^2$, is given by

$$\mathbf{F}_k(z) = \begin{cases} P_k(z-\rho_k^2) + c_k'(z-\rho_k^2)^{((k-1)^2+(k-1)/2)-1}\log(z-\rho_k^2)\,(1+o(1)) \\ P_k(z-\rho_k^2) + c_k'(z-\rho_k^2)^{((k-1)^2+(k-1)/2)-1}\,(1+o(1))\,, \end{cases}$$

depending on whether k is odd or even and where $P_k(z)$ are polynomials of degree $\leq (k-1)^2 + (k-1)/2 - 1$, c_k' is some constant, and $\rho_k = 1/2(k-1)$. By assumption, $\gamma(s)$ is the unique analytic solution of $\psi(\gamma(s),s) = \rho_k^2$ and by construction $\mathbf{F}_k(\psi(\gamma(s)z,s)) = \mathbf{F}_k(\widetilde{\psi}(z,s))$. In view of eq. (2.35), we have for $z \to 1$ the expansion

$$\widetilde{\psi}(z,s) - \rho_k^2 = \sum_{n\geq 1} \widetilde{\psi}_n(s)(1-z)^n = \widetilde{\psi}_1(s)(1-z)(1+o(1)), \tag{2.36}$$

that is uniform in s since $\widetilde{\psi}_n(s)$ is analytic for $|s| < \widetilde{\epsilon}$ and $\widetilde{\psi}_0(s) = \psi(\gamma(s), s) = \rho_k^2$. As for the singular expansion of $\mathbf{F}_k(\widetilde{\psi}(z,s))$ we derive, substituting the eq. (2.36) into the singular expansion of $\mathbf{F}_k(z)$, for $z \to 1$,

$$\begin{cases} \widetilde{P}_k(z,s) + c_k(s)(1-z)^{((k-1)^2+(k-1)/2)-1}\log(1-z)\,(1+o(1)) & \text{for } k \text{ odd,} \\ \widetilde{P}_k(z,s) + c_k(s)(1-z)^{((k-1)^2+(k-1)/2)-1}\,(1+o(1)) & \text{for } k \text{ even} \end{cases}$$

where $\widetilde{P}_k(z,s) = P_k(\widetilde{\psi}(z,s) - \rho_k^2)$ and $c_k(s) = c_k' \widetilde{\psi}_1(s)^{((k-1)^2+(k-1)/2)-1}$ and

$$\widetilde{\psi}_1(s) = \partial_z \widetilde{\psi}(z,s)|_{z=1} = \gamma(s)\partial_z \psi(\gamma(s), s) \neq 0 \quad \text{for } |s| < \epsilon.$$

Furthermore $\widetilde{P}_k(z,s)$ is analytic at $|z| \leq 1$, whence $[z^n]\widetilde{P}_k(z,s)$ is exponentially small compared to 1. Therefore, we arrive at

$$[z^n]\mathbf{F}_k(\widetilde{\psi}(z,s)) \sim \begin{cases} [z^n]c_k(s)(1-z)^{((k-1)^2+(k-1)/2)-1}\log(1-z)\,(1+o(1)) \\ [z^n]c_k(s)(1-z)^{((k-1)^2+(k-1)/2)-1}\,(1+o(1))\,, \end{cases} \tag{2.37}$$

depending on k being odd or even and uniformly in $|s| < \widetilde{\epsilon}$. We observe that $c_k(s)$ is analytic in $|s| < \widetilde{\epsilon}$. Note that a dependency in the parameter s is only given in the coefficients $c_k(s)$ that are analytic in s. The transfer Theorem 2.20 and eq. (2.37) imply that

$$[z^n]\mathbf{F}_k(\widetilde{\psi}(z,s)) \sim A(s)\, n^{-((k-1)^2+(k-1)/2)} \quad \text{for some } A(s) \in \mathbb{C},$$

uniformly in s contained in a small neighborhood of 0. Finally, as mentioned in the beginning of the proof, we use the scaling property of Taylor expansions in order to derive

$$[z^n]\mathbf{F}_k(\psi(z,s)) = (\gamma(s))^{-n}\,[z^n]\mathbf{F}_k(\widetilde{\psi}(z,s))$$

and the proof of the theorem is complete.

2.5 n-Cubes

In this section we deal with a formalization of the space of all sequences. For this purpose we regard the nucleotides an element of an arbitrary finite set (alphabet), A. The existence of the so-called point-mutations, that is mutations of individual nucleotides, see Fig. 2.14, suggests to consider two sequences to be adjacent, if they differ in exactly one position. This point of view gives rise to consider sequence space as a graph. In this graph each $\mathbf{A}, \mathbf{U}, \mathbf{G}, \mathbf{C}$ sequence of n nucleotides has $3n$ neighbors.

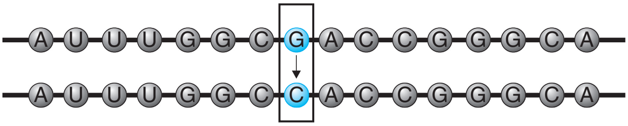

Fig. 2.14. Single point mutations.

k	
2	$(4\,x-1)\,xf''\,(x)+(10\,x-2)\,f'\,(x)+2\,f\,(x)=0$
3	$\left(16\,x^3-x^2\right)f^{(3)}\,(x)+\left(96\,x^2-8\,x\right)f''\,(x)+(108\,x-12)\,f'\,(x)+12\,f\,(x)=0$
4	$\left(144\,x^5-40\,x^4+x^3\right)f^{(4)}\,(x)+\left(1584\,x^4-556\,x^3+20\,x^2\right)f^{(3)}\,(x)$ $+\left(4428\,x^3-1968\,x^2+112\,x\right)f''\,(x)+\left(3024\,x^2-1728\,x+168\right)f'\,(x)$ $+(216\,x-168)\,f\,(x)=0$
5	$\left(1024\,x^6-80\,x^5+x^4\right)f^{(5)}\,(x)+\left(20,480\,x^5-2256\,x^4+40\,x^3\right)f^{(4)}\,(x)$ $+\left(121,600\,x^4-19,380\,x^3+532\,x^2\right)f^{(3)}\,(x)+\left(241,920\,x^3-56,692\,x^2+2728\,x\right)$ $f''\,(x)+\left(130,560\,x^2-46,048\,x+4400\right)f'\,(x)+(7680\,x-4400)\,f\,(x)=0$
6	$\left(14,400\,x^8-4144\,x^7+140\,x^6-x^5\right)f^{(6)}\,(x)$ $+\left(367,200\,x^7-148,368\,x^6+7126\,x^5-70\,x^4\right)f^{(5)}\,(x)$ $+\left(3,078,000\,x^6-1,728,900\,x^5+123,850\,x^4-1792\,x^3\right)f^{(4)}\,(x)$ $+\left(10,179,000\,x^5-7,880,640\,x^4+880,152\,x^3-20,704\,x^2\right)f^{(3)}\,(x)$ $+\left(12,555,000\,x^4-13,367,880\,x^3+2,399,184\,x^2-106,016\,x\right)f''\,(x)$ $+\left(4,374,000\,x^3-6,475,680\,x^2+1,922,736\,x-187,200\right)f'\,(x)$ $+\left(162,000\,x^2-350,640\,x+187,200\right)f\,(x)=0$
7	$\left(147,456\,x^9-12,544\,x^8+224\,x^7-x^6\right)f^{(7)}\,(x)$ $+\left(6,193,152\,x^8-757,760\,x^7+18,816\,x^6-112\,x^5\right)f^{(6)}\,(x)$ $+\left(89,800,704\,x^7-16,035,456\,x^6+582,280\,x^5-4872\,x^4\right)f^{(5)}\,(x)$ $+\left(561,254,400\,x^6-146,691,840\,x^5+8,254,664\,x^4-104,480\,x^3\right)f^{(4)}\,(x)$ $+\left(1,535,708,160\,x^5-585,419,280\,x^4+54,069,792\,x^3-1,151,984\,x^2\right)f^{(3)}\,(x)$ $+\left(1,651,829,760\,x^4-916,833,600\,x^3+144,777,216\,x^2-6,094,528\,x\right)f''\,(x)$ $+\left(516,741,120\,x^3-421,901,280\,x^2+117,590,208\,x-11,797,632\right)f'\,(x)$ $+\left(17,418,240\,x^2-22,034,880\,x+11,797,632\right)f\,(x)=0$
8	$\left(2,822,400\,x^{11}-826,624\,x^{10}+31,584\,x^9-336\,x^8+x^7\right)f^{(8)}\,(x)$ $+\left(129,830,400\,x^{10}-55,968,384\,x^9+3,026,208\,x^8-43,512\,x^7+168\,x^6\right)f^{(7)}\,(x)$ $+\left(2,202,883,200\,x^9-1,363,532,352\,x^8+107,691,912\,x^7-2,188,752\,x^6\right.$ $\left.+11,424\,x^5\right)$ $f^{(6)}\,(x)+(17455132800\,x^8-15,140,260,128\,x^7+1,789,953,376\,x^6$ $-54349,728\,x^5+405,200\,x^4)f^{(5)}\,(x)$ $+(67,586,778,000\,x^7-80,551,356,480\,x^6+14,421,855,200\,x^5$ $-698,609,104\,x^4+8,035,104\,x^3)f^{(4)}\,(x)$ $+(122,393,376,000\,x^6-197,784,236,160\,x^5+53,661,386,080\,x^4$ $-4437573,920\,x^3+88,180,864\,x^2)f^{(3)}\,(x)$

Table 2.1. The differential equations for $\mathbf{F}_k(z)(2 \le k \le 9)$, obtained by Maple package `gfun`.

	$-4437573,920\,x^3 + 88,180,864\,x^2)f^{(3)}\,(x)$
	$+(90,239,184,000\,x^5 - 196,676,000,640\,x^4 + 80,758,975,680\,x^3$
	$-11,973,419,104\,x^2 + 488,846,272\,x)f''\,(x)$
	$+(19,559,232,000\,x^4 - 57,892,907,520\,x^3 + 35,467,753,520\,x^2$
	$-9,969,500,032\,x + 1,033,305,728)f'\,(x)$
	$+\left(444,528,000\,x^3 - 1,852,865,280\,x^2 + 186,993,760\,x - 1,033,305,728\right)f\,(x) = 0$
9	$\left(37,748,736\,x^{12} - 3,358,720\,x^{11} + 69,888\,x^{10} - 480\,x^9 + x^8\right)f^{(9)}\,(x)$
	$+\left(2,717,908,992\,x^{11} - 351,387,648\,x^{10} + 10,065,408\,x^9 - 90,912\,x^8\right.$
	$\left.+240\,x^7\right)f^{(8)}\,(x)$
	$+(72,873,934,848\,x^{10} - 1,378,440,8064\,x^9$
	$+563,449,728\,x^8 - 6,950,616\,x^7 + 24,024\,x^6)f^{(7)}\,(x)$
	$+(940,566,380,544\,x^9 - 258,478,202,880\,x^8 + 15,638,941,312\,x^7$
	$-2,368,505,160\,x^6 + 1,304,336\,x^5)f^{(6)}\,(x)$
	$+(6,273,464,795,136\,x^8 - 2,467,959,432,192\,x^7 + 227,994,061,392\,x^6$
	$-18,674,432,128\,x^5 + 41,782,224\,x^4)f^{(5)}\,(x)$
	$+(21,523,928,186,880\,x^7 - 119,317,461,350,40\,x^6 + 17,131,29,509,184\,x^5$
	$-75,115,763,872\,x^4 + 802,970,368\,x^3)f^{(4)}\,(x)$
	$+(35,583,374,131,200\,x^6 - 27,454,499,6659,20\,x^5 + 614,7724,228,704\,x^4$
	$-475,182,777,504\,x^3 + 8,956,331,968\,x^2)f^{(3)}\,(x)$
	$+(24,400,027,975,680\,x^5 - 26,056,335,882,240\,x^4 + 9,086,553,292,608\,x^3$
	$-1,308,864,283,488\,x^2 + 52,313,960,192\,x)f''\,(x)$
	$+(4,976,321,495,040\,x^4 - 740,2528,051,200\,x^3 + 4,051,342,551,744\,x^2$
	$-1,122,348,764,928\,x + 120,086,385,408)f'\,(x)$
	$+\left(107,017,666,560\,x^3 - 230,051,819,520\,x^2 + 208,033,076,736\,x - 120,\right.$
	$\left.086,385,408\right)f\,(x) = 0$

Table 2.1. continued

2.5.1 Some basic facts

The n-cube, Q_α^n, is a combinatorial graph with vertex set A^n, where A is some finite alphabet of size $\alpha \geq 2$. Without loss of generality we will assume $\mathbb{F}_2 \subset A$ (here $\mathbb{F}_2$ denotes the field having the two elements $0, 1$) and call Q_2^n the binary n-cube. In an n-cube two vertices are adjacent if they differ in exactly one coordinate; see Fig. 2.15.

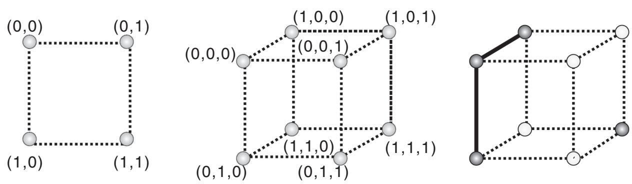

Fig. 2.15. The n-cubes Q_2^n for $n = 2$ (*left*) and $n = 3$ (*middle*). On the RHS we display an induced Q_2^3-subgraph, induced by the gray vertices.

Let $d(v, v')$ be the number of coordinates by which v and v' differ. $d(v, v')$ is oftentimes referred to as Hamming metric. We set $\forall\, C \subset A^n$, $j \le n$

$$\begin{aligned} \mathsf{B}(C, j) &= \{v \in \mathbb{A}^n \mid \exists\, a \in C;\, d(v, a) \le j\} \\ \mathsf{S}(C, j) &= \mathsf{B}(C, j) \setminus \mathsf{B}(C, j-1) \\ \mathsf{d}(C) &= \mathsf{B}(C, 1) \setminus C \end{aligned}$$

and call $\mathsf{B}(C, j)$ and $\mathsf{d}(C)$ the ball of radius j around C and the vertex boundary of C in Q_α^n, respectively. If $C = \{v\}$, we simply write $\mathsf{B}(v, j)$. Let $B, C \subset A^n$, we call B ℓ-dense in C if $\mathsf{B}(v, \ell) \cap B \neq \varnothing$ for any $v \in C$.

Q_2^n can also be viewed as the Cayley graph $\mathsf{Cay}(\mathbb{F}_2^n, \{e_i \mid i = 1, \dots, n\})$, where e_i is the canonical base vector. We will view $\mathbb{F}_2^n$ as a $\mathbb{F}_2$-vectorspace and denote the linear hull over $\{v_1, \dots, v_h\}$, $v_j \in \mathbb{F}_2^n$ by $\langle v_1, v_2, \dots, v_h\rangle$.

There exists a natural linear order $\le$ over Q_2^n given by

$$v \le v' \quad \Longleftrightarrow \quad (d(v, 0) < d(v', 0)) \;\vee\; (d(v, 0) = d(v', 0) \;\wedge\; v \le_{\text{lex}} v'), \quad (2.38)$$

where $\le_{\text{lex}}$ denotes the lexicographical order. Any notion of minimal element or smallest element in $A \subset Q_2^n$ is considered with respect to the linear order $\le$ of eq. (2.38).

Each $B \subset A^n$ induces a unique induced subgraph in Q_α^n, denoted by $Q_\alpha^n[B]$, in which $b_1, b_2 \in B$ are adjacent iff b_1, b_2 are adjacent in Q_α^n.

We next prove a combinatorial lemma, which is a slightly stronger version of a result in [14].

Lemma 2.25. *Let $d \in \mathbb{N}$, $d \ge 2$ and let v, v' be two Q_2^n-vertices where $d(v, v') = d$. Then any Q_2^n-path from v to v' has length $2\ell + d$ and there are at most*

$$\binom{2\ell + d}{\ell + d}\binom{\ell + d}{\ell}\, n^\ell\, \ell!\, d!$$

Q_2^n-paths from v to v' of length $2\ell + d$.

Proof. Without loss of generality, we can assume $v = (0, \dots, 0)$ and $v' = (x_i)_i$, where $x_i = 1$ for $1 \le i \le d$ and $x_i = 0$, otherwise. Each path of length m induces the family of steps $(\epsilon_s)_{1 \le s \le m}$, where $\epsilon_s \in \{e_j \mid 1 \le j \le n\}$. Since each path ends at v', we have for fixed $1 \le i \le n$

$$\sum_{\{\epsilon_s \mid \epsilon_s = e_i\}} \epsilon_s = \begin{cases} 1 & \text{for } \; 1 \le i \le d, \\ 0 & \text{otherwise.} \end{cases}$$

Hence the families induced by these paths contain necessarily the set $\{e_1, \dots, e_d\}$. Let $(\epsilon'_s)_{1 \le s \le m'}$ be the family obtained from $(\epsilon_s)_{1 \le s \le m}$ by removing the steps $e_1, \dots, e_d$, at the smallest index at which they occur. Then $(\epsilon'_s)_{1 \le s \le m'}$ represents a cycle starting and ending at v. Furthermore, we have for all i; $\sum_{\{\epsilon'_s \mid \epsilon'_s = e_i\}} \epsilon'_s = 0$, i.e., all steps must come in up-step/down-step pairs. As a result we derive $m = 2\ell + d$ and there are exactly ℓ steps of the form e_j that can be freely chosen (free up-steps). We proceed by counting the number of the $(2\ell + d)$-tuples $(\epsilon_s)_{1 \le s \le 2\ell+d}$. There are exactly $\binom{2\ell+d}{\ell+d}$ ways to select the $(\ell+d)$ indices for the up-steps within the set of all $2\ell+d$ indices. Furthermore, there are at most $\binom{\ell+d}{\ell}$ ways to select the positions for the ℓ up-steps and at most n^ℓ ways to choose the free up-steps themselves (once their positions are fixed). Since a free up-step is paired with a unique down-step reversing it, the ℓ free up-steps determine all ℓ down-steps. Clearly, there are at most $\ell!$ ways to assign the down-steps to their ℓ indices. Finally, there are at most $d!$ ways to assign the fixed up-steps and the lemma follows.

2.5.2 Random subgraphs of the *n*-cube

Let Q^n_{α,λ_n} be the random graph consisting of Q^n_α-subgraphs, Γ_n, induced by selecting each Q^n_α-vertex with independent probability λ_n; see Fig. 2.16. Q^n_{α,λ_n} is the finite probability space

$$(\{Q^n_\alpha[B] \mid B \subset \mathbb{A}^n\}, \mathbb{P}_n),$$

with the probability measure $\mathbb{P}_n(B) = \lambda_n^{|B|}\,(1-\lambda_n)^{\alpha^n - |B|}$.

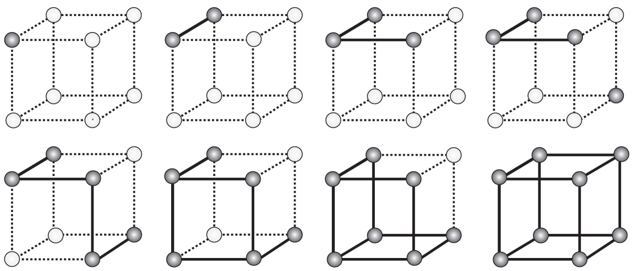

Fig. 2.16. Eight random-induced subgraphs of Q^3_2

A property M_n is a subset of induced subgraphs of Q^n_α closed under graph isomorphisms. The terminology "M_n holds a.s." is equivalent to

$$\lim_{n \to \infty} \mathbb{P}(\mathsf{M}_n) = 1.$$

We use the notation

$$B_m(\ell, \lambda_n) = \binom{m}{\ell} \lambda_n^\ell \,(1-\lambda_n)^{m-\ell}$$

and write $g(n) = O(f(n))$ and $g(n) = o(f(n))$ for $g(n)/f(n) \to \kappa$ as $n \to \infty$ and $g(n)/f(n) \to 0$ as $n \to \infty$, respectively.

A component of Γ_n is a maximal connected induced Γ_n-subgraph, C_n. The largest Γ_n-component is denoted by $C_n^{(1)}$. Analogously, the second largest component is denoted by $C_n^{(2)}$. The largest Γ_n-component $C_n^{(1)}$ is called a giant component or giant if and only if

$$|C_n^{(2)}| = o(|C_n^{(1)}|).$$

Furthermore, we write $x_n \sim y_n$ if and only if (a) $\lim_{n\to\infty} x_n/y_n$ exists and (b) $\lim_{n\to\infty} x_n/y_n = 1$.

Let $Z_n = \sum_{i=1}^n \xi_i$ be a sum of mutually independent indicator random variables (r.v.), ξ_i having values in $\{0, 1\}$. Then we have, [58], for $\eta > 0$ and $c_\eta = \min\{-\ln(e^\eta[1+\eta]^{-[1+\eta]}), \frac{\eta^2}{2}\}$

$$\mathsf{Prob}(\,|\,Z_n - \mathbb{E}[Z_n]\,|\, > \eta\,\mathbb{E}[Z_n]\,) \le 2e^{-c_\eta \mathbb{E}[Z_n]}\,. \tag{2.39}$$

n is always assumed to be sufficiently large and ϵ is a positive constant satisfying $0 < \epsilon < 1$.

2.5.3 Vertex boundaries

In this section we present some generic results on vertex boundaries, which are instrumental for our analysis of connectivity, large components, and distances in n-cubes. The first result is due to [7] used for Sidon sets in groups in the context of Cayley graphs. In the following G denotes a finite group and M a finite set acted upon by G.

Proposition 2.26. *Suppose G act transitively on M and let $A \subset M$, then we have*

$$\frac{1}{|G|}\sum_{g\in G} |A \cap gA| = |A|^2/|M|. \tag{2.40}$$

Proof. We prove eq. (2.40) by induction on $|A|$. For $A = \{x\}$ we derive $\frac{1}{|G|}\sum_{gx=x} 1 = |G_x|/|G|$, since $|M| = |G|/|G_x|$. We next prove the induction step. We write $A = A_0 \cup \{x\}$ and compute

$$\begin{aligned}\frac{1}{|G|}\sum_{g} |A \cap gA| &= \frac{1}{|G|}\sum_{g}(|A_0 \cap gA_0| + |\{gx\} \cap A_0| + \\ &\qquad |\{x\} \cap gA_0| + |\{gx\} \cap \{x\}| \\ &= \frac{1}{|G|}(|A_0|^2|G_x| + 2|A_0||G_x| + |G_x|) \\ &= \frac{1}{|G|}((|A_0|+1)^2|G_x|) = \frac{|A|^2}{|M|}.\end{aligned}$$

Aldous [4, 6] observed how to use Proposition 2.26 for deriving a very general lower bound for vertex boundaries in Cayley graphs:

Theorem 2.27. *Suppose G acts transitively on M and let $A \subset M$, and let S be a generating set of the Cayley graph $\mathsf{Cay}(G,S)$ where $|S| = n$. Then we have*

$$\exists\, s \in S; \quad |sA \setminus A| \geq \frac{1}{n}|A|\left(1 - \frac{|A|}{|M|}\right).$$

Proof. We compute

$$|A| = \frac{1}{|G|}\sum_{g}(|gA \setminus A| + |A \cap gA|) = \frac{1}{|G|}\sum_{g}|gA \setminus A| + |A|\frac{|A|}{|M|}$$

and hence $|A|(1 - \frac{|A|}{|M|}) = \frac{1}{|G|}\sum_g |gA \setminus A|$. From this we can immediately conclude

$$\exists\, g \in G; \quad |gA \setminus A| \geq |A|\left(1 - \frac{|A|}{|M|}\right).$$

Let $g = \prod_{j=1}^{k} s_j$. Since each element of $gA \setminus A$ is contained in at least one set $s_j A \setminus A$ we obtain

$$|gA \setminus A| \leq \sum_{j=1}^{k} |s_j A \setminus A|.$$

Hence there exists some $1 \leq j \leq k$ such that $|s_j A \setminus A| \geq \frac{1}{k}|gA \setminus A|$ and the lemma follows.

2.5.4 Branching processes and Janson's inequality

Let us next recall some basic facts about branching processes [62, 83]. Suppose ξ is a random variable and $(\xi_i^{(t)})$, $i, t \in \mathbb{N}$ are random variables that count the number of offspring of the ith individual at generation $t-1$. We consider the family of r.v. $Z = (Z_i)_{i \in \mathbb{N}_0}$, given by

$$Z_0 = 1 \quad \text{and} \quad Z_t = \sum_{i=1}^{Z_{t-1}} \xi_i^{(t)}, \text{ for } t \geq 1$$

and interpret Z_t as the number of individuals "alive" in generation t. We will be interested in the limit probability $\lim_{t\to\infty} \mathsf{Prob}(Z_t > 0)$, i.e., the probability of infinite survival.

In the following, we distinguish three branching processes:

- Suppose the r.v.s ξ and $\xi_i^{(t)}$ are all $B_m(\ell, p)$-distributed. We denote this process by Z^* and its survival probability by

$$\pi_m(p) = \lim_{t\to\infty} \mathsf{Prob}(Z_t^* > 0).$$

- Let Z^0 denote the branching process in which ξ is $B_m(\ell,p)$-distributed and all subsequent r.vs. $\xi_i^{(t)}$ are $B_{m-1}(\ell,p)$-distributed and

$$\pi_0(p) = \lim_{t\to\infty} \mathsf{Prob}(Z_t^0 > 0).$$

- Let Z^P denote the branching process in which the individuals generate offspring according to the Poisson distribution, i.e.,

$$\mathsf{Prob}(\xi_i^{(t)} = j) = \frac{\lambda^j}{j!}e^{-\lambda},$$

  where $\lambda > 0$ and let

$$\pi_P(\lambda) = \lim_{t\to\infty} \mathsf{Prob}(Z_t^P > 0).$$

Lemma 2.28. (Bollobas et al. [14])

(1) *For all $0 \le p \le 1$, we have $\pi_{n-1}(p) \le \pi_0(p) \le \pi_n(p)$.*

(2) *If $\lambda > 1$ is fixed, then $\pi_P(\lambda)$ is the unique solution of $x + e^{-\lambda x} = 1$ in the interval $0 < x < 1$.*

(3) *Let $p = \frac{\lambda_n}{n}$ where $\lambda_n = 1 + \epsilon_n$ and $0 < \epsilon_n = o(1)$. Then*

$$\pi_n(p) = \frac{2n\epsilon_n}{n-1} + O(\epsilon_n^2).$$

In particular, if $r = n - s$ then

$$\pi_r(p) = 2\epsilon_n + O(\epsilon_n/n) + O(s/n) + O(\epsilon_n^2);$$

and hence if $s = o(\epsilon_n\, n)$ then $\pi_r(p) = (1 + o(1))\pi_0(p)$.

Corollary 2.29. *Let $p = \lambda/n$.*

(1) *If $\lambda > 1$ is fixed, then $\pi_0(p) = (1 + o(1))\pi_P(\lambda)$.*

(2) *Let $\lambda_n = 1 + \epsilon_n$, where $0 < \epsilon_n = o(1)$. Then, if $r = n - s$ and $s = o(n\epsilon_n)$,*

$$\pi_0(p) = (1 + o(1))\pi_r(p) = (2 + o(1))\epsilon_n.$$

In Chapter 7 we need the following particular formulation of Corollary 2.29.

Corollary 2.30. *Let $u_n = n^{-\frac{1}{3}}$, $\lambda_n = \frac{1+\chi_n}{n}$, $m = n - \lfloor \frac{3}{4}u_n n \rfloor$, and*

$$\mathsf{Prob}(\xi = \ell) = B_m(\ell, \lambda_n).$$

Then for $\chi_n = \epsilon$ *the r.v.* ξ *becomes asymptotically Poisson, i.e.,* $\mathbb{P}(\xi = \ell) \sim \frac{(1+\epsilon)^\ell}{\ell!} e^{-(1+\epsilon)}$ *and*

$$0 < \lim_{t\to\infty} \mathsf{Prob}(Z_t > 0) = \alpha(\epsilon) < 1,$$

where $0 < \alpha(\epsilon) < 1$ *is the unique solution of the equation* $x + e^{-(1+\epsilon)x} = 1$. *For* $o(1) = \chi_n \geq n^{-\frac{1}{3}+\delta}$, $\delta > 0$ *we have*

$$\lim_{t\to\infty} \mathsf{Prob}(Z_t > 0) = (2 + o(1))\,\chi_n.$$

The next theorem, used in Chapter 7, is Janson's inequality [75]. It facilitates the proof of Theorem 7.15 and Theorem 7.13. Intuitively, Janson's inequality can be viewed as a large deviation result in the presence of correlation.

Theorem 2.31. *Let* R *be a random subset of some set* $[V] = \{1, \ldots, V\}$ *obtained by selecting each element* $v \in V$ *independently with probability* λ. *Let* $S_1, \ldots, S_s$ *be subsets of* $[V]$ *and* X *be the r.v. counting the number of* S_i *for which* $S_i \subset R$. *Let furthermore*

$$\Omega = \sum_{(i,j);\, S_i \cap S_j \neq \varnothing} \mathbb{P}(S_i \cup S_j \subset R),$$

where the sum is taken over all ordered pairs (i, j). *Then for any* $\gamma > 0$, *we have*

$$\mathbb{P}(X \leq (1-\gamma)\mathbb{E}[X]) \leq e^{-\frac{\gamma^2 \mathbb{E}[X]}{2+2\Omega/\mathbb{E}[X]}}.$$

2.6 Exercises

2.1. Prove Lemma 2.9 via symbolic enumeration. Consider the mapping that assigns to each partial k-noncrossing matching a k-noncrossing matching by removing all isolated vertices. Note that given a k-noncrossing matching, there are exactly $2n+1$ positions in which an arbitrary sequence of isolated vertices can be inserted.

2.2. Compute the generating function of secondary structures with minimum arc length λ and minimum stack-length σ. Hint: Compute the bivariate generating function of noncrossing matchings in which each stack has size exactly one, having exactly m 1-arcs (i.e., arcs of the form $(i, i+1)$). Then use symbolic enumeration and the fact that each secondary structure is mapped into exactly one such matching.

2.3. We analyze the case $k = 2$, i.e., RNA secondary structures. Here the generating function itself coincides with its singular expansion. The particular approach offers a great simplification of the proof in [69] and easily extends to all subclasses of secondary structures, considered there. Prove: The number of RNA secondary, i.e., 2-noncrossing RNA, structures is asymptotically given by

$$\mathsf{T}_2^{[2]}(n) \sim \frac{1.9572}{\sqrt{n}} \left(\frac{1}{n+1} - \frac{1}{8n(n+1)} + \frac{1}{128n^2(n+1)} + O(n^{-4}) \right) \times \left(\frac{3+\sqrt{5}}{2} \right)^n .$$

2.4. An $*$-tableaux is called irreducible if its only two empty shapes are λ^0 and λ^n. Let $\mathbf{Irr}_k^*(z)$ denote the generating function of irreducible $*$-tableaux. Prove

$$\mathbf{Irr}_k^*(z) = 1 - z - \frac{1}{\frac{1}{1-z}\mathbf{F}_k\left(\frac{z}{1-z}\right)}.$$

Furthermore, prove that

$$[z^n]\mathbf{Irr}_k^*(z) \ \sim \ \tilde{c}_k n^{-\mu-1} \left(\frac{\rho_k}{1-\rho_k} \right)^{-n} (1 + o(1)),$$

where $\tilde{c}_k$ is some computable positive constant, $\mu = (k-1)^2 + \frac{k-1}{2} - 1$, and ρ_k is the real positive dominant singularity of $\mathbf{F}_k(z)$.

2.5. Show: suppose $\lambda > 1$, then $\pi_P(\lambda)$ is the unique solution of $x + e^{-\lambda x} = 1$ in the interval $0 < x < 1$.

2.6. Prove: The number of isolated vertices is asymptotically Poisson distributed in $Q_{2,\lambda}^n$, where $0 < \lambda$.

2.7. Let S_n be the symmetric group and $T_n \subset S_n$ be a minimal generating set of transpositions. We consider the Cayley graph $\Gamma(S_n, T_n)$, having vertex set S_n and edges (v, v') where $v^{-1}v' \in T_n$. Suppose one selects permutations with probability $\frac{1+\epsilon}{n}$. Compute the probability of a cycle of length ℓ, $\mathcal{O}_\ell$, that contains a given permutation.

3

Tangled diagrams

Most of the material presented in this chapter is derived from [27, 28].

3.1 Tangled diagrams and vacillating tableaux

A tangled diagram, or tangle, is a labeled graph over the vertex set $[n] = \{1, \ldots, n\}$, with vertices of degree at most 2, drawn in increasing order in a horizontal line. Their arcs are drawn in the upper half plane. In general, a tangled diagram has isolated points and other types of degree 2 vertices, as displayed in Fig. 3.1.

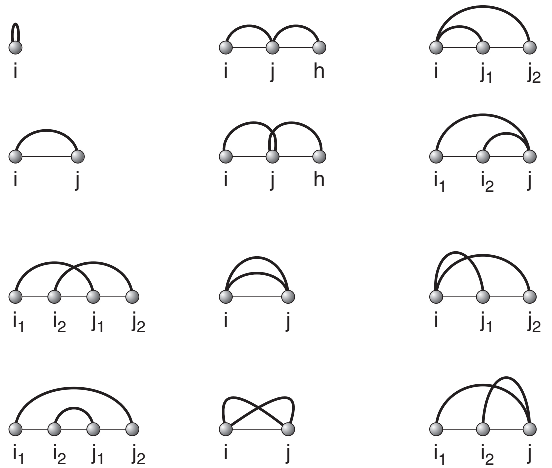

Fig. 3.1. All types of vertices with degree ≥ 1 in tangled diagrams.

Important subclasses of tangles are given as follows: (1) partial matchings, i.e., tangles in which each vertex has degree at most 1; (2) partitions,

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i.e., tangles in which any vertex of degree 2, j, is incident to the arcs (i, j) and (j, s), where $i < j < s$. Furthermore, partitions without arcs of the form $(i, i+1)$ are called 2-regular partitions. (3) Braids, i.e., tangled diagrams in which all vertices of degree 2, j, are either incident to loops (j, j), or crossing arcs (i, j) and (j, h), where $i < j < h$; see Fig. 3.2.

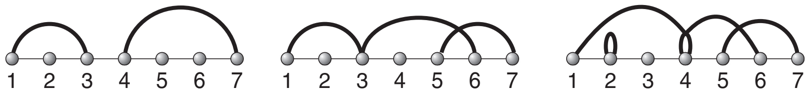

Fig. 3.2. From *left* to *right*: a partial matching, a partition, and a braid, respectively.

In order to describe the geometric crossings in tangled diagrams we map a tangled diagram into a partial matching. This mapping is called inflation. The inflation "splits" each vertex of degree 2, j, into two vertices j and j' having degree 1; see Fig. 3.3.

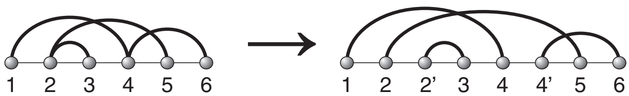

Fig. 3.3. The inflation of the first tangled diagram in Fig. 1.21 into its corresponding partial matching over eight vertices.

Accordingly, a tangle with ℓ vertices of degree 2 over n vertices is expanded into a diagram over $n+\ell$ vertices via inflation. The inflation map has a unique inverse, obtained by simply identifying the vertices j, j'. As RSK insertion refers implicitly a linear order, for this purpose, we consider the following linear ordering on $\{1, 1', \ldots, n, n'\}$:

$$1 < 1' < 2 < 2' < \cdots < n < n'.$$

Let G_n be a tangled diagram with exactly ℓ vertices of degree 2. Then the inflation of G_n, $\eta(G_n)$, is a labeled graph on $\{1, \ldots, n+\ell\}$ vertices with degree less than or equal to 1, obtained as follows:

Suppose first we have $i < j_1 < j_2$. If the arcs (i, j_1), (i, j_2) are crossing, then we map $((i, j_1), (i, j_2))$ into $((i, j_1), (i', j_2))$ and if (i, j_1), (i, j_2) are nesting then $((i, j_1), (i, j_2))$ is mapped into $((i, j_2), (i', j_1))$; see Fig. 3.4.

Second, let $i_1 < i_2 < j$. If (i_1, j), (i_2, j) are crossing, then we map $((i_1, j), (i_2, j))$ into $((i_1, j), (i_2, j'))$. If (i_1, j), (i_2, j) are nesting then we map $((i_1, j), (i_2, j))$ into $((i_1, j'), (i_2, j))$; see Fig. 3.5

Third suppose $i < j$. If $(i, j), (i, j)$ are crossing arcs, then $((i, j), (i, j))$ is mapped into $((i, j), (i', j'))$. If $(i, j), (i, j)$ are nesting arcs, then we map

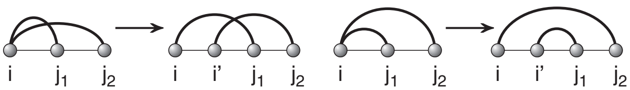

Fig. 3.4. The case $i < j_1 < j_2$: crossing (*left*) and nesting (*right*).

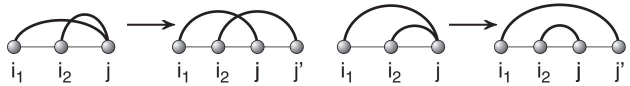

Fig. 3.5. The case $i_1 < i_2 < j$: crossing (*left*) and nesting (*right*).

$((i,j),(i,j))$ into $((i,j'),(i',j))$. Finally, if (i,i) is a loop we map (i,i) into (i,i'); see Fig. 3.6.

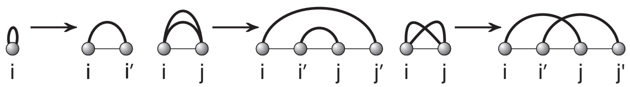

Fig. 3.6. The cases (i,i) and $i < j$: we resolve loops as arcs (*left*) and in case of $i < j$ we distinguish nesting (*middle*) and crossing (*right*).

Lastly, suppose we have $i < j < h$. If (i,j), (j,h) are crossing, then we map $((i,j),(j,h))$ into $((i,j'),(j,h))$ and we map $((i,j),(j,h))$ into $((i,j),(j',h))$, otherwise, see Fig. 3.7.

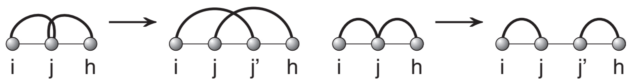

Fig. 3.7. The case $i < j < h$: crossing (*left*) and nesting (*right*).

As mentioned above, identifying all vertex-pairs (i,i') recovers the original tangle, whence we have the bijection

$$\eta\colon \mathcal{G}_n \longrightarrow \eta(\mathcal{G}_n).$$

The mapping η preserves by definition the maximal number of crossing and nesting arcs, respectively. Equivalently, a tangle G_n is k-noncrossing or k-nonnesting if and only if its inflation $\eta(G_n)$ is k-noncrossing or k-nonnesting, respectively. We have accordingly shown that the notion of crossings and nestings in tangles coincides with the notation of crossings and nestings in partial matchings.

A vacillating tableau V_λ^{2n} of shape λ and length $2n$ is a sequence of shapes $(\lambda^0,\lambda^1,\ldots,\lambda^{2n})$ such that (i) $\lambda^0=\varnothing$ and $\lambda^{2n}=\lambda$ and (ii) $(\lambda^{2i-1},\lambda^{2i})$ is derived from λ^{2i-2}, for $1 \le i \le n$, by one of the following operations. $(\varnothing,\varnothing)$:

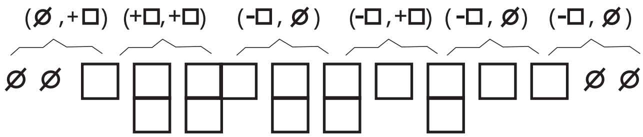

Fig. 3.8. A vacillating tableaux of shape $\varnothing$ and length 12.

do nothing twice; $(-\Box, \varnothing)$: first remove a square then do nothing; $(\varnothing, +\Box)$: first do nothing then add a square; $(\pm\Box, \pm\Box)$: add/remove a square at the odd and even steps, respectively. We denote the set of vacillating tableaux by $\mathcal{V}_\lambda^{2n}$; see Fig. 3.8.

3.2 The bijection

Lemma 3.1. *Any vacillating tableaux of shape* $\varnothing$ *and length* $2n$, $V_\varnothing^{2n}$, *induces a unique inflation of some tangled diagram on* $[n]$, $\phi(V_\varnothing^{2n})$, *namely, we have the mapping*

$$\phi\colon V_\varnothing^{2n} \longrightarrow \eta(\mathcal{G}_n).$$

Proof. In order to define ϕ, we recursively define a sequence of triples

$$((P_0, T_0, V_0), (P_1, T_1, V_1), \ldots, (P_{2n}, T_{2n}, V_{2n})),$$

where P_i is a set of arcs, T_i is a tableau of shape λ^i, and

$$V_i \subset \{1, 1', 2, 2', \ldots, n, n'\}$$

is a set of vertices. $P_0 = \varnothing$, $T_0 = \varnothing$, and $V_0 = \varnothing$. We assume that the left and right endpoints of all P_i-arcs and the entries of the tableau T_i are contained in $\{1, 1', \ldots, n, n'\}$. Once given $(P_{2j-2}, T_{2j-2}, V_{2j-2})$, we derive $(P_{2j-1}, T_{2j-1}, V_{2j-1})$ and (P_{2j}, T_{2j}, V_{2j}) as follows:

(I) $(+\Box, +\Box)$. If $\lambda^{2j-1} \supsetneq \lambda^{2j-2}$ and $\lambda^{2j} \supsetneq \lambda^{2j-1}$, we set $P_{2j-1} = P_{2j-2}$, and T_{2j-1} is obtained from T_{2j-2} by adding the entry j in the square $\lambda^{2j-1} \setminus \lambda^{2j-2}$. Furthermore we set $P_{2j} = P_{2j-1}$ and T_{2j} is obtained from T_{2j-1} by adding the entry j' in the square $\lambda^{2j} \setminus \lambda^{2j-1}$, $V_{2j-1} = V_{2j-2} \cup \{j\}$, and $V_{2j} = V_{2j-1} \cup \{j'\}$; see Fig. 3.9.

(II) $(\varnothing, +\Box)$. If $\lambda^{2j-1} = \lambda^{2j-2}$ and $\lambda^{2j} \supsetneq \lambda^{2j-1}$, then $(P_{2j-1}, T_{2j-1}) = (P_{2j-2}, T_{2j-2})$, $P_{2j} = P_{2j-1}$, and T_{2j} is obtained from T_{2j-1} by adding the

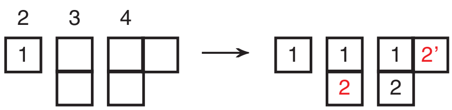

Fig. 3.9. From vacillating tableaux to tangles: in case of $\{+\Box, +\Box\}$, we have $V_3 = V_2 \cup \{2\}$ and $V_4 = V_3 \cup \{2'\}$.

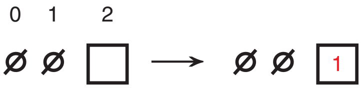

Fig. 3.10. $(\varnothing, +\Box)$: here we have $V_1 = V_0 = \varnothing$ and $V_2 = V_1 \cup \{1\}$.

entry j in the square $\lambda^{2j} \setminus \lambda^{2j-1}$, $V_{2j-1} = V_{2j-2}$, and $V_{2j} = V_{2j-1} \cup \{j\}$; see Fig. 3.10.

(III) $(+\Box, -\Box)$. If $\lambda^{2j-2} \subsetneq \lambda^{2j-1}$ and $\lambda^{2j} \subsetneq \lambda^{2j-1}$ then T_{2j-1} is obtained from T_{2j-2} by adding the entry j in the square $\lambda^{2j-1} \setminus \lambda^{2j-2}$ and the tableau T_{2j} is the unique tableau of shape λ^{2j} such that T_{2j-1} is obtained from T_{2j} by RSK inserting the unique number i. We then set $P_{2j-1} = P_{2j-2}$, $P_{2j} = P_{2j-1} \cup \{(i, j')\}$, $V_{2j-1} = V_{2j-2} \cup \{j\}$, and $V_{2j} = V_{2j-1} \cup \{j'\}$; see Fig. 3.11.

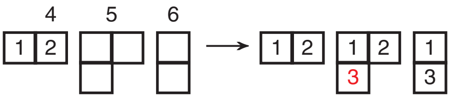

Fig. 3.11. $(+\Box, -\Box)$: here we have $P_5 = P_4$, $P_6 = P_5 \cup \{(2, 3')\}$, $V_5 = V_4 \cup \{3\}$, and $V_6 = V_5 \cup \{3'\}$.

(IV) $(-\Box, \varnothing)$. If $\lambda^{2j-1} \subsetneq \lambda^{2j-2}$ and $\lambda^{2j} = \lambda^{2j-1}$, then T_{2j-1} is the unique tableau of shape λ^{2j-1} such that T_{2j-2} is obtained by RSK inserting the unique number i into T_{2j-1}, $P_{2j-1} = P_{2j-2} \cup \{(i, j)\}$, $(P_{2j}, T_{2j}) = (P_{2j-1}, T_{2j-1})$, $V_{2j-1} = V_{2j-2} \cup \{j\}$, and $V_{2j} = V_{2j-1}$; see Fig. 3.12.

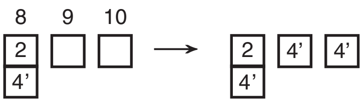

Fig. 3.12. $(-\Box, \varnothing)$: here we have $P_5 = P_4 \cup \{(2, 5)\}$, $P_6 = P_5$, $V_5 = V_4 \cup \{5\}$, and $V_6 = V_5$.

(V) $(-\Box, -\Box)$. If $\lambda^{2j-1} \subsetneq \lambda^{2j-2}$ and $\lambda^{2j} \subsetneq \lambda^{2j-1}$, let T_{2j-1} be the unique tableau of shape λ^{2j-1} such that T_{2j-2} is obtained from T_{2j-1} by RSK inserting i_1 and T_{2j} be the unique tableau of shape λ^{2j} such that T_{2j-1} is obtained from T_{2j} by RSK inserting i_2, $P_{2j-1} = P_{2j-2} \cup \{(i_1, j)\}$, $P_{2j} = P_{2j-1} \cup \{(i_2, j')\}$, $V_{2j-1} = V_{2j-2} \cup \{j\}$, and $V_{2j} = V_{2j-1} \cup \{j'\}$; see Fig. 3.13.

(VI) $(-\Box, +\Box)$. If $\lambda^{2j-1} \subsetneq \lambda^{2j-2}$ and $\lambda^{2j} \supsetneq \lambda^{2j-1}$, then T_{2j-1} is the unique tableau of shape λ^{2j-1} such that T_{2j-2} is obtained from T_{2j-1} by

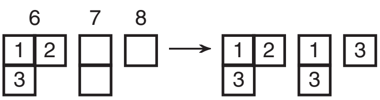

Fig. 3.13. $(-\Box, -\Box)$: here we have $P_7 = P_6 \cup \{(2, 4)\}$, $P_8 = P_7 \cup \{(1, 4')\}$, $V_7 = V_6 \cup \{4\}$, and $V_8 = V_7 \cup \{4'\}$.

RSK inserting the unique number i. Then we set $P_{2j-1} = P_{2j-2} \cup \{(i,j)\}$, $P_{2j} = P_{2j-1}$, and T_{2j} is obtained from T_{2j-1} by adding the entry j' in the square $\lambda^{2j} \setminus \lambda^{2j-1}$, $V_{2j-1} = V_{2j-2} \cup \{j\}$, and $V_{2j} = V_{2j-1} \cup \{j'\}$; see Fig. 3.14.

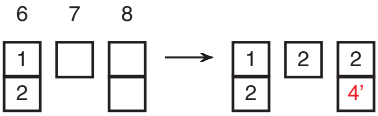

Fig. 3.14. $(-\square, +\square)$: we have $P_7 = P_6 \cup \{(1,4)\}$, $P_8 = P_7$, $V_7 = V_6 \cup \{4\}$, and $V_8 = V_7 \cup \{4'\}$.

(VII) $(\varnothing, \varnothing)$. If $\lambda^{2j-1} = \lambda^{2j-2}$ and $\lambda^{2j} = \lambda^{2j-1}$, we have $(P_{2j-1}, T_{2j-1}) = (P_{2j-2}, T_{2j-2})$, $(P_{2j}, T_{2j}) = (P_{2j-1}, T_{2j-1})$, $V_{2j-1} = V_{2j-2} \cup \{j\}$, and $V_{2j} = V_{2j-1}$.

Claim. The image $\phi(V_\varnothing^{2n})$ is the inflation of a tangled diagram.
First, if $(i,j) \in P_{2n}$, then $i < j$. Second, any vertex j can occur only as either a left or right endpoint of an arc, whence $\phi(V_\varnothing^{2n})$ is a 1-diagram. Each step $(+\square, +\square)$ induces a pair of arcs of the form (i, j_1), (i', j_2) and each step $(-\square, -\square)$ induces a pair of arcs of the form (i_1, j), (i_2, j'). Each step $(-\square, +\square)$ corresponds to a pair of arcs (h, j), (j', s) where $h < j < j' < s$, and each step $(+\square, -\square)$ induces a pair of arcs of the form (j, s), (h, j'), where $h < j < j' < s$ or a 1-arc of the form (i, i').

Let ℓ be the number of steps not containing $\varnothing$. By construction each of these steps adds the 2-set $\{j, j'\}$, whence (V_{2n}, P_{2n}) corresponds to the inflation of a unique tangled diagram with ℓ vertices of degree 2 and the claim follows.

We remark that, if squares are added, then the corresponding numbers are inserted. If squares are deleted Lemma 2.1 is used to extract a unique number, which then forms the left endpoint of the so-derived arcs; see Fig. 3.15. We proceed by explicitly constructing the inverse of ϕ.

Lemma 3.2. *Any inflation of a tangled diagram on n vertices, $\eta(G_n)$, induces the vacillating tableaux of shape $\varnothing$ and length $2n$, $\psi(\eta(G_n))$, namely, we have the mapping*

$$\psi \colon \eta(\mathcal{G}_n) \longrightarrow \mathcal{V}_\varnothing^{2n}. \tag{3.1}$$

Proof. We define ψ as follows. Let $\eta(G_n)$ be the inflation of the tangle G_n. We set

$$\eta_i = \begin{cases} (i, i'), & \text{iff } i \text{ has degree 2 in } G_n, \\ i, & \text{otherwise.} \end{cases}$$

Let $T_{2n} = \varnothing$ be the empty tableau. We will construct a sequence of tableaux T_h of shape $\lambda^h_{\eta(G_n)}$, where $h \in \{0, 1, \ldots 2n\}$ by considering η_i for $i = n, n-1, n-2, \ldots, 1$. For each η_j we inductively define the pair of tableaux (T_{2j}, T_{2j-1}):

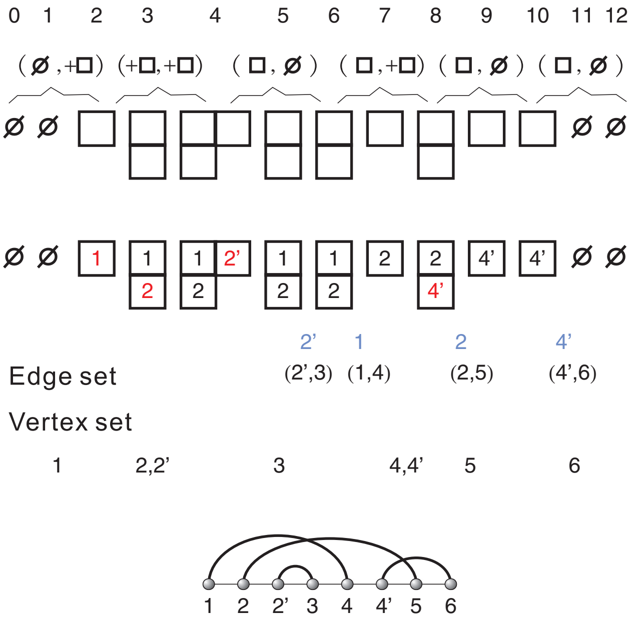

Fig. 3.15. Lemma 3.1: from vacillating tableaux to inflated tangles.

(I) j is a left endpoint of degree 2, then we have the two $\eta(G_n)$-arcs (j, r) and (j', h). T_{2j-1} is obtained by removing the square with entry j' from the tableau T_{2j} and T_{2j-2} is obtained by removing the square with entry j from T_{2j-1}. Then we have $\lambda^{2j-1}_{\eta(G_n)} \subsetneq \lambda^{2j}_{\eta(G_n)}$ and $\lambda^{2j-2}_{\eta(G_n)} \subsetneq \lambda^{2j-1}_{\eta(G_n)}$ (left to right: $(+\square, +\square)$); see Fig. 3.16.

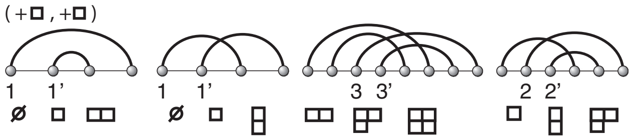

Fig. 3.16. All the possible cases for $(+\square, +\square)$ in case of 3-noncrossing tangles.

(II) j is the left endpoint of exactly one arc (j, k) but not a right endpoint, then first set T_{2j-1} to be the tableau obtained by removing the square with entry j from T_{2j} and let $T_{2j-2} = T_{2j-1}$. Therefore $\lambda^{2j-1}_{\eta(G_n)} \subsetneq \lambda^{2j}_{\eta(G_n)}$ and $\lambda^{2j-2}_{\eta(G_n)} = \lambda^{2j-1}_{\eta(G_n)}$ (left to right: $(\varnothing, +\square)$).

(III) j is a left and right endpoint of crossing arcs or a loop, then we have the two $\eta(G_n)$-arcs (j, s) and (h, j'), $h < j < j' < s$ or an arc of the form (j, j'), respectively. T_{2j-1} is obtained by RSK-inserting h into the tableau T_{2j} and T_{2j-2} is obtained by removing the square with entry j from the T_{2j-1}

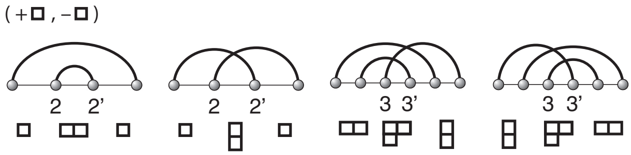

Fig. 3.17. All the possible cases for $(+\square, -\square)$ in case of 3-noncrossing tangles.

or T_{2j-1} is obtained by RSK-inserting j into the tableau T_{2j} and T_{2j-2} is obtained by removing the square with entry j from the T_{2j-1}, respectively (left to right: $(+\square, -\square)$); see Fig. 3.17.

(IV) $\eta_j = j$ is the right endpoint of exactly one arc (i, j) but not a left endpoint, then we set $T_{2j-1} = T_{2j}$ and obtain T_{2j-2} by RSK-inserting i into T_{2j-1}. Consequently we have $\lambda^{2j-1}_{\eta(G_n)} = \lambda^{2j}_{\eta(G_n)}$ and $\lambda^{2j-2}_{\eta(G_n)} \supsetneq \lambda^{2j-1}_{\eta(G_n)}$ (left to right: $(-\square, \varnothing)$).

(V) j is a right endpoint of degree 2, then we have the two $\eta(G_n)$-arcs (i, j) and (h, j'). T_{2j-1} is obtained by RSK-inserting h into T_{2j} and T_{2j-2} is obtained by RSK-inserting i into T_{2j-1}. We derive $\lambda^{2j-1}_{\eta(G_n)} \supsetneq \lambda^{2j}_{\eta(G_n)}$ and $\lambda^{2j-2}_{\eta(G_n)} \supsetneq \lambda^{2j-1}_{\eta(G_n)}$ (left to right: $(-\square, -\square)$); see Fig. 3.18.

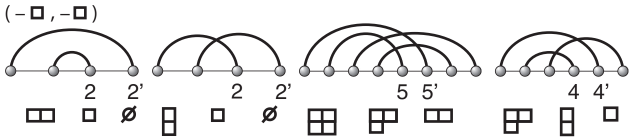

Fig. 3.18. All the possible cases for $(-\square, -\square)$ in case of 3-noncrossing tangles.

(VI) j is a left and right endpoint, then we have the two $\eta(G_n)$-arcs (i, j) and (j', h), where $i < j < j' < h$. First, the tableaux T_{2j-1} is obtained by removing the square with entry j' in T_{2j}. Second, the RSK insertion of i into T_{2j-1} generates the tableau T_{2j-2}. Accordingly, we derive the shapes $\lambda^{2j-1}_{\eta(G_n)} \subsetneq \lambda^{2j}_{\eta(G_n)}$ and $\lambda^{2j-2}_{\eta(G_n)} \supsetneq \lambda^{2j-1}_{\eta(G_n)}$ (left to right: $(-\square, +\square)$); see Fig. 3.19.

(VII) $\eta_j = j$ is an isolated vertex in $\eta(G_n)$, then we set $T_{2j-1} = T_{2j}$ and $T_{2j-2} = T_{2j-1}$. Accordingly, $\lambda^{2j-1}_{\eta(G_n)} = \lambda^{2j}_{\eta(G_n)}$ and $\lambda^{2j-2}_{\eta(G_n)} = \lambda^{2j-1}_{\eta(G_n)}$ (left to right: $(\varnothing, \varnothing)$).

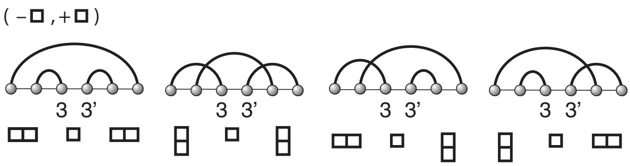

Fig. 3.19. All the possible cases for $(-\square, +\square)$ when restricted to 3-noncrossing tangles.

Therefore, ψ maps the inflation of a tangled diagram into a vacillating tableau and the lemma follows.

As an illustration of Lemma 3.2, see Fig. 3.20: starting from right to left the vacillating tableaux is obtained via the RSK algorithm as follows: if j is a

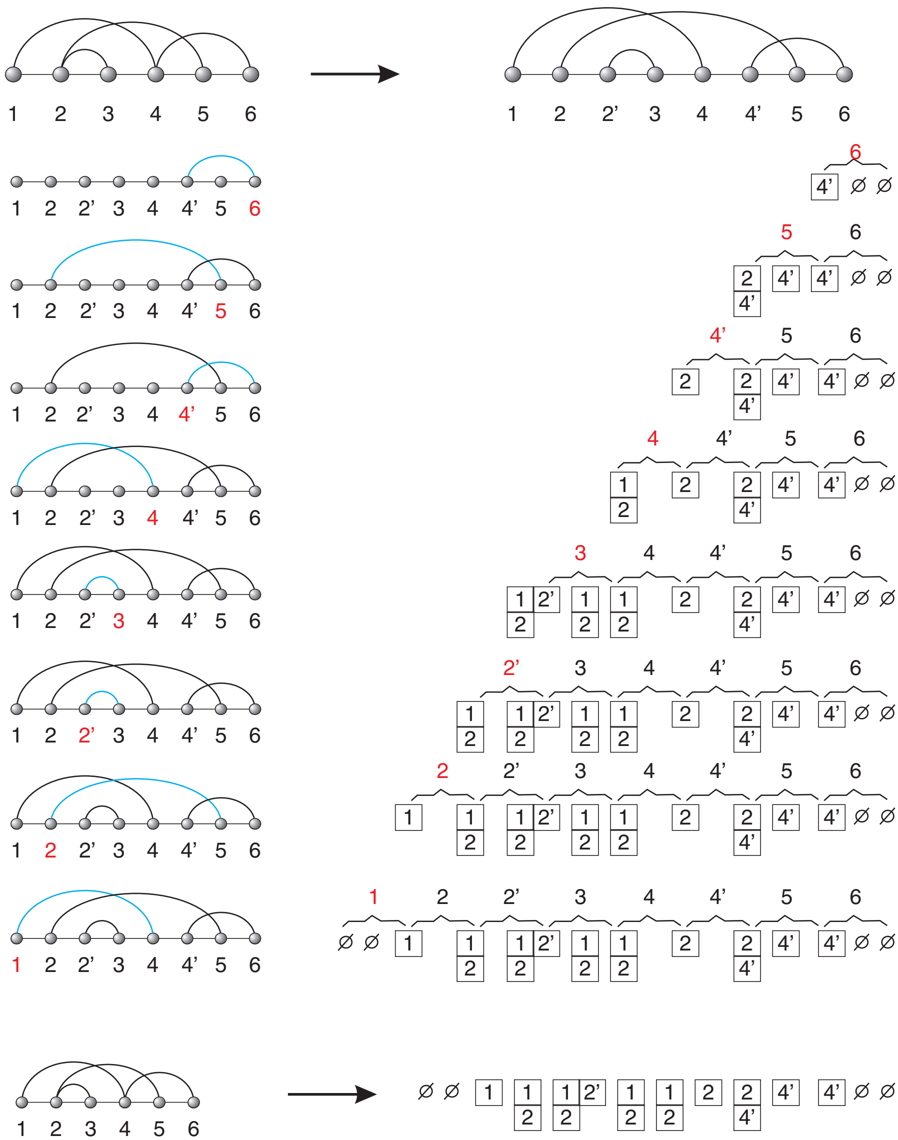

Fig. 3.20. An illustration of Lemma 3.2: how to map a tangle into a vacillating tableaux via ψ.

right endpoint it gives rise to RSK insertion of its (unique) left endpoint and if j is a left endpoint the square filled with j is removed.

Theorem 3.3. *There exists a bijection between the set of vacillating tableaux of shape $\varnothing$ and length $2n$, $\mathcal{V}_{\varnothing}^{2n}$, and the set of tangles on n vertices, $\mathcal{G}_n$,*

$$\beta\colon \mathcal{V}_{\varnothing}^{2n} \longrightarrow \mathcal{G}_n.$$

Proof. According to Lemmas 3.1 and 3.2, we have the mappings $\phi\colon \mathcal{V}_{\varnothing}^{2n} \longrightarrow \eta(\mathcal{G}_n)$ and $\psi\colon \eta(\mathcal{G}_n) \longrightarrow \mathcal{V}_{\varnothing}^{2n}$. We next show that ϕ and ψ are indeed inverses of each other. By definition, the mapping ϕ generates arcs whose left endpoints, when RSK inserted into T_i, recover the tableaux T_{i-1}. We observe that by definition, the mapping ψ reverses this extraction: it is constructed via the RSK insertion of the left endpoints. Therefore we have the following relations:

$$\phi \circ \psi(\eta(G_n)) = \phi((\lambda^h_{\eta(G_n)})_0^{2n}) = \eta(G_n) \quad \text{and} \quad \psi \circ \phi(V_{\varnothing}^{2n}) = V_{\varnothing}^{2n},$$

from which we conclude that ϕ and ψ are bijective. Since G_n is in one-to-one correspondence with $\eta(G_n)$, the proof of the theorem is complete.

By construction, the bijection $\eta\colon \mathcal{G}_n \longrightarrow \eta(\mathcal{G}_n)$ preserves the maximal number crossing and nesting arcs, respectively. Equivalently, a tangled diagram G_n is k-noncrossing or k-nonnesting if and only if its inflation $\eta(G_n)$ is k-noncrossing or k-nonnesting [25]. Indeed, this follows immediately from the definition of the inflation. Accordingly the next result is directly implied by Theorem 2.2:

Theorem 3.4. *A tangled diagram G_n is k-noncrossing if and only if all shapes λ^i in the corresponding vacillating tableau have less than k rows, i.e., $\phi\colon \mathcal{V}_{\varnothing}^{2n} \longrightarrow \mathcal{G}_n$ maps vacillating tableaux having less than k rows into k-noncrossing tangles. Furthermore, there is a bijection between the set of k-noncrossing and k-nonnesting tangles.*

Restricting the steps for vacillating tableaux produces the bijection of Chen et al. [25]. Let $\mathcal{M}_k^{\dagger}(n)$, $\mathcal{P}_k(n)$, and $\mathcal{B}_k(n)$ denote the set of k-noncrossing matchings, partitions, and braids. Theorem 3.3 implies that the tableaux sequences of $\mathcal{M}_k^{\dagger}(n)$, $\mathcal{P}_k(n)$, and $\mathcal{B}_k(n)$ are composed by the elements in $S_{\mathcal{M}_k^{\dagger}}$, $S_{\mathcal{P}_k}$, and $S_{\mathcal{B}_k}$, respectively, where $1 \le h, l \le k-1$ and

$$\begin{aligned} S_{\mathcal{M}_k^{\dagger}} &= \{(-\square_h, \varnothing), (\varnothing, +\square_h)\}, \\ S_{\mathcal{P}_k} &= \{(\varnothing, \varnothing), (-\square_h, \varnothing), (\varnothing, +\square_h), (-\square_h, +\square_l)\}, \\ S_{\mathcal{B}_k} &= \{(\varnothing, \varnothing), (-\square_h, \varnothing), (\varnothing, +\square_h), (+\square_h, -\square_l)\}, \end{aligned}$$

where we use the following notation: if λ_{i+1} is obtained from λ_i by adding, removing a square from the jth row, or doing nothing we write $\lambda_{i+1} \backslash \lambda_i = +\square_j$, $\lambda_{i+1} \setminus \lambda_i = -\square_j$ or $\lambda_{i+1} \setminus \lambda_i = \varnothing$, respectively; see Fig. 3.21.

The enumeration of 3-noncrossing partitions and 3-noncrossing enhanced partitions has been studied by Xin and Bousquet-Mélou [17]. The authors obtain their results by solving a functional equation of walks in the first quadrant using the reflection principle [149] and the kernel method [92].

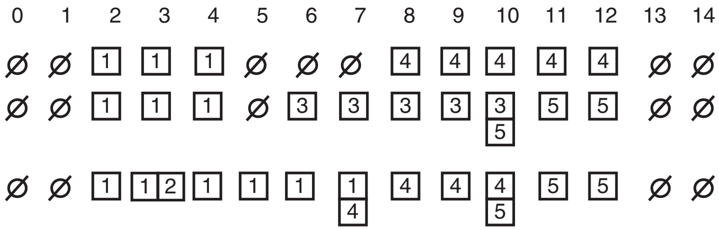

Fig. 3.21. The corresponding tableaux sequences for the partial matching, partition, and braid shown in Fig. 3.2.

A 2-regular, k-noncrossing partition is a k-noncrossing partition without arcs of the form $(i, i+1)$. We denote the set of 2-regular, k-noncrossing partitions by $\mathcal{P}_{k,2}(n)$. There exists a bijection between 2-regular, k-noncrossing partitions and k-noncrossing braids without isolated points, denoted by $\mathcal{B}_k^\dagger(n)$, i.e., k-noncrossing enhanced partitions[25]. This bijection is obtained as follows: for $\delta \in \mathcal{B}_k^\dagger(n)$, we identify loops with isolated points and crossing arcs (i,j) and (j,h), where $i < j < h$, by noncrossing arcs. This identification produces a mapping from $\mathcal{P}_{k,2}(n)$ into a subset of partitions $\mathcal{P}_k^*(n)$, which we refer to as ϑ; see Fig. 3.22.

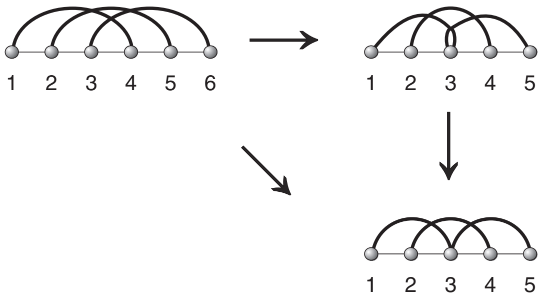

Fig. 3.22. An illustration of Theorem 3.5: the bijection ϑ

Theorem 3.5. *Let $k \in \mathbb{N}$, $k \geq 3$. Then we have a bijection*

$$\vartheta \colon \mathcal{P}_{k,2}(n) \longrightarrow \mathcal{B}_k^\dagger(n-1), \qquad \vartheta((i,j)) = (i, j-1).$$

Proof. By construction, ϑ maps tangled diagrams on $[n]$ to tangled diagrams on $[n-1]$. Since there does not exist any arc of the form $(i, i+1)$, for any $\pi \in \mathcal{P}_{k,2}(n)$, $\vartheta(\pi)$ is loop free. By construction, ϑ preserves the orientation of arcs, whence $\vartheta(\pi)$ is a partition.

Claim 1. $\vartheta \colon \mathcal{P}_{k,2}(n) \longrightarrow \mathcal{B}_k^\dagger(n-1)$ is well defined.
We first prove that $\vartheta(\pi)$ is k-noncrossing. Suppose there exist k mutually crossing arcs, $\{(i_s, j_s)\}_{s=1}^{s=k}$ in $\vartheta(\pi)$. Since $\vartheta(\pi)$ is a partition, we have

$i_1 < \cdots < i_k < j_1 < \cdots < j_k$. So, we obtain for the partition $\pi \in \mathcal{P}_{k,2}(n)$ the k arcs $(i_s, j_s + 1)$, $s = 1, \dots, k$, where $i_1 < \cdots < i_k < j_1 + 1 < \cdots < j_k + 1$, which is impossible since π is k-noncrossing. We next show that $\vartheta(\pi)$ is a k-noncrossing braid. If $\vartheta(\pi)$ is not a k-noncrossing braid, then it contains k arcs of the form $(i_1, j_1), \dots, (i_k, j_k)$ such that $i_1 < \cdots < i_k = j_1 < \cdots < j_k$. Then π contains the arcs $(i_1, j_1 + 1)$, $(i_k, j_k + 1)$ where $i_1 < \cdots < i_k < j_1 + 1 < \cdots < j_k + 1$, which is impossible since these arcs are a set of k mutually crossing arcs and Claim 1 follows.

Claim 2. ϑ is bijective.
Clearly ϑ is injective and it remains to prove surjectivity. For any k-noncrossing braid δ there exists 2-regular partition π such that $\vartheta(\pi) = \delta$. We have to show that π is k-noncrossing. Suppose that there exists some partition π with k mutually crossing arcs such that $\vartheta(\pi) = \delta$. Let $M' = \{(i_1, j_1), \dots, (i_k, j_k)\}$ be a set of k mutually crossing arcs in the standard representation of π, i.e., $i_1 < \cdots < i_k < j_1 < \cdots < j_k$. Then we have in $\vartheta(\pi)$ the arcs $(i_s, j_s - 1)$, $s = 1, \dots, k$, such that

$$i_1 < \cdots < i_k \le j_1 - 1 < \cdots < j_k - 1.$$

Since $M = \{(i_1, j_1 - 1), \dots, (i_k, j_k - 1)\}$ is k-noncrossing, we conclude $i_k = j_1 - 1$. This is impossible in k-noncrossing braids. By transposition, we have proved that any ϑ-preimage is necessarily a k-noncrossing partition, whence Claim 2 and the proof of the theorem is complete.

In Fig. 3.22 we give an illustration of the bijection $\vartheta\colon \mathcal{P}_{k,2}(n) \longrightarrow \mathcal{B}_k^{\dagger}(n-1)$.

3.3 Enumeration

Let $t_k(n)$ and $\tilde{t}_k(n)$ denote the numbers of k-noncrossing tangles and k-noncrossing tangles without isolated points on $[n]$, respectively. Recall that $f_k(2n, 0)$ is the number of k-noncrossing matchings on $2n$ vertices. In the following we will illustrate that the enumeration of tangles could be reduced to the enumeration of matchings via the inflation map. Without loss of generality we can restrict our analysis to the case of tangles without isolated points since the number of tangled diagrams on $[n]$ is given by

$$t_k(n) = \sum_{i=0}^{n} \binom{n}{i} \tilde{t}_k(n - i). \tag{3.2}$$

Theorem 3.6. *The number of k-noncrossing tangles without isolated points on $[n]$ is given by*

$$\tilde{t}_k(n) = \sum_{\ell=0}^{n} \binom{n}{\ell} f_k(2n - \ell, 0).$$

In particular, for $k=3$ we have

$$\tilde{t}_3(n) = \sum_{\ell=0}^{n} \binom{n}{\ell} \left(C_{\frac{2n-\ell}{2}} \, C_{\frac{2n-\ell}{2}+2} - C^2_{\frac{2n-\ell}{2}+1} \right),$$

where C_m denotes the mth Catalan number $\frac{1}{m+1}\binom{2m}{m}$.

Proof. Let $\tilde{\mathcal{T}}_k(n,V)$ be the set of tangles without isolated points where $V = \{i_1,\dots,i_h\}$ is the set of vertices of degree 1 (where $h \equiv 0 \mod 2$ by definition of $\tilde{\mathcal{T}}_k(n,V)$) and let $\mathcal{M}_k^{\dagger}(\{1,1',\dots,n,n'\}\backslash V')$, where $V' = \{i'_1,\dots,i'_h\}$ denotes the set of matchings on $\{1,1',\dots,n,n'\} \setminus V'$. By construction, the inflation $\eta\colon \mathcal{G}_n \longrightarrow \eta(\mathcal{G}_n)$ induces a well-defined mapping

$$\hat{\eta}\colon \tilde{\mathcal{T}}_k(n,V) \longrightarrow \mathcal{M}_k^{\dagger}(\{1,1',\dots,n,n'\} \setminus V')$$

with inverse κ defined by identifying all pairs (y,y'), where $y,y' \in \{1,1',\dots,n,n'\} \setminus V'$. Obviously, we have $|\mathcal{M}_k^{\dagger}(\{1,1',\dots,n,n'\} \setminus V')| = f_k(2n-h,0)$ and

$$\tilde{t}_k(n) = \sum_{V \subset [n]} \tilde{t}_k(n,V) = \sum_{\ell=0}^{n} \binom{n}{\ell} f_k(2n-\ell,0). \tag{3.3}$$

Suppose $n \equiv 0 \mod 2$. Let C_m denote the mth Catalan number. Then we have [53]

$$f_3(n,0) = C_{\frac{n}{2}} \, C_{\frac{n}{2}+2} - C^2_{\frac{n}{2}+1},$$

and the theorem follows.

The first five numbers of 3-noncrossing tangles are given by 2, 7, 39, 292, 2635.

In eq. (3.3) we relate the generating functions of k-noncrossing tangles $\mathbf{T}_k(z) = \sum_n t_k(n) z^n$ and k-noncrossing matchings $\mathbf{F}_k(z) = \sum_n f_k(2n,0)\, z^n$. We derive the functional equation which is instrumental to prove eq. (3.6) for $2 \le k \le 9$.

For this purpose we employ Cauchy's integral formula: let D be a simply connected domain and let C be a simple closed positively oriented contour that lies in D. If f is analytic inside C and on C, except at the vertices $z_1, z_2, \dots, z_n$ that are in the interior of C, then we have Cauchy's integral formula

$$\int_C f(z)dz = 2\pi i \sum_{k=1}^{n} Res[f, z_k]. \tag{3.4}$$

In particular, if f has a simple pole at z_0, then $Res[f,z_0] = \lim_{z \to z_0} (z-z_0) f(z)$.

Lemma 3.7. *Let $k \in \mathbb{N}$, $k \ge 2$. Then we have*

$$\mathbf{T}_k\left(\frac{z^2}{1+z+z^2}\right) = \frac{1+z+z^2}{z+2}\, \mathbf{F}_k(z^2)\,. \tag{3.5}$$

Proof. The relation between the number of k-noncrossing tangles, $t_k(n)$, and k-noncrossing matchings, $f_k(2n,0)$, given in eq. (2.7), which implies

$$t_k(n) = \sum_{r,\ell} \binom{n}{r}\binom{n-r}{\ell} f_k(2n-2r-\ell,0).$$

Substituting the combinatorial terms with the contour integrals we derive

$$\begin{aligned}
\binom{n}{r} &= \frac{1}{2\pi i}\oint_{|u|=\alpha}(1+u)^n u^{-r-1}du,\\
f_k(2n-2r-\ell,0) &= \frac{1}{2\pi i}\oint_{|z|=\beta_3}\mathbf{F}_k(z^2)z^{-(2n-2r-\ell)-1}dz,\\
t_k(n) &= \sum_{r,\ell}\binom{n}{r}\binom{n-r}{\ell}f_k(2n-2r-\ell,0)\\
&= \frac{1}{(2\pi i)^3}\sum_{r,\ell}\oint_{\substack{|v|=\beta_1\\|z|=\beta_2\\|u|=\beta_3}}(1+u)^n u^{-r-1}(1+v)^{n-r}v^{-\ell-1}\ \times\\
&\qquad\qquad\qquad\qquad \mathbf{F}_k(z^2)\,z^{-(2n-2r-\ell)-1}dv\,du\,dz,
\end{aligned}$$

where $\alpha,\beta_1,\beta_2,\beta_3$ are arbitrary small positive numbers. Since the series are absolute convergent, we obtain

$$\begin{aligned}
t_k(n) = \frac{1}{(2\pi i)^3}\sum_r\oint_{\substack{|v|=\beta_1\\|z|=\beta_2\\|u|=\beta_3}}&(1+u)^n u^{-r-1}\mathbf{F}_k(z^2)\,z^{-2n+2r-1}(1+v)^{n-r}v^{-1}\ \times\\
&\sum_\ell\left(\frac{z}{v}\right)^\ell dv\,du\,dz,
\end{aligned}$$

which gives rise to

$$\begin{aligned}
t_k(n) = \frac{1}{(2\pi i)^3}\sum_r\oint_{\substack{|u|=\beta_3\\|z|=\beta_2}}&(1+u)^n u^{-r-1}\mathbf{F}_k(z^2)\,z^{-2n+2r-1}\ \times\\
&\left(\oint_{|v|=\beta_1}\frac{(1+v)^{n-r}}{v-z}dv\right)du\,dz.
\end{aligned}$$

Since $v=z$ is the unique (simple) pole in the integral domain, eq. (3.4) implies

$$\oint_{|v|=\beta_1}\frac{(1+v)^{n-r}}{v-z}dv = 2\pi i\,(1+z)^{n-r}.$$

We accordingly have

$$t_k(n) = \frac{1}{(2\pi i)^2}\sum_r\oint_{\substack{|u|=\beta_3\\|z|=\beta_2}}(1+u)^n u^{-r-1}\mathbf{F}_k(z^2)\,z^{-2n+2r-1}(1+z)^{n-r}du\,dz.$$

Proceeding analogously with respect to the summation over r yields

$$\begin{aligned} t_k(n) &= \frac{1}{(2\pi i)^2} \oint_{\substack{|u|=\beta_3 \\ |z|=\beta_2}} (1+u)^n \mathbf{F}_k(z^2)\, z^{-2n-1}(1+z)^n u^{-1} \sum_r \frac{z^{2r}}{u^r(1+z)^r} du\, dz \\ &= \frac{1}{(2\pi i)^2} \oint_{|z|=\beta_2} \mathbf{F}_k(z^2)\, z^{-2n-1}(1+z)^n \left(\oint_{|u|=\beta_3} (1+u)^n \frac{1}{u - \frac{z^2}{1+z}} du \right) dz. \end{aligned}$$

Since $u = \frac{z^2}{1+z}$ is the only pole in the integral domain, Cauchy's integral formula implies

$$\oint_{|u|=\beta_3} (1+u)^n \frac{1}{u - \frac{z^2}{1+z}} du = 2\pi i \left(1 + \frac{z^2}{1+z}\right)^n .$$

Now we compute

$$\begin{aligned} t_k(n) &= \frac{1}{2\pi i} \oint_{|z|=\beta_2} \mathbf{F}_k(z^2)\, z^{-1} z^{-2n} (1+z)^n \left(1 + \frac{z^2}{1+z}\right)^n dz \\ &= \frac{1}{2\pi i} \oint_{|z|=\beta_2} \mathbf{F}_k(z^2)\, z^{-1} \left(\frac{1+z+z^2}{z^2}\right)^n dz \\ &= \frac{1}{2\pi i} \oint_{|z|=\beta_2} \frac{1+z+z^2}{z+2} \mathbf{F}_k(z^2) \left(\frac{z^2}{1+z+z^2}\right)^{-n-1} d\left(\frac{z^2}{1+z+z^2}\right) \end{aligned}$$

from which

$$\mathbf{T}_k\left(\frac{z^2}{1+z+z^2}\right) = \frac{1+z+z^2}{z+2} \mathbf{F}_k(z^2)$$

follows and the theorem is proved.

Lemma 3.7, Theorem 2.8, and Proposition 2.24 imply for the asymptotics of tangles.

Theorem 3.8. *For $2 \leq k \leq 9$ the number of k-noncrossing tangles is asymptotically given by*

$$t_k(n) \sim c_k\, n^{-((k-1)^2 + \frac{k-1}{2})} \left(4(k-1)^2 + 2(k-1) + 1\right)^n \quad \textit{where } c_k > 0. \quad (3.6)$$

Proof. According to Lemma 3.7, we have the functional equation

$$\mathbf{T}_k\left(\frac{z^2}{z^2+z+1}\right) = \frac{z^2+z+1}{z+2}\, \mathbf{F}_k(z^2), \quad (3.7)$$

where $|z| \leq \rho_k < 1$ and the function $\vartheta(z) = \frac{z^2}{z^2+z+1}$ is regular at $z = \pm\rho_k$ and $\rho_k = 1/2(k-1)$. Then

$$\vartheta(\rho_k) = \frac{\rho_k^2}{\rho_k^2 + \rho_k + 1} \quad \text{and} \quad \vartheta(-\rho_k) = \frac{\rho_k^2}{\rho_k^2 - \rho_k + 1}$$

are both singularities of $\mathbf{T}_k(z)$. We claim that $\vartheta(\rho_k)$ is the unique dominant positive real singularity of $\mathbf{T}_k(z)$. Indeed, $\vartheta(z)$ is strictly monotonously increasing and continuous for $0 < z \le 1$, and $0 < \vartheta(z) \le 1/3$. If there is a positive singularity γ of $\mathbf{T}_k(z)$

$$\gamma < \vartheta(\rho_k) \le \vartheta\left(\frac{1}{2}\right) = \frac{1}{7},$$

there would exist $\vartheta^{-1}(\gamma) < \rho_k$ which is a contradiction to ρ_k being the dominant singularity of $\mathbf{T}_k(\vartheta(z))$. Next we show that $\vartheta(\rho_k)$ is unique. Suppose there exists a dominant singularity η different from $\vartheta(\rho_k)$, where $|\eta| = \vartheta(\rho_k)$. Then there exists $z_\eta \in \mathbb{C}$ such that $\vartheta(z_\eta) = \eta$ and $z_\eta \neq \rho_k$. Since $|\vartheta(z_\eta)| = \vartheta(\rho_k)$,

$$(\rho_k^2 + \rho_k + 1)|z_\eta|^2 = |z_\eta^2 + z_\eta + 1|\rho_k^2 \le \left(|z_\eta^2| + |z_\eta| + 1\right)\rho_k^2,$$

whence $|z_\eta| \le \rho_k$. Accordingly, z_η is a dominant singularity of $\mathbf{T}_k(\vartheta(z))$ which is a contradiction to eq. (3.7) which implies that $\mathbf{T}_k(\vartheta(z))$ has only the dominant singularities $\pm\rho_k$. Consequently, $\vartheta(\rho_k)$ is the unique dominant singularity of $\mathbf{T}_k(z)$.

According to Corollary 2.14, the generating function, $\mathbf{F}_k(z)$, is D-finite. Theorem 2.13 shows that the composition $F(G(z))$ of a D-finite function F and a rational function G, where $G(0) = 0$, is again D-finite, and the product of two D-finite functions is also D-finite, whence $\mathbf{T}_k(z)$ and $\mathbf{T}_k(\vartheta(z))$ are D-finite and accordingly have singular expansions. Let $S_{\mathbf{T}_k}(z - \vartheta(\rho_k))$ denote the singular expansion of $\mathbf{T}_k(z)$ at $z = \vartheta(\rho_k)$. Since $\vartheta(z)$ is regular at $z = \rho_k$ and $\vartheta'(\rho_k) \neq 0$, see Table 3.1, we are given the supercritical paradigm [42]. Indeed, we have $\vartheta'(\rho_k) \neq 0$, see Table 3.1 and derive

$$\begin{aligned} \mathbf{T}_k(\vartheta(z)) &\sim S_{\mathbf{T}_k}(\vartheta(z) - \vartheta(\rho_k)) && \text{as } \vartheta(z) \to \vartheta(\rho_k) \\ &= \Theta(S_{\mathbf{T}_k}(z - \rho_k)) && \text{as } z \to \rho_k. \end{aligned}$$

Proposition 2.24 implies that for $z \to \rho_k^2$

$$\mathbf{F}_k(z) = \begin{cases} P_k(z - \rho_k^2) + c_k'(z - \rho_k^2)^{\left((k-1)^2 + (k-1)/2\right) - 1} \ln(z - \rho_k^2)\,(1 + o(1)) \\ P_k(z - \rho_k^2) + c_k'(z - \rho_k^2)^{\left((k-1)^2 + (k-1)/2\right) - 1}\,(1 + o(1)) \end{cases}$$

depending on k being odd and even. Here the terms $P_k(z)$ are polynomials of degree $\le (k-1)^2 + (k-1)/2 - 1$ and c_k' is some constant. Let $S_{\mathbf{F}_k}(z - \rho_k^2)$

k	2	3	4	5	6	7	8	9
$\vartheta'(\rho_k)$	0.4082	0.3265	0.2531	0.2042	0.1704	0.1461	0.1277	0.1134

Table 3.1. The values of $\vartheta'(\rho_k)$ for $2 \le k \le 9$.

denote the singular expansion of $\mathbf{F}_k(z)$ at $z = \rho_k^2$. Equation (3.7) implies for $z \longrightarrow \rho_k$

$$\mathbf{T}_k(\vartheta(z)) \sim \frac{\rho_k^2 + \rho_k + 1}{\rho_k + 2} S_{\mathbf{F}_k}(z^2 - \rho_k^2)$$

and thus

$$S_{\mathbf{T}_k}(z - \rho_k) = \Theta\left(S_{\mathbf{F}_k}(z - \rho_k)\right) \quad \text{as } z \longrightarrow \rho_k.$$

Therefore, $\mathbf{T}_k(z)$ has at $v = \vartheta(\rho_k)$ exactly the same subexponential factors as $\mathbf{F}_k(z)$ at ρ_k^2, i.e., we have

$$[z^n]\,\mathbf{T}_k(z) \sim c_k\, n^{-\left((k-1)^2 + \frac{k-1}{2}\right)} \left(\frac{\rho_k^2}{\rho_k^2 + \rho_k + 1}\right)^{-n} \qquad \text{for some } t_k > 0$$

and the theorem is proved.

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