Supplemental Materials for Shapes of RNA pseudoknot structures

In [3], we have the following four generating function equations to do singularity analysis for $2 \leq k \leq 9$, $1 \leq \sigma \leq 10$

$$\begin{aligned}
\mathbf{I}_k(z) &= \mathbf{F}_k\left(\frac{z}{1+z}\right), & (1)\\
\mathbf{J}_k(z) &= \frac{(1+z)(1+z^2)}{z^3+2z^2+1}\mathbf{F}_k\left(\frac{(1+z)^2(1+z^2)z^2}{(z^3+2z^2+1)^2}\right), & (2)\\
\mathbf{Lv}^1_{k,\sigma}(z) &= \frac{(1+z)(1+z^{2\sigma})}{(1-z)(z^{2\sigma+1}+2z^{2\sigma}+1)}\mathbf{F}_k\left(\frac{(1+z)^2 z^{2\sigma}(1+z^{2\sigma})}{\left(z^{2\sigma+1}+2z^{2\sigma}+1\right)^2}\right), & (3)\\
\mathbf{Lv}^5_{k,\sigma}(z) &= \frac{(1+z^{2\sigma})}{(1-z)(1+2z^{2\sigma}-z^{2\sigma+1})}\mathbf{F}_k\left(\frac{z^{2\sigma}(1+z^{2\sigma})}{\left(1+2z^{2\sigma}-z^{2\sigma+1}\right)^2}\right), & (4)
\end{aligned}$$

where $\mathbf{F}_k(z) = \sum_{n\geq 0} f_k(2n,0)z^n$. In [3], we have that $\mathbf{F}_k(z)$ is D-finite [2], i.e. there exists some $e \in \mathbb{N}$ such that

$$q_{0,k}(z)\frac{d^e}{dz^e}\mathbf{F}_k(z) + q_{1,k}(z)\frac{d^{e-1}}{dz^{e-1}}\mathbf{F}_k(z) + \cdots + q_{e,k}(z)\mathbf{F}_k(z) = 0, \qquad (5)$$

where $q_{j,k}(z)$ are polynomials. Any singularity of $\mathbf{F}_k(z)$ is contained in the set of roots of $q_{0,k}(z)$ [2]. Observing the Table 1, we find that the singularities set of $F_k(z)(2 \leq k \leq 9)$ is contained in the set

$$\{\rho_i^2 | \rho_i = 1/(2i-2),\ i \equiv k \mod 2,\ 2 \leq i \leq k\}. \qquad (6)$$

Furthermore, $\mathbf{F}_k(z)$ has unique dominant singularity ρ_k^2, where $\rho_k = 1/(2k-2)$, $2 \leq k \leq 9$. Our four generating functions (eq.(1)-(4)) are all the compositions of $\mathbf{F}_k(z)$. We denote that

$$h_1(z) = 1, \qquad h_2(z) = \frac{(1+z)(1+z^2)}{z^3+2z^2+1},$$
$$h_{3,\sigma}(z) = \frac{(1+z)(1+z^{2\sigma})}{(1-z)(z^{2\sigma+1}+2z^{2\sigma}+1)}, \qquad h_{4,\sigma}(z) = \frac{(1+z^{2\sigma})}{(1-z)(1+2z^{2\sigma}-z^{2\sigma+1})}.$$

and

$$g_1(z) = \frac{z}{1+z}, \qquad g_2(z) = \frac{(1+z)^2(1+z^2)z^2}{(z^3+2z^2+1)^2},$$
$$g_{3,\sigma}(z) = \frac{(1+z)^2 z^{2\sigma}(1+z^{2\sigma})}{\left(z^{2\sigma+1}+2z^{2\sigma}+1\right)^2}, \qquad g_{4,\sigma}(z) = \frac{z^{2\sigma}(1+z^{2\sigma})}{\left(1+2z^{2\sigma}-z^{2\sigma+1}\right)^2}.$$

k	$q_{0,k}(z)$	R_k
2	$(4z-1)z$	$\{\frac{1}{4}\}$
3	$(16z-1)z^2$	$\{\frac{1}{16}\}$
4	$(144z^2-40z+1)z^3$	$\{\frac{1}{4},\frac{1}{36}\}$
5	$(1024z^2-80z+1)z^4$	$\{\frac{1}{16},\frac{1}{64}\}$
6	$(14400z^3-4144z^2+140z-1)z^5$	$\{\frac{1}{4},\frac{1}{36},\frac{1}{100}\}$
7	$(147456z^3-12544z^2+224z-1)z^6$	$\{\frac{1}{16},\frac{1}{64},\frac{1}{144}\}$
8	$(2822400z^4-826624z^3+31584z^2-336z+1)z^7$	$\{\frac{1}{4},\frac{1}{36},\frac{1}{100},\frac{1}{196}\}$
9	$(37748736z^4-3358720z^3+69888z^2-480z+1)z^8$	$\{\frac{1}{16},\frac{1}{64},\frac{1}{144},\frac{1}{256}\}$

Table 1: The polynomials $q_{0,k}(z)$ and their nonzero roots obtained by the MAPLE package `GFUN`.

When $j=1,2$, $g_j(0)=0$ and $g_j(z)$ are all rational functions. For fixed σ, $g_{j,\sigma}(0)=0$ and $g_{j,\sigma}(z)$ are rational functions when $j=3,4$. The four generating functions (eq.(1)-(4)) are of the form $h_j(z)\mathbf{F}_k(g_j(z))(j=1,2)$ and $h_{j,\sigma}(z)\mathbf{F}_k(g_{j,\sigma}(z))(j=3,4)$.

In the following, we will discuss the dominant singularities of our four generating functions (eq. (1)-(4)) by the following two propositions, when $2\le k\le 9, 1\le\sigma\le 10$. The Proposition 1 and Proposition 2 are vital tools for our singularity analysis in [3].

Proposition 1 *The four generating functions are all supercritical case [1], i.e. the singularities of* $h_j(z)$ $(h_{j,\sigma}(z))$ *and* $g_j(z)$ $(g_{j,\sigma}(z))$ *are not the dominant singularities of* $h_j(z)\mathbf{F}_k(g_j(z))(h_{j,\sigma}(z)\mathbf{F}_k(g_{j,\sigma}(z)))$*, when* $2\le k\le 9, 1\le\sigma\le 10$*.*

Proposition 2 *The minimum positive real solutions of the equations*

$$g_j(z)=\rho_k^2 \text{ and } g_{j,\sigma}(z)=\rho_k^2 \tag{7}$$

are respectively the unique dominant singularities of

$$h_j(z)\mathbf{F}_k(g_j(z)) \text{ and } h_{j,\sigma}(z)\mathbf{F}_k(g_{j,\sigma}(z)), \tag{8}$$

when $2\le k\le 9, 1\le\sigma\le 10$*.*

Proof of Proposition 1.

We observe that $h_1(z)$ is analytic and all the poles of $h_2(z)$ are the poles of $g_2(z)$. All the poles of $h_{j,\sigma}(z)$ are the poles of $g_{j,\sigma}(z)(j=3,4)$ except at $z=1$. Let $\gamma_{k_{j,\sigma}}$ be the minimum positive real solution of $g_{j,\sigma}(z)=\rho_k^2$ and it's a singularity of $h_{j,\sigma}(z)\mathbf{F}_k(g_{j,\sigma}(z))$. In Table 4-5, we find that $\gamma_{k_{j,\sigma}}$ are all smaller than 1, where $2\le k\le 9, 1\le\sigma\le 10$. Then $z=1$ can not be the dominant singularity of $h_{j,\sigma}(z)\mathbf{F}_k(g_{j,\sigma}(z))(j=3,4)$. So we only have to discuss the poles of $g_j(z)(j=1,2)$ and $g_{j,\sigma}(z)(j=3,4)$. Observing Table 2 and Table 3-5, the poles of $g_j(z)(j=1,2)$ and $g_{j,\sigma}(z)(j=3,4)$ are all with larger module than the minimum positive solutions of $g_j(z)=\rho_k^2$ and $g_{j,\sigma}(z)=\rho_k^2$ except $g_{4,\sigma}(z)$ when $k=2$. When $k=2$, we have that

$$\mathbf{F}_2(z)=\sum_{n\ge 0} f_2(2n,0)z^n=\frac{2}{1+\sqrt{1-4\,z}}. \tag{9}$$

and then

$$\begin{aligned} h_{4,\sigma}(z)\mathbf{F}_2(g_{4,\sigma}(z)) &= \frac{(1+z^{2\sigma})}{(1-z)(1+2z^{2\sigma}-z^{2\sigma+1})}\mathbf{F}_2\left(\frac{z^{2\sigma}(1+z^{2\sigma})}{(1+2z^{2\sigma}-z^{2\sigma+1})^2}\right) \\ &= \frac{1+2z^{2\sigma}-z^{2\sigma+1}-\sqrt{(1+2z^{2\sigma}-z^{2\sigma+1})^2-4z^{2\sigma}(1+z^{2\sigma})}}{2(1-z)z^{2\sigma}}. \end{aligned}$$

Following the above equations, the poles of $g_{4,\sigma}(z)$ are not the singularities of $h_{4,\sigma}(z)\mathbf{F}_2(g_{4,\sigma}(z))$. Thus the poles of $g_j(z)(j=1,2)$ and $g_{j,\sigma}(z)(j=3,4)$ can not be dominant singularities of $h_j(z)\mathbf{F}_k(g_j(z))$ and $h_{j,\sigma}(z)\mathbf{F}_k(g_{j,\sigma}(z))$.

Proof of Proposition 2.

Proposition 1 implies that the dominant singularities of the generating functions eq.(1)-(4) are from the solutions of $g_j(z)=\rho$, where ρ is a singularity of $F_k(z)$. The singularities set of $F_k(z)(2\le k\le 9)$ is contained in the set

$$\{\rho_i^2|\rho_i=1/(2i-2),\, i\equiv k \mod 2,\, 2\le i\le k\}.$$

Observing Table 3-5, all the minimum positive solutions of

$$g_j(z)=\rho_i^2(j=1,2) \text{ and } g_{j,\sigma}(z)=\rho_i^2(j=3,4)$$

are decreasing as i increases when $2\le i\le 9$. All the minimum positive solutions of

$$g_j(z)=\rho_i^2(j=1,2) \text{ and } g_{j,\sigma}(z)=\rho_i^2(j=3,4)$$

are also the solutions of minimum module. We have checked it by the MAPLE for $2 \leq k \leq 9$ and $1 \leq \sigma \leq 10$. Here we only show the checking result for $g_{4,2}(z)$ as an example in Table 6. Thus the Proposition follows.

$g_1(z)$	1	$g_2(z)$	0.67335		
σ	1	2	3	4	5
$g_{j,\sigma}(z)(j=3,4)$	0.67335	0.78486	0.84380	0.87789	0.89990
σ	6	7	8	9	10
$g_{j,\sigma}(z)(j=3,4)$	0.91523	0.92651	0.93515	0.94198	0.94751

Table 2: The minimum modules of the poles of $g_j(z)(j=1,2)$ and $g_{j,\sigma}(z)(j=3,4)$ obtained by the MAPLE.

j/k	2	3	4	5	6	7	8	9
1	0.33333	0.06667	0.02857	0.01587	0.01010	0.00699	0.00513	0.00392
2	0.47804	0.22160	0.15024	0.11452	0.09276	0.07804	0.06739	0.05932

Table 3: The minimum positive solution of $g_j(z) = \rho_k^2$ obtained by the MAPLE.

σ/k	2	3	4	5	6	7	8	9
1	0.47804	0.22160	0.15024	0.11452	0.09276	0.07804	0.06739	0.05932
2	0.63716	0.43147	0.35576	0.31135	0.28095	0.25835	0.24064	0.22627
3	0.72215	0.55430	0.48638	0.44451	0.41480	0.39208	0.37386	0.35877
4	0.77494	0.63386	0.57388	0.53595	0.50855	0.48729	0.47005	0.45562
5	0.81088	0.68943	0.63619	0.60198	0.57699	0.55744	0.54147	0.52802
6	0.83693	0.73040	0.68271	0.65173	0.62893	0.61099	0.59626	0.58380
7	0.85668	0.76184	0.71873	0.69051	0.66962	0.65311	0.63951	0.62798
8	0.87216	0.78672	0.74743	0.72155	0.70232	0.68707	0.67447	0.66377
9	0.88462	0.80690	0.77083	0.74696	0.72917	0.71502	0.70330	0.69333
10	0.89487	0.82360	0.79027	0.76814	0.75159	0.73840	0.72747	0.71814

Table 4: The minimum positive solution of $g_{3,\sigma}(z) = \rho_k^2$ obtained by the MAPLE.

σ/k	2	3	4	5	6	7	8	9
1	0.66119	0.27209	0.17322	0.12778	0.10143	0.08417	0.07196	0.06285
2	0.78998	0.51681	0.41468	0.35679	0.31813	0.28990	0.26811	0.25061
3	0.84798	0.64205	0.55530	0.50265	0.46578	0.43787	0.41568	0.39742
4	0.88090	0.71631	0.64286	0.59674	0.56367	0.53819	0.51763	0.50049
5	0.90211	0.76521	0.70201	0.66151	0.63206	0.60912	0.59045	0.57477
6	0.91691	0.79979	0.74450	0.70859	0.68223	0.66155	0.64461	0.63032
7	0.92782	0.82552	0.77644	0.74427	0.72049	0.70174	0.68632	0.67326
8	0.93620	0.84540	0.80132	0.77221	0.75060	0.73349	0.71937	0.70738
9	0.94284	0.86122	0.82123	0.79468	0.77489	0.75917	0.74617	0.73511
10	0.94823	0.87411	0.83753	0.81313	0.79489	0.78037	0.76833	0.75808

Table 5: The minimum positive solution of $g_{4,\sigma}(z) = \rho_k^2$ obtained by the MAPLE.

k	$g_{4,2}(z)=\rho_k^2$	$\lvert z\rvert$
2	0.7899834629	0.7899834629
	4.007748508	4.007748508
	$0.1741659102 \pm 0.7791518559i$	0.7983804725
	$-0.7489564472 \pm 0.3474880105i$	0.8256413733
	$-0.5194671926 \pm 0.7094460554i$	0.8792950982
	$0.6953917442 \pm 0.6757271017i$	0.9696271417
3	0.5168065030	0.5168065030
	-0.5403154532	0.5403154532
	-2.054586126	2.054586126
	6.002310955	6.002310955
	$0.01143117447 \pm 0.5262310009i$	0.5263551444
	$0.7062440430 \pm 0.6980608304i$	0.9930103581
	$-0.6797831569 \pm 0.7751476138i$	1.030999012
4	0.4146753010	0.4146753010
	-0.4201242326	0.4201242326
	-4.007741068	4.007741068
	8.000976041	8.000976041
	$0.002717904815 \pm 0.4172390276i$	0.4172478798
	$0.7069347120 \pm 0.7030499483i$	0.9970134988
	$-0.7035456379 \pm 0.7344425990i$	1.017045916
5	0.3567930712	0.3567930712
	-0.3589278368	0.3589278368
	-6.002310659	6.002310659
	10.00049989	10.00049989
	$0.001066847717 \pm 0.3578317116i$	0.3578333020
	$0.7070522457 \pm 0.7048209520i$	0.9983463590
	$-0.7061463261 \pm 0.7215825908i$	1.009615803
6	0.3181284151	0.3181284151
	-0.3191862050	0.3191862050
	-8.000976012	8.000976012
	12.00028932	12.00028932
	$0.0005288129886 \pm 0.3186493927i$	0.3186498315
	$0.7070844327 \pm 0.7056430846i$	0.9989497274
	$-0.7067410054 \pm 0.7161041474i$	1.006125240
7	0.2899027828	0.2899027828
	-0.2905043531	0.2905043531
	-10.00049989	10.00049989
	14.00018221	14.00018221
	$0.0003007669815 \pm 0.2902007580i$	0.2902009139
	$0.7070960016 \pm 0.7060901061i$	0.9992737330
	$-0.7069371435 \pm 0.7132554379i$	1.004237743

Table 6: The solutions of $g_{4,2}(z)=\rho_k^2 (2\le k\le 7)$ and their modulus.

References

[1] P. Flajolet, R. Sedgewick, Analytic combinatorics, Cambridge University Press, New York, 2009.

[2] R. Stanley, Differentiably finite power series, Europ. J. Combinatorics, 1 (1980) 175–188.

[3] C.M. Reidys, R.R. Wang, Shapes of RNA pseudoknot structures, submitted.