

**(\* Asymptotic expected number of hairpins in saturated structures, theta=1,p=1,using results from earlier version of paper \*)**

**(\*We first compute the dominant singularity and asymptotic number of saturated structures, using Drmota–Lalley–Woods Theorem. \*)**

```
eqn = {S == DO + NO, DO == z + z^2,
      NO == R DO + DO z^2 + NO z^2 + S DO z^2 + S NO z^2, R == DO z^2 + NO z^2 + R DO z^2 + R NO z^2};
Last[First[First[Solve[eqn, {S, DO, NO, R}]]]];
Eliminate[eqn, {NO, DO, R}]
F = S^3 z^4 + S (1 - z^2) + S^2 z^2 (-2 + z^2) - z (1 + z) + S;
NSolve[{F == S, D[F, S] == 1}, {z, S}]
z0 = 0.42468731042028074^;
y0 = 1.6568963458689865^;
dFdzOfz0S0 = D[F, z] /. {z -> z0, S -> y0}
d2FdYOfz0S0 = D[F, {S, 2}] /. {z -> z0, S -> y0}
c = Sqrt[z0 dFdzOfz0S0 / (2 Pi d2FdYOfz0S0)]
AsymptoticValue = c * (1 / z0) ^ n n ^ (-3 / 2)
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**(\*Now, we compute mean,variance using Drmota's Theorem\*)**

```
(*S = z + z^2 + R*(z+z^2) + (z+z^2)u z^2 + (S-z-z^2)z^2 + S(z+z^2) u z^2 + S
(S-z -z^2) z^2;
R = u z^2(z+z^2) + z^2 (S-z-z^2) +R(z+z^2)u z^2 + R(S-z-z^2) z^2;
*)
Clear[R, F, S, eqn, NO, DO, F, z0, y0, c];
(*Equation (5) from paper, written in form R = .... *)
sol =
  Solve[R == u z^2 (z + z^2) + z^2 (S - z - z^2) + R (z + z^2) u z^2 + R (S - z - z^2) z^2, R];
(* Now it follows that R = Last[Last[Last[sol]]]*)
(* Equation (4) from paper, written in form S = .... *)
rightSideOfS = z + z^2 + R * (z + z^2) +
  (z + z^2) u z^2 + (S - z - z^2) z^2 + S (z + z^2) u z^2 + S (S - z - z^2) z^2
(* Now replace R in right side of equation by previous expression "sol"*)
rightSideOfS /. R -> Last[Last[Last[sol]]]
(* The following is the functional relation which satisfies y =
  F(z,y,u) where y is S*)
(* We now follow Drmota's paper "Systems of Functional Equations",
  where his x,y,z are our z,S,u*)
F = %
f = (F /. S -> s)
s - f
(* express over a common denominator*)
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```

Together[s - f]
dfs = D[f, s]
1 - dfs
(* express over a common denominator*)
Together[1 - dfs]
(* a is numerator of s-f, and b is numerator of 1-dfs,
where both have identical denominators *)
a = (-1 + s z^2 - z^3 + u z^3 - z^4 + u z^4)
(-s + z + z^2 + s z^2 + 2 s^2 z^2 - z^3 - 2 s z^3 + u z^3 + 2 s u z^3 - z^4 - 2 s z^4 - s^2 z^4 - s^3 z^4 + u z^4 + 2 s u z^4 +
2 s z^5 + 2 s^2 z^5 - 2 s u z^5 - 2 s^2 u z^5 - z^6 + s z^6 + 2 s^2 z^6 + 2 u z^6 - 2 s^2 u z^6 - u^2 z^6 - s u^2 z^6 -
2 z^7 - 2 s z^7 + 4 u z^7 + 4 s u z^7 - 2 u^2 z^7 - 2 s u^2 z^7 - z^8 - s z^8 + 2 u z^8 + 2 s u z^8 - u^2 z^8 - s u^2 z^8);
b = (1 - z^2 - 4 s z^2 + 2 z^3 - 3 u z^3 + 2 z^4 + 2 s z^4 + 5 s^2 z^4 - 3 u z^4 - 2 z^5 - 8 s z^5 + 2 u z^5 + 8 s u z^5 +
z^6 - 8 s z^6 - s^2 z^6 - 2 s^3 z^6 - 4 u z^6 + 8 s u z^6 + 3 u^2 z^6 + 6 z^7 + 2 s z^7 + 5 s^2 z^7 - 12 u z^7 - 2 s u z^7 -
5 s^2 u z^7 + 6 u^2 z^7 + 2 z^8 - 2 s z^8 + 5 s^2 z^8 - 4 u z^8 + 6 s u z^8 - 5 s^2 u z^8 + 2 u^2 z^8 - 4 s u^2 z^8 - z^9 -
8 s z^9 + u z^9 + 16 s u z^9 + u^2 z^9 - 8 s u^2 z^9 - u^3 z^9 + 2 z^10 - 4 s z^10 - 7 u z^10 + 8 s u z^10 + 8 u^2 z^10 -
4 s u^2 z^10 - 3 u^3 z^10 + 3 z^11 - 9 u z^11 + 9 u^2 z^11 - 3 u^3 z^11 + z^12 - 3 u z^12 + 3 u^2 z^12 - u^3 z^12);
CellPrint["Now compute the resultant of numerators a,b to get relation between S,u,z"]

(*We compute resultant of numerators,
since we have Resultant[S-F,1-D[F,S],S]=0 which is not much use.*)
res = Resultant[a, b, s]
(* Replace z by z[u], a function of u *)
res /. z -> z[u];
(* Now compute z'[u] *)
dres = D[%, u]
dzu = Last[Last[Last[Solve[dres == 0, z'[u]]]]];
(*z[1] equals rho, the dominant singularity *)
rho = 0.42468731042028074`
dzuEvaluatedAt1 = (dzu /. u -> 1) /. z[1] -> rho
CellPrint[
"According to Drmota's Theorem 1, the mean equals -z'[1]/z[1], computed next. "]
mu = ((-dzu / z[u] /. u -> 1) /. z[1] -> rho)

(*Variance computation *)
CellPrint["Now compute variance, which by Drmota is -z''[1]/z[1] + mu^2 + mu"]
(* d2zu is z''[1] *)
d2zu = (((D[dzu, u] /. u -> 1) /. z[1] -> rho) /. z'[1] -> dzuEvaluatedAt1)
var = -d2zu / rho + mu * mu + mu

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$$S^3 z^4 + S(1 - z^2) + S^2 z^2(-2 + z^2) = z(1 + z)$$

```

{{z -> 3.2141, S -> -0.587227}, {z -> -0.854537, S -> 0.988667},
{z -> 0.424687, S -> 1.6569}, {z -> -2.29493, S -> -0.513379},
{z -> -1., S -> 0.}, {z -> -0.244657 + 0.5601 i, S -> -0.741229 + 0.680476 i},
{z -> -0.244657 - 0.5601 i, S -> -0.741229 - 0.680476 i}}

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-5.68551

-0.33299

1.07427

1.07427 × 2.35467<sup>n</sup>

$n^{3/2}$

$$z + z^2 + z^2(S - z - z^2) + S z^2(S - z - z^2) + R(z + z^2) + u z^2(z + z^2) + S u z^2(z + z^2)$$

$$z + z^2 + z^2(S - z - z^2) + S z^2(S - z - z^2) +$$

$$u z^2(z + z^2) + S u z^2(z + z^2) + \frac{(z + z^2)(-S z^2 + z^3 - u z^3 + z^4 - u z^4)}{-1 + S z^2 - z^3 + u z^3 - z^4 + u z^4}$$

$$\begin{aligned}
 & z + z^2 + z^2 (S - z - z^2) + S z^2 (S - z - z^2) + \\
 & u z^2 (z + z^2) + S u z^2 (z + z^2) + \frac{(z + z^2) (-S z^2 + z^3 - u z^3 + z^4 - u z^4)}{-1 + S z^2 - z^3 + u z^3 - z^4 + u z^4} \\
 & z + z^2 + z^2 (s - z - z^2) + s z^2 (s - z - z^2) + \\
 & u z^2 (z + z^2) + s u z^2 (z + z^2) + \frac{(z + z^2) (-s z^2 + z^3 - u z^3 + z^4 - u z^4)}{-1 + s z^2 - z^3 + u z^3 - z^4 + u z^4} \\
 & s - z - z^2 - z^2 (s - z - z^2) - s z^2 (s - z - z^2) - \\
 & u z^2 (z + z^2) - s u z^2 (z + z^2) - \frac{(z + z^2) (-s z^2 + z^3 - u z^3 + z^4 - u z^4)}{-1 + s z^2 - z^3 + u z^3 - z^4 + u z^4} \\
 & \frac{1}{-1 + s z^2 - z^3 + u z^3 - z^4 + u z^4} \\
 & (-s + z + z^2 + s z^2 + 2 s^2 z^2 - z^3 - 2 s z^3 + u z^3 + 2 s u z^3 - z^4 - 2 s z^4 - s^2 z^4 - s^3 z^4 + u z^4 + 2 s u z^4 + \\
 & 2 s z^5 + 2 s^2 z^5 - 2 s u z^5 - 2 s^2 u z^5 - z^6 + s z^6 + 2 s^2 z^6 + 2 u z^6 - 2 s^2 u z^6 - u^2 z^6 - s u^2 z^6 - \\
 & 2 z^7 - 2 s z^7 + 4 u z^7 + 4 s u z^7 - 2 u^2 z^7 - 2 s u^2 z^7 - z^8 - s z^8 + 2 u z^8 + 2 s u z^8 - u^2 z^8 - s u^2 z^8) \\
 & \frac{z^2 + s z^2 + z^2 (s - z - z^2) + u z^2 (z + z^2) - z^2 (z + z^2) (-s z^2 + z^3 - u z^3 + z^4 - u z^4)}{(-1 + s z^2 - z^3 + u z^3 - z^4 + u z^4)^2} - \frac{z^2 (z + z^2)}{-1 + s z^2 - z^3 + u z^3 - z^4 + u z^4} \\
 & \frac{1 - z^2 - s z^2 - z^2 (s - z - z^2) - u z^2 (z + z^2) + z^2 (z + z^2) (-s z^2 + z^3 - u z^3 + z^4 - u z^4)}{(-1 + s z^2 - z^3 + u z^3 - z^4 + u z^4)^2} + \frac{z^2 (z + z^2)}{-1 + s z^2 - z^3 + u z^3 - z^4 + u z^4} \\
 & \frac{1}{(-1 + s z^2 - z^3 + u z^3 - z^4 + u z^4)^2} \\
 & (1 - z^2 - 4 s z^2 + 2 z^3 - 3 u z^3 + 2 z^4 + 2 s z^4 + 5 s^2 z^4 - 3 u z^4 - 2 z^5 - 8 s z^5 + 2 u z^5 + 8 s u z^5 + z^6 - \\
 & 8 s z^6 - s^2 z^6 - 2 s^3 z^6 - 4 u z^6 + 8 s u z^6 + 3 u^2 z^6 + 6 z^7 + 2 s z^7 + 5 s^2 z^7 - 12 u z^7 - 2 s u z^7 - \\
 & 5 s^2 u z^7 + 6 u^2 z^7 + 2 z^8 - 2 s z^8 + 5 s^2 z^8 - 4 u z^8 + 6 s u z^8 - 5 s^2 u z^8 + 2 u^2 z^8 - 4 s u^2 z^8 - z^9 - \\
 & 8 s z^9 + u z^9 + 16 s u z^9 + u^2 z^9 - 8 s u^2 z^9 - u^3 z^9 + 2 z^{10} - 4 s z^{10} - 7 u z^{10} + 8 s u z^{10} + 8 u^2 z^{10} - \\
 & 4 s u^2 z^{10} - 3 u^3 z^{10} + 3 z^{11} - 9 u z^{11} + 9 u^2 z^{11} - 3 u^3 z^{11} + z^{12} - 3 u z^{12} + 3 u^2 z^{12} - u^3 z^{12})
 \end{aligned}$$

Now compute the resultant of numerators a,b to get relation between S,u,z

$$\begin{aligned}
 & (z^9 + z^{10}) \\
 & (4 z^{18} + 9 z^{19} - z^{20} - 29 z^{21} - 12 u z^{21} - 57 z^{22} - 38 u z^{22} - 46 z^{23} - 46 u z^{23} + 18 z^{24} - 58 u z^{24} + 12 u^2 z^{24} + \\
 & 91 z^{25} - 132 u z^{25} + 49 u^2 z^{25} + 135 z^{26} - 218 u z^{26} + 87 u^2 z^{26} + 139 z^{27} - 246 u z^{27} + 111 u^2 z^{27} - 4 u^3 z^{27} + \\
 & 117 z^{28} - 242 u z^{28} + 145 u^2 z^{28} - 20 u^3 z^{28} + 88 z^{29} - 216 u z^{29} + 168 u^2 z^{29} - 40 u^3 z^{29} + 52 z^{30} - 144 u z^{30} + \\
 & 132 u^2 z^{30} - 40 u^3 z^{30} + 20 z^{31} - 60 u z^{31} + 60 u^2 z^{31} - 20 u^3 z^{31} + 4 z^{32} - 12 u z^{32} + 12 u^2 z^{32} - 4 u^3 z^{32})
 \end{aligned}$$

$$\begin{aligned}
& (4 z[u]^{18} + 9 z[u]^{19} - z[u]^{20} - 29 z[u]^{21} - 12 u z[u]^{21} - 57 z[u]^{22} - 38 u z[u]^{22} - 46 z[u]^{23} - 46 u z[u]^{23} + \\
& 18 z[u]^{24} - 58 u z[u]^{24} + 12 u^2 z[u]^{24} + 91 z[u]^{25} - 132 u z[u]^{25} + 49 u^2 z[u]^{25} + 135 z[u]^{26} - \\
& 218 u z[u]^{26} + 87 u^2 z[u]^{26} + 139 z[u]^{27} - 246 u z[u]^{27} + 111 u^2 z[u]^{27} - 4 u^3 z[u]^{27} + \\
& 117 z[u]^{28} - 242 u z[u]^{28} + 145 u^2 z[u]^{28} - 20 u^3 z[u]^{28} + 88 z[u]^{29} - 216 u z[u]^{29} + \\
& 168 u^2 z[u]^{29} - 40 u^3 z[u]^{29} + 52 z[u]^{30} - 144 u z[u]^{30} + 132 u^2 z[u]^{30} - 40 u^3 z[u]^{30} + 20 z[u]^{31} - \\
& 60 u z[u]^{31} + 60 u^2 z[u]^{31} - 20 u^3 z[u]^{31} + 4 z[u]^{32} - 12 u z[u]^{32} + 12 u^2 z[u]^{32} - 4 u^3 z[u]^{32}) \\
& (9 z[u]^8 \text{Derivative}[1][z][u] + 10 z[u]^9 \text{Derivative}[1][z][u]) + \\
& (z[u]^9 + z[u]^{10}) (-12 z[u]^{21} - 38 z[u]^{22} - 46 z[u]^{23} - 58 z[u]^{24} + 24 u z[u]^{24} - 132 z[u]^{25} + \\
& 98 u z[u]^{25} - 218 z[u]^{26} + 174 u z[u]^{26} - 246 z[u]^{27} + 222 u z[u]^{27} - 12 u^2 z[u]^{27} - 242 z[u]^{28} + \\
& 290 u z[u]^{28} - 60 u^2 z[u]^{28} - 216 z[u]^{29} + 336 u z[u]^{29} - 120 u^2 z[u]^{29} - 144 z[u]^{30} + \\
& 264 u z[u]^{30} - 120 u^2 z[u]^{30} - 60 z[u]^{31} + 120 u z[u]^{31} - 60 u^2 z[u]^{31} - 12 z[u]^{32} + 24 u z[u]^{32} - \\
& 12 u^2 z[u]^{32} + 72 z[u]^{17} \text{Derivative}[1][z][u] + 171 z[u]^{18} \text{Derivative}[1][z][u] - \\
& 20 z[u]^{19} \text{Derivative}[1][z][u] - 609 z[u]^{20} \text{Derivative}[1][z][u] - \\
& 252 u z[u]^{20} \text{Derivative}[1][z][u] - 1254 z[u]^{21} \text{Derivative}[1][z][u] - \\
& 836 u z[u]^{21} \text{Derivative}[1][z][u] - 1058 z[u]^{22} \text{Derivative}[1][z][u] - \\
& 1058 u z[u]^{22} \text{Derivative}[1][z][u] + 432 z[u]^{23} \text{Derivative}[1][z][u] - \\
& 1392 u z[u]^{23} \text{Derivative}[1][z][u] + 288 u^2 z[u]^{23} \text{Derivative}[1][z][u] + \\
& 2275 z[u]^{24} \text{Derivative}[1][z][u] - 3300 u z[u]^{24} \text{Derivative}[1][z][u] + \\
& 1225 u^2 z[u]^{24} \text{Derivative}[1][z][u] + 3510 z[u]^{25} \text{Derivative}[1][z][u] - \\
& 5668 u z[u]^{25} \text{Derivative}[1][z][u] + 2262 u^2 z[u]^{25} \text{Derivative}[1][z][u] + \\
& 3753 z[u]^{26} \text{Derivative}[1][z][u] - 6642 u z[u]^{26} \text{Derivative}[1][z][u] + \\
& 2997 u^2 z[u]^{26} \text{Derivative}[1][z][u] - 108 u^3 z[u]^{26} \text{Derivative}[1][z][u] + \\
& 3276 z[u]^{27} \text{Derivative}[1][z][u] - 6776 u z[u]^{27} \text{Derivative}[1][z][u] + \\
& 4060 u^2 z[u]^{27} \text{Derivative}[1][z][u] - 560 u^3 z[u]^{27} \text{Derivative}[1][z][u] + \\
& 2552 z[u]^{28} \text{Derivative}[1][z][u] - 6264 u z[u]^{28} \text{Derivative}[1][z][u] + \\
& 4872 u^2 z[u]^{28} \text{Derivative}[1][z][u] - 1160 u^3 z[u]^{28} \text{Derivative}[1][z][u] + \\
& 1560 z[u]^{29} \text{Derivative}[1][z][u] - 4320 u z[u]^{29} \text{Derivative}[1][z][u] + \\
& 3960 u^2 z[u]^{29} \text{Derivative}[1][z][u] - 1200 u^3 z[u]^{29} \text{Derivative}[1][z][u] + \\
& 620 z[u]^{30} \text{Derivative}[1][z][u] - 1860 u z[u]^{30} \text{Derivative}[1][z][u] + \\
& 1860 u^2 z[u]^{30} \text{Derivative}[1][z][u] - 620 u^3 z[u]^{30} \text{Derivative}[1][z][u] + \\
& 128 z[u]^{31} \text{Derivative}[1][z][u] - 384 u z[u]^{31} \text{Derivative}[1][z][u] + \\
& 384 u^2 z[u]^{31} \text{Derivative}[1][z][u] - 128 u^3 z[u]^{31} \text{Derivative}[1][z][u])
\end{aligned}$$

0.424687

-0.0523188

According to Drmota's Theorem 1, the mean equals  $-z'[1]/z[1]$ , computed next.

0.123194

Now compute variance, which by Drmota is  $-z''[1]/z[1] + \mu^2 + \mu$

0.0442454

0.0341867