

(* Asymptotic expected number of hairpins in saturated structures with theta=1 and p=1/2 *)

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

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Clear["*"]
Clear[p, S, D0, N0, z, R, eqn0, eqn, F, z0, y0, dFdzoFz0S0, d2FdzoFz0S0];
p = 1 / 2;
eqn = {S == D0 + N0, D0 == z + z^2, N0 == R D0 + p D0 z^2 + p N0 z^2 + p S D0 z^2 + p S N0 z^2,
  R == p D0 z^2 + p N0 z^2 + p R D0 z^2 + p R N0 z^2}
Eliminate[eqn, {N0, D0, R}]
F = (S^3 z^4 + S^2 z^2 (-4 + z^2) - z (4 + 4 z)) / (-1 (4 - 2 z^2))
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NSolve[{F == S, D[F, S] == 1}, {z, S}];
z0 = 0.5343653037924583`
y0 = 2.1489053808896275`
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dFdzoFz0S0 = D[F, z] /. {z -> z0, S -> y0}
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d2FdzoFz0S0 = D[F, {S, 2}] /. {z -> z0, S -> y0}
c = Sqrt[z0 dFdzoFz0S0 / (2 Pi d2FdzoFz0S0)]
c * (1 / z0)^n n^(-3 / 2)
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$$\left\{ S = D0 + N0, D0 = z + z^2, N0 = D0 R + \frac{D0 z^2}{2} + \frac{N0 z^2}{2} + \frac{1}{2} D0 S z^2 + \frac{1}{2} N0 S z^2, \right.$$

$$\left. R = \frac{D0 z^2}{2} + \frac{N0 z^2}{2} + \frac{1}{2} D0 R z^2 + \frac{1}{2} N0 R z^2 \right\}$$

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

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

0.534365

2.14891

6.92169

0.312055

1.37347

$$\frac{1.37347 \times 1.87138^n}{n^{3/2}}$$

(*Now, we compute mean, variance using Drmota's Theorem*)

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Clear["*"]
Clear[p, rho, z0, y0, eqn, F, f, S, s, D0, N0, z, R, dfs, a, b]
p = 1/2;
eqn = {S == D0 + N0, D0 == z + z^2, N0 == R D0 + p u D0 z^2 + p N0 z^2 + p u S D0 z^2 + p S N0 z^2,
  R == p u D0 z^2 + p N0 z^2 + p u R D0 z^2 + p R N0 z^2}

CellPrint["Eliminate all variables except S,u,z"]
Eliminate[eqn, {D0, N0, R}]
Collect[%, S, Simplify]
F = (S^3 z^4 + S^2 z^2 (-4 + z^2 + 2 (-1 + u) z^3 + 2 (-1 + u) z^4) +
  z (1 + z) (-4 - 2 (-1 + u) z^2 + (-1 + u)^2 z^5 + (-1 + u)^2 z^6)) /
  (- (4 - 2 z^2 - 4 (-1 + u) z^3 - 4 (-1 + u) z^4 + 2 (-1 + u) z^5 + (-1 + u)^2 z^6 + 2 (-1 + u)^2 z^7 + (-1 + u)^2 z^8))

f = (F /. S -> s)
s - f
(* express over a common denominator*)
Together[s - f]
a = Numerator[%]

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 *)
b = Numerator[%]
(* a is numerator of s-f, and b is numerator of 1-dfs,
where both have identical denominators *)

If[Denominator[Together[s - f]] == Denominator[Together[1 - dfs]],
  CellPrint["Denominator of (s-f) same as that of (1-dfs)"],
  CellPrint["Denominator of (s-f) different than than of (1-dfs)"]]

(* NOTE: denominators of both expressions s-f and 1-dfs is the same *)
CellPrint["Now compute the resultant of numerators a,b to get relation between S,u,z"]

(* res =Resultant[s-f,1-dfs,s] *)

(*We compute resultant of numerators,
since we have Resultant[S-F,1-D[F,S],S]=0 which is not much use.*)
CellPrint["Express S-F and 1-D[F,S] as fractions over the same common denominator"]
CellPrint["Then compute the resultant of the numerators of these expressions"]
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]
Simplify[Collect[dres, z'[u]]]
Solve[dres == 0, z'[u]]
dzu = Last[Last[Last[Solve[dres == 0, z'[u]]]]];
(*z[1] equals rho, the dominant singularity *)

rho = 0.5343653037924583`;
(* value of z0 in the first part of this file, the dominant singularity*)
dzuEvaluatedAt1 = (dzu /. u -> 1) /. z[1] -> rho
CellPrint[

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

$\mu = ((-dz[u] / z[u] /. u \rightarrow 1) /. z[1] \rightarrow \rho)$

(*Variance computation *)

(* d2zu is z''[1] *)

$d2zu = ((D[dz[u], u] /. u \rightarrow 1) /. z[1] \rightarrow \rho) /. z'[1] \rightarrow dz[u]_{evaluatedAt1}$

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

$var = -d2zu / \rho + \mu * \mu + \mu$

$$\left\{ \begin{aligned} S &= D0 + N0, D0 = z + z^2, N0 = D0 R + \frac{N0 z^2}{2} + \frac{1}{2} N0 S z^2 + \frac{1}{2} D0 u z^2 + \frac{1}{2} D0 S u z^2, \\ R &= \frac{N0 z^2}{2} + \frac{1}{2} N0 R z^2 + \frac{1}{2} D0 u z^2 + \frac{1}{2} D0 R u z^2 \end{aligned} \right\}$$

Eliminate all variables except S,u,z

$$\begin{aligned} &S^3 z^4 + S^2 z^2 (-4 + z^2 - 2 z^3 + 2 u z^3 - 2 z^4 + 2 u z^4) + \\ &S (4 - 2 z^2 + 4 z^3 - 4 u z^3 + 4 z^4 - 4 u z^4 - 2 z^5 + 2 u z^5 - z^6 + \\ &u^2 z^6 + 2 z^7 - 4 u z^7 + 2 u^2 z^7 + z^8 - 2 u z^8 + u^2 z^8) = \\ &z (4 + 4 z - 2 z^2 + 2 u z^2 - 2 z^3 + 2 u z^3 - z^5 + 2 u z^5 - u^2 z^5 - 2 z^6 + 4 u z^6 - 2 u^2 z^6 - z^7 + 2 u z^7 - u^2 z^7) \\ &S^3 z^4 + S^2 z^2 (-4 + z^2 + 2 (-1 + u) z^3 + 2 (-1 + u) z^4) + \\ &S (4 - 2 z^2 - 4 (-1 + u) z^3 - 4 (-1 + u) z^4 + 2 (-1 + u) z^5 + (-1 + u^2) z^6 + 2 (-1 + u)^2 z^7 + (-1 + u)^2 z^8) = \\ &-z (1 + z) (-4 - 2 (-1 + u) z^2 + (-1 + u)^2 z^5 + (-1 + u)^2 z^6) \\ &(S^3 z^4 + S^2 z^2 (-4 + z^2 + 2 (-1 + u) z^3 + 2 (-1 + u) z^4) + \\ &z (1 + z) (-4 - 2 (-1 + u) z^2 + (-1 + u)^2 z^5 + (-1 + u)^2 z^6)) / \\ &(-4 + 2 z^2 + 4 (-1 + u) z^3 + 4 (-1 + u) z^4 - 2 (-1 + u) z^5 - (-1 + u^2) z^6 - 2 (-1 + u)^2 z^7 - (-1 + u)^2 z^8) \\ &(s^3 z^4 + s^2 z^2 (-4 + z^2 + 2 (-1 + u) z^3 + 2 (-1 + u) z^4) + \\ &z (1 + z) (-4 - 2 (-1 + u) z^2 + (-1 + u)^2 z^5 + (-1 + u)^2 z^6)) / \\ &(-4 + 2 z^2 + 4 (-1 + u) z^3 + 4 (-1 + u) z^4 - 2 (-1 + u) z^5 - (-1 + u^2) z^6 - 2 (-1 + u)^2 z^7 - (-1 + u)^2 z^8) \\ &s - (s^3 z^4 + s^2 z^2 (-4 + z^2 + 2 (-1 + u) z^3 + 2 (-1 + u) z^4) + \\ &z (1 + z) (-4 - 2 (-1 + u) z^2 + (-1 + u)^2 z^5 + (-1 + u)^2 z^6)) / \\ &(-4 + 2 z^2 + 4 (-1 + u) z^3 + 4 (-1 + u) z^4 - 2 (-1 + u) z^5 - (-1 + u^2) z^6 - 2 (-1 + u)^2 z^7 - (-1 + u)^2 z^8) \\ &(4 s - 4 z - 4 z^2 - 2 s z^2 - 4 s^2 z^2 + 2 z^3 + 4 s z^3 - 2 u z^3 - 4 s u z^3 + 2 z^4 + 4 s z^4 + s^2 z^4 + s^3 z^4 - 2 u z^4 - \\ &4 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) / \\ &(4 - 2 z^2 + 4 z^3 - 4 u z^3 + 4 z^4 - 4 u z^4 - 2 z^5 + 2 u z^5 - z^6 + u^2 z^6 + 2 z^7 - 4 u z^7 + 2 u^2 z^7 + z^8 - 2 u z^8 + u^2 z^8) \\ &4 s - 4 z - 4 z^2 - 2 s z^2 - 4 s^2 z^2 + 2 z^3 + 4 s z^3 - 2 u z^3 - 4 s u z^3 + 2 z^4 + 4 s z^4 + s^2 z^4 + s^3 z^4 - 2 u z^4 - \\ &4 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) \\ &(3 s^2 z^4 + 2 s z^2 (-4 + z^2 + 2 (-1 + u) z^3 + 2 (-1 + u) z^4)) / \\ &(-4 + 2 z^2 + 4 (-1 + u) z^3 + 4 (-1 + u) z^4 - 2 (-1 + u) z^5 - (-1 + u^2) z^6 - 2 (-1 + u)^2 z^7 - (-1 + u)^2 z^8) \\ &1 - (3 s^2 z^4 + 2 s z^2 (-4 + z^2 + 2 (-1 + u) z^3 + 2 (-1 + u) z^4)) / \\ &(-4 + 2 z^2 + 4 (-1 + u) z^3 + 4 (-1 + u) z^4 - 2 (-1 + u) z^5 - (-1 + u^2) z^6 - 2 (-1 + u)^2 z^7 - (-1 + u)^2 z^8) \end{aligned}$$

$$\frac{(4 - 2z^2 - 8sz^2 + 4z^3 - 4uz^3 + 4z^4 + 2sz^4 + 3s^2z^4 - 4uz^4 - 2z^5 - 4sz^5 + 2uz^5 + 4su^2z^5 - z^6 - 4sz^6 + 4su^2z^6 + u^2z^6 + 2z^7 - 4uz^7 + 2u^2z^7 + z^8 - 2uz^8 + u^2z^8)}{(4 - 2z^2 + 4z^3 - 4uz^3 + 4z^4 - 4uz^4 - 2z^5 + 2uz^5 - z^6 + u^2z^6 + 2z^7 - 4uz^7 + 2u^2z^7 + z^8 - 2uz^8 + u^2z^8)} \\ 4 - 2z^2 - 8sz^2 + 4z^3 - 4uz^3 + 4z^4 + 2sz^4 + 3s^2z^4 - 4uz^4 - 2z^5 - 4sz^5 + 2uz^5 + 4su^2z^5 - z^6 - 4sz^6 + 4su^2z^6 + u^2z^6 + 2z^7 - 4uz^7 + 2u^2z^7 + z^8 - 2uz^8 + u^2z^8$$

Denominator of (s-f) same as that of (1-dfs)

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

Express S-F and 1-D[F,S] as fractions over the same common denominator

Then compute the resultant of the numerators of these expressions

$$\begin{aligned} & -128z^{11} - 144z^{12} + 96z^{13} + 352z^{14} + 192uz^{14} + 512z^{15} + 400uz^{15} + 220z^{16} + 256uz^{16} - 216z^{17} + \\ & 296uz^{17} - 96u^2z^{17} - 412z^{18} + 688uz^{18} - 292u^2z^{18} - 440z^{19} + 784uz^{19} - 344u^2z^{19} - 308z^{20} + \\ & 584uz^{20} - 292u^2z^{20} + 16u^3z^{20} - 208z^{21} + 480uz^{21} - 336u^2z^{21} + 64u^3z^{21} - 144z^{22} + 384uz^{22} - \\ & 336u^2z^{22} + 96u^3z^{22} - 64z^{23} + 192uz^{23} - 192u^2z^{23} + 64u^3z^{23} - 16z^{24} + 48uz^{24} - 48u^2z^{24} + 16u^3z^{24} \\ & -128z[u]^{11} - 144z[u]^{12} + 96z[u]^{13} + 352z[u]^{14} + 192uz[u]^{14} + 512z[u]^{15} + 400uz[u]^{15} + \\ & 220z[u]^{16} + 256uz[u]^{16} - 216z[u]^{17} + 296uz[u]^{17} - 96u^2z[u]^{17} - 412z[u]^{18} + \\ & 688uz[u]^{18} - 292u^2z[u]^{18} - 440z[u]^{19} + 784uz[u]^{19} - 344u^2z[u]^{19} - 308z[u]^{20} + \\ & 584uz[u]^{20} - 292u^2z[u]^{20} + 16u^3z[u]^{20} - 208z[u]^{21} + 480uz[u]^{21} - 336u^2z[u]^{21} + \\ & 64u^3z[u]^{21} - 144z[u]^{22} + 384uz[u]^{22} - 336u^2z[u]^{22} + 96u^3z[u]^{22} - 64z[u]^{23} + \\ & 192uz[u]^{23} - 192u^2z[u]^{23} + 64u^3z[u]^{23} - 16z[u]^{24} + 48uz[u]^{24} - 48u^2z[u]^{24} + 16u^3z[u]^{24} \\ & 192z[u]^{14} + 400z[u]^{15} + 256z[u]^{16} + 296z[u]^{17} - 192uz[u]^{17} + 688z[u]^{18} - 584uz[u]^{18} + 784z[u]^{19} - \\ & 688uz[u]^{19} + 584z[u]^{20} - 584uz[u]^{20} + 48u^2z[u]^{20} + 480z[u]^{21} - 672uz[u]^{21} + 192u^2z[u]^{21} + \\ & 384z[u]^{22} - 672uz[u]^{22} + 288u^2z[u]^{22} + 192z[u]^{23} - 384uz[u]^{23} + 192u^2z[u]^{23} + 48z[u]^{24} - \\ & 96uz[u]^{24} + 48u^2z[u]^{24} - 1408z[u]^{10} \text{Derivative}[1][z][u] - 1728z[u]^{11} \text{Derivative}[1][z][u] + \\ & 1248z[u]^{12} \text{Derivative}[1][z][u] + 4928z[u]^{13} \text{Derivative}[1][z][u] + \\ & 2688uz[u]^{13} \text{Derivative}[1][z][u] + 7680z[u]^{14} \text{Derivative}[1][z][u] + \\ & 6000uz[u]^{14} \text{Derivative}[1][z][u] + 3520z[u]^{15} \text{Derivative}[1][z][u] + \\ & 4096uz[u]^{15} \text{Derivative}[1][z][u] - 3672z[u]^{16} \text{Derivative}[1][z][u] + \\ & 5032uz[u]^{16} \text{Derivative}[1][z][u] - 1632u^2z[u]^{16} \text{Derivative}[1][z][u] - \\ & 7416z[u]^{17} \text{Derivative}[1][z][u] + 12384uz[u]^{17} \text{Derivative}[1][z][u] - \\ & 5256u^2z[u]^{17} \text{Derivative}[1][z][u] - 8360z[u]^{18} \text{Derivative}[1][z][u] + \\ & 14896uz[u]^{18} \text{Derivative}[1][z][u] - 6536u^2z[u]^{18} \text{Derivative}[1][z][u] - \\ & 6160z[u]^{19} \text{Derivative}[1][z][u] + 11680uz[u]^{19} \text{Derivative}[1][z][u] - \\ & 5840u^2z[u]^{19} \text{Derivative}[1][z][u] + 320u^3z[u]^{19} \text{Derivative}[1][z][u] - \\ & 4368z[u]^{20} \text{Derivative}[1][z][u] + 10080uz[u]^{20} \text{Derivative}[1][z][u] - \\ & 7056u^2z[u]^{20} \text{Derivative}[1][z][u] + 1344u^3z[u]^{20} \text{Derivative}[1][z][u] - \\ & 3168z[u]^{21} \text{Derivative}[1][z][u] + 8448uz[u]^{21} \text{Derivative}[1][z][u] - \\ & 7392u^2z[u]^{21} \text{Derivative}[1][z][u] + 2112u^3z[u]^{21} \text{Derivative}[1][z][u] - \\ & 1472z[u]^{22} \text{Derivative}[1][z][u] + 4416uz[u]^{22} \text{Derivative}[1][z][u] - \\ & 4416u^2z[u]^{22} \text{Derivative}[1][z][u] + 1472u^3z[u]^{22} \text{Derivative}[1][z][u] - \\ & 384z[u]^{23} \text{Derivative}[1][z][u] + 1152uz[u]^{23} \text{Derivative}[1][z][u] - \\ & 1152u^2z[u]^{23} \text{Derivative}[1][z][u] + 384u^3z[u]^{23} \text{Derivative}[1][z][u] \end{aligned}$$

$$\begin{aligned}
 & 8 z[u]^{10} (6 (-1 + u)^2 z[u]^{14} - 176 \text{Derivative}[1][z][u] - 216 z[u] \text{Derivative}[1][z][u] + \\
 & 156 z[u]^2 \text{Derivative}[1][z][u] + 56 (11 + 6 u) z[u]^3 \text{Derivative}[1][z][u] + \\
 & 24 (-1 + u)^2 z[u]^{13} (1 + 2 (-1 + u) \text{Derivative}[1][z][u]) + \\
 & 4 (-1 + u) z[u]^{12} (-12 + 9 u + 46 (-1 + u)^2 \text{Derivative}[1][z][u]) + \\
 & z[u]^{10} (73 - 73 u + 6 u^2 + 42 (-1 + u)^2 (-13 + 4 u) \text{Derivative}[1][z][u]) + \\
 & 6 z[u]^4 (4 + 5 (32 + 25 u) \text{Derivative}[1][z][u]) + z[u]^5 (50 + 8 (55 + 64 u) \text{Derivative}[1][z][u]) + \\
 & 12 (-1 + u) z[u]^{11} (-5 + 2 u + 11 (3 - 5 u + 2 u^2) \text{Derivative}[1][z][u]) + \\
 & z[u]^6 (32 - 17 (27 - 37 u + 12 u^2) \text{Derivative}[1][z][u]) + \\
 & z[u]^8 (86 - 73 u - 19 (55 - 98 u + 43 u^2) \text{Derivative}[1][z][u]) + \\
 & z[u]^7 (37 - 24 u - 9 (103 - 172 u + 73 u^2) \text{Derivative}[1][z][u]) + \\
 & 2 z[u]^9 (49 - 43 u + 5 (-77 + 146 u - 73 u^2 + 4 u^3) \text{Derivative}[1][z][u])
 \end{aligned}$$

$$\begin{aligned}
 & \{ \{ \text{Derivative}[1][z][u] \rightarrow \\
 & (-24 z[u]^4 - 50 z[u]^5 - 32 z[u]^6 - 37 z[u]^7 + 24 u z[u]^7 - 86 z[u]^8 + 73 u z[u]^8 - \\
 & 98 z[u]^9 + 86 u z[u]^9 - 73 z[u]^{10} + 73 u z[u]^{10} - 6 u^2 z[u]^{10} - 60 z[u]^{11} + \\
 & 84 u z[u]^{11} - 24 u^2 z[u]^{11} - 48 z[u]^{12} + 84 u z[u]^{12} - 36 u^2 z[u]^{12} - \\
 & 24 z[u]^{13} + 48 u z[u]^{13} - 24 u^2 z[u]^{13} - 6 z[u]^{14} + 12 u z[u]^{14} - 6 u^2 z[u]^{14}) / \\
 & (-176 - 216 z[u] + 156 z[u]^2 + 616 z[u]^3 + 336 u z[u]^3 + 960 z[u]^4 + 750 u z[u]^4 + \\
 & 440 z[u]^5 + 512 u z[u]^5 - 459 z[u]^6 + 629 u z[u]^6 - 204 u^2 z[u]^6 - 927 z[u]^7 + 1548 u z[u]^7 - \\
 & 657 u^2 z[u]^7 - 1045 z[u]^8 + 1862 u z[u]^8 - 817 u^2 z[u]^8 - 770 z[u]^9 + 1460 u z[u]^9 - \\
 & 730 u^2 z[u]^9 + 40 u^3 z[u]^9 - 546 z[u]^{10} + 1260 u z[u]^{10} - 882 u^2 z[u]^{10} + 168 u^3 z[u]^{10} - \\
 & 396 z[u]^{11} + 1056 u z[u]^{11} - 924 u^2 z[u]^{11} + 264 u^3 z[u]^{11} - 184 z[u]^{12} + 552 u z[u]^{12} - \\
 & 552 u^2 z[u]^{12} + 184 u^3 z[u]^{12} - 48 z[u]^{13} + 144 u z[u]^{13} - 144 u^2 z[u]^{13} + 48 u^3 z[u]^{13}) \} \}
 \end{aligned}$$

-0.0664001

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

0.12426

0.0564015

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

0.0341517