(*Computation of values for canonical sec str Nov 23, 2008 *)

```
Clear[R, S, P, Q, F, K1, K2];
```

```
eqn = {S == z + S z + R z^2 + R S z^2, R == z^3 + S z^3 + R S z^4 }
sol = Solve[eqn, S, R]
```

$\{S == z + S z + R z^2 + R S z^2,\ R == z^3 + S z^3 + R S z^4\}$

$$\left\{\left\{S \to \frac{1 - z - z^5 - \sqrt{4 z^5 \left(-1 - z^4\right) + \left(-1 + z + z^5\right)^2}}{2 z^4}\right\}, \left\{S \to \frac{1 - z - z^5 + \sqrt{4 z^5 \left(-1 - z^4\right) + \left(-1 + z + z^5\right)^2}}{2 z^4}\right\}\right\}$$

```
sol1 = Last[ Extract[sol, {1}]]
```

$$S \to \frac{1 - z - z^5 - \sqrt{4 z^5 \left(-1 - z^4\right) + \left(-1 + z + z^5\right)^2}}{2 z^4}$$

Series$\left[4 z^5 \left(-1 - z^4\right) + \left(-1 + z + z^5\right)^2,\ \{z, 0, 40\}\right]$

$1 - 2 z + z^2 - 6 z^5 + 2 z^6 - 4 z^9 + z^{10} + O[z]^{41}$

F $= 1 - 2 z + z^2 - 6 z^5 + 2 z^6 - 4 z^9 + z^{10}$

$1 - 2 z + z^2 - 6 z^5 + 2 z^6 - 4 z^9 + z^{10}$

```
solset = NSolve[F == 0, z]
```

{{z → -0.732124 - 0.553742 i}, {z → -0.732124 + 0.553742 i}, {z → -0.65691 - 0.784684 i},
{z → -0.65691 + 0.784684 i}, {z → 0.350788 - 0.589081 i}, {z → 0.350788 + 0.589081 i},
{z → 0.530953}, {z → 0.776693 - 0.730796 i}, {z → 0.776693 + 0.730796 i}, {z → 3.99215}}

```
rho = 0.5309527613419542`

(* dominant singularity *)
```

0.530953

```
(* Now rho is dominant singularity.Want to factor (1-z/rho) from P.*)
```

```
growth = 1 / rho
Q = Series[F / (1 - z / rho), {z, 0, 10}]

Print[F]
Expand[Series[Q, {z, 0, 10}] * (1 - z / rho)]
```

1.88341

$1 - 0.116593\, z + 0.780407\, z^2 + 1.46982\, z^3 + 2.76828\, z^4 - 0.786207\, z^5 + 0.519252\, z^6 + 0.977962\, z^7 + 1.8419\, z^8 - 0.530953\, z^9 + 1.13687 \times 10^{-13}\, z^{10} + O[z]^{11}$

$1 - 2\, z + z^2 - 6\, z^5 + 2\, z^6 - 4\, z^9 + z^{10}$

$1 - 2.\, z + z^2 - 6.66134 \times 10^{-16}\, z^3 + 1.33227 \times 10^{-15}\, z^4 - 6.\, z^5 + 2.\, z^6 - 3.04201 \times 10^{-14}\, z^7 + 5.08482 \times 10^{-14}\, z^8 - 4.\, z^9 + 1.\, z^{10} + O[z]^{11}$

```
(*So F=Q(1-z/rho) *)
(* Q0 is approximation to Q, which is F with (1-z/rho) factored out*)
Q0 = 1 - 0.11659327757792548` z + 0.7804074372205121` z^2 + 1.469824613489295` z^3 +
  2.768277557827167` z^4 - 0.7862074380581525` z^5 + 0.5192516259430491` z^6 +
  0.9779620029297007` z^7 + 1.8419002105912057` z^8 - 0.5309527613419505` z^9
K0 = Q0 /. z → rho
```

$1 - 0.116593\, z + 0.780407\, z^2 + 1.46982\, z^3 + 2.76828\, z^4 - 0.786207\, z^5 + 0.519252\, z^6 + 0.977962\, z^7 + 1.8419\, z^8 - 0.530953\, z^9$

1.59806

```
K1 = -Sqrt[K0] / (2 z^4) /. z → rho
```

-7.95321

```
K2 = K1 / Gamma[-1 / 2]
```

2.24356

```
(* asymptotic function *)

K[n_] := K2 * n^(-3 / 2) * (1 / rho)^n
For[i = 1, i ≤ 50, i++, Print[i, "  ", K[i]]]

(* Compute average number of base pairs in sat str, where theta is 0*)
s = 1 / (1 - u z^2 )
Series[D[s, u] /. u → 1, {z, 0, 30}]
Series[s, {z, 0, 50}]
```

1 4.22553

2 2.81372

3 2.88462

4 3.52877

5 4.75557

6 6.81358

7	10.1835
8	15.6984
9	24.7783
10	39.8454
11	65.048
12	107.521
13	179.596
14	302.666
15	513.999
16	878.746
17	1511.17
18	2612.3
19	4536.75
20	7911.79
21	13 849.5
22	24 326.2
23	42 860.8
24	75 732.
25	134 162.
26	238 245.
27	424 017.
28	756 198.
29	1.3512×10^{6}
30	2.41868×10^{6}
31	4.33673×10^{6}
32	7.78797×10^{6}
33	1.40063×10^{7}
34	2.52243×10^{7}
35	4.54862×10^{7}
36	8.21243×10^{7}
37	1.48446×10^{8}
38	2.6862×10^{8}
39	4.86588×10^{8}
40	8.82291×10^{8}
41	1.60129×10^{9}

42	2.90882×10^{9}
43	5.28849×10^{9}
44	9.62276×10^{9}
45	1.75228×10^{10}
46	3.19323×10^{10}
47	5.82323×10^{10}
48	1.06266×10^{11}
49	1.94046×10^{11}
50	3.54559×10^{11}

$$\frac{1}{1-u\,z^2}$$

$$z^2+2\,z^4+3\,z^6+4\,z^8+5\,z^{10}+6\,z^{12}+7\,z^{14}+8\,z^{16}+9\,z^{18}+10\,z^{20}+11\,z^{22}+12\,z^{24}+13\,z^{26}+14\,z^{28}+15\,z^{30}+O[z]^{31}$$

$1+u z^2+u^2 z^4+u^3 z^6+u^4 z^8+u^5 z^{10}+u^6 z^{12}+u^7 z^{14}+u^8 z^{16}+u^9 z^{18}+u^{10} z^{20}+u^{11} z^{22}+u^{12} z^{24}+u^{13} z^{26}+u^{14} z^{28}+u^{15} z^{30}+u^{16} z^{32}+u^{17} z^{34}+u^{18} z^{36}+u^{19} z^{38}+u^{20} z^{40}+u^{21} z^{42}+u^{22} z^{44}+u^{23} z^{46}+u^{24} z^{48}+u^{25} z^{50}+O[z]^{51}$

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Canonical structures, comparison with Hofacker et al;

Here we get the same dominant singularity as in Table 1 on page 15 of Hofacker et al. where value of L is 2,minimum stack size, and value of m is 1,minimum number of unpaired bases in hairpin loop.

**)

$$-S+\frac{1-z-z^5-\sqrt{4 z^5\left(-1-z^4\right)+\left(-1+z+z^5\right)^2}}{2 z^4}=0$$

$$S*2 z^4-1+z+z^5+\sqrt{4 z^5\left(-1-z^4\right)+\left(-1+z+z^5\right)^2}=0$$

$$F=\text{Expand}\left[\left(S*2 z^4-1+z+z^5+\sqrt{4 z^5\left(-1-z^4\right)+\left(-1+z+z^5\right)^2}\right)^2\right]$$

```
Fx =
  D[F, z] = -4 S z^3 (-S + z + S z) + (z^2 + S z^2) (3 z^2 + 3 S z^2) + (2 z + 2 S z) (z^3 + S z^3) - (1 + S) (-1 + S z^4);
Fyy = D[D[F, S], S] = -2 (-1 + z) z^4 + 2 z^5;
alpha = 0.5081
beta = (1 / alpha^2) * Sqrt[1 - alpha^2 + alpha^4]
FxEval = Fx /. {z → alpha, S → beta}
FyyEval = Fyy /. {z → alpha, S → beta}
gAlpha = -Sqrt[(alpha * FxEval) / (2 * Pi * FyyEval)]
growthRate = 1 / alpha
constant = -gAlpha / (2 Sqrt[Pi])


F = Resultant[-S + z + S z + R z^2 + S R z^2, -R + z^3 + R z^2 + S R z^4 + S z^3, R];
F = (z^2 + S z^2) (z^3 + S z^3) - (-S + z + S z) (-1 + z^2 + S z^4);
Fx = D[F, z] =
   (z^2 + S z^2) (3 z^2 + 3 S z^2) + (2 z + 2 S z) (z^3 + S z^3) - (-S + z + S z) (2 z + 4 S z^3) - (1 + S) (-1 + z^2 + S z^4);
Fyy = D[D[F, S], S] = -2 (-1 + z) z^4 + 2 z^5;
alpha = 0.5081
beta = (1 / alpha^2) * Sqrt[1 - alpha^2 + alpha^4]
FxEval = Fx /. {z → alpha, S → beta}
FyyEval = Fyy /. {z → alpha, S → beta}
gAlpha = -Sqrt[2 alpha * FxEval / FyyEval]
growthRate = 1 / alpha
constant = -gAlpha / (2 Sqrt[Pi])

Eliminate[{S == z + S z + R z^2 + S R z^2, R == z^3 + R z^2 + S R z^4 + S z^3}, R]
F = S^2 z^4 + S (-1 + z + z^2 - z^3 + z^5) - z (-1 + z^2 - z^4)
Fx = D[F, z]
Fyy = D[D[F, S], S]
alpha = 0.5081
beta = (1 / alpha^2) * Sqrt[1 - alpha^2 + alpha^4]
FxEval = Fx /. {z → alpha, S → beta}
FyyEval = Fyy /. {z → alpha, S → beta}
gAlpha = -Sqrt[2 alpha * FxEval / FyyEval]
```

```
growthRate = 1 / alpha
constant = -gAlpha / (2 Sqrt[Pi])
```

(***
By taking F defined by solution of equations or resultant
or from elimination of variables I get in both cases that constant
is 2.7437038542949987` rather than the real value 2.1614.
***)