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Highlights:

* Mixed numeric and analytic methods are applied to determine polymer shape parameters. \\
* Semi-analytic and simulational results compare favorably. \\
* The method may easily be applied to other branched polymer structures.\\

The two dimensional shapes of simple three and four junction ideal comb polymers

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Abstract

We redesign and apply a scheme originally proposed by G. Wei [Physica A **222**, 152 (1995); Physica A **222**, 155 (1995)] to produce numerical shape parameters with high precision for arbitrary tree-branched polymers based on their Kirchhoff matrix eigenvalue spectrum. This algorithm and a Monte Carlo growth method on square and triangular lattices are employed to investigate the shapes of ideal three and four junction two dimensional comb polymers. We find that the extrapolated values obtained by all of these methods are in excellent agreement with each other and the available theory. We confirm that polymers with a complete set of interior branches display a more circular shape.

Introduction

In a previous publication von Ferber et al[1] investigated the shapes of three and four junction comb polymers by redesigning a scheme originally proposed by G. Wei [2,3] to produce numerical shape parameters of arbitrary tree-branched polymers based on the Kirchhoff matrix eigenvalue spectrum. The predictions of this method and the simulation results of two different Monte Carlo (MC) techniques (pivot and growth) were compared for 5, 7, 8, 9 and 11 branch combs. See Figure 1 which illustrates the connectivity of the branches. In all of these uniform comb structures, if m is the number of monomers ("beads") in a branch and b is the number of branches, there are a total of $N = bm + 1$ units. It was found that the extrapolated property values obtained by all the methods were in excellent agreement with each other and the available theory in the ideal regime. This paper further tests the redesigned scheme by examining corresponding two dimensional systems.

An overall polymer size can be measured by the mean-square radius of gyration, $\langle S^2 \rangle$, where $\langle\ \rangle$ denotes an average over the polymer configurations. It is well-known[4] that for large polymers, with or without branches, $\langle S^2 \rangle$ follows a scaling law:

$$\langle S^2 \rangle = C(N-1)^{2\nu} \tag{1}$$

The coefficient, C, is a model dependent amplitude but the exponent, 2ν, is universal and equal to 1.0 for all ideal polymers in two dimensions.

If $\langle S^2 \rangle_b$ and $\langle S^2 \rangle_l$ are the mean-square radii of gyration of a branched and linear structure with an identical number of monomers then the g-ratio, a useful parameter for comparing the compactness of linear and branched polymers, is defined as

$$g = \frac{\langle S^2 \rangle_b}{\langle S^2 \rangle_l} \tag{2}$$

Casassa and Berry[5] obtained a general equation for the g-ratio of uniform, ideal comb

polymers with f three-functional junctions regularly spaced along the backbone:

$$g = 1 - r - \frac{r^2(1-r)}{(f+1)} + \frac{2r(1-r)^2}{f} + \frac{(3f-2)(1-r)^3}{f^2} \tag{3}$$

Here, r is the ratio of the number of units in the comb backbone to the total number of units in the polymer. In the case of five branch combs, $r = 3/5$ and $f = 2$, so $g = 89/125$ (0.7120). In the seven branch case $r = 4/7$, $f = 3$ and $g = 229/343$ (0.6676) whereas for nine branches $r = 5/9$, $f = 4$ and $g = 155/243$ (0.6379). The g-gratios of ideal eight and eleven branch polymers were determined by von Ferber et al [6] from the form factor. These values are 37/64 (0.5781) and 683/1331 (0.5131) for eight and eleven branches, respectively. Note that all of these results are independent of the spatial dimension.

The shape of any polymer composed of N units can be determined from the matrix representation of the radius of gyration tensor, $\overleftrightarrow{T}$. If X_j^α denotes the α component of the two dimensional position vector of the $j-th$ polymer bead, then the center of mass coordinates, $X_{CM}^{(\alpha)}$, of a given configuration are given by

$$X_{CM}^{(\alpha)} = \frac{1}{N}\sum_{j=1}^{N} X_j^{(\alpha)}, \text{ where } \alpha = 1 \text{ or } 2 \tag{4}$$

and the matrix components of $\overleftrightarrow{T}$ may be written in the form

$$T_{\alpha\beta} = \frac{1}{N}\sum_{j=1}^{N}(X_j^{(\alpha)} - X_{CM}^{(\alpha)})(X_j^{(\beta)} - X_{CM}^{(\beta)}) \tag{5}$$

This tensor has eigenvalues e_1 and e_2, which are the principal moments of gyration along the principal orthogonal axes[7]. The average trace of this tensor, $e_1 + e_2$, is equal to $\langle S^2 \rangle$. The eigenvalues of each configuration are ordered by magnitude, $e_1 \geq e_2$. Rudnick and Gaspari[8,9] have defined the average asphericity, $\langle A \rangle$, of polymers in two dimensions as

$$\langle A \rangle \;=\; \langle \frac{(e_1 - e_2)^2}{(e_1 + e_2)^2} \rangle \tag{6}$$

These averages are over all sets of eigenvalues determined from the simulated configuration. Note that in these equations $\langle A \rangle$ involves the average of a ratio and not the ratio of an average.

The shape of a two dimensional linear polymer can vary from a fully extended rod in which e_2 essentially vanishes so that $\langle A \rangle$ has unit value, to a circle for which $e_2 = e_1$. In the latter case $\langle A \rangle$ is zero. More complex polymer structures such as those studied here can obtain a fully extended rod shape in the ideal regime because the units can overlap each other. In between the extremes of a rod and a circle, a polymer configuration can be imagined[10] as approximately enclosed inside an ellipse with semi-major axis equal to e_1 and semi-minor axis equal to e_2.

In this article we compute a variety of two dimensional ideal branched comb properties by both theoretical and MC approaches and find excellent agreement between the values obtained.

Methods

Redesigned Wei Scheme

Various universal ratios for Gaussian (ideal) tree-branched macromolecules may be computed by a method originally developed by Wei[2,3]. This approach is exact in two dimensions. In general, Wei's method can be applied to any structure for which the Kirchhoff matrix and its corresponding eigenvalues are known. Here, this method is employed to predict universal ratios of two dimensional branched combs. A specific feature of the present implementation is that universal ratios are determined by extrapolating to infinite size branches.

von Ferber et al[1] found that the asphericity, $\langle A \rangle$, in two dimensions is given by

$$\langle A \rangle = 4 \int_0^\infty \mathrm{d}y \sum_{j=1}^{N-1} \frac{y^3}{(\lambda_j + y^2)^2} \left[\prod_{k=1}^{N-1} \frac{\lambda_k}{\lambda_k + y^2} \right]. \tag{7}$$

where $\lambda_1, \ldots, \lambda_{N-1}$ are the N - 1 non-zero eigenvalues of the $N \times N$ Kirchhoff matrix of a Gaussian structure with N beads.

Independent of the dimension, the g-ratio of the radius of gyration of the branched structure with respect to that of a linear chain with the same number of beads is given by

$$g = \sum_{j=1}^{N-1} \lambda_j^{-1} / \sum_{k=1}^{N-1} \hat{\lambda}_k^{-1}. \tag{8}$$

Here, the $\hat{\lambda}_k$ are the non-zero eigenvalues of the Kirchhoff matrix of a linear chain with N beads.

Wei's method is applied to determine the shape parameters of the given structures as a function of N. The extrapolated value for a shape parameter is determined in the limit of $1/N \to 0$. The results scale perfectly with $1/N$ and thus extrapolated results may be extracted from these series. This procedure is illustrated in Fig. 2 for the g-ratio, in Fig. 3 for the asphericity, and in Fig. 4 for the shape factor δ_1 which is calculated as the ratio of two averages,

$$\delta_1 = \frac{\langle e_1 \rangle}{\langle S^2 \rangle}. \tag{9}$$

The final results concerning the combs discussed in this paper are given in Table III for the g-ratio, in Table IV for the average asphericity, $\langle A \rangle$, and in Table V for the shape factor, δ_1. Estimated errors given for the Wei method in the tables are based on the statistical error taken from the extrapolation.

Monte Carlo Growth Algorithms

Two dimensional polymers are constructed on an integer coordinate system. Given the numbers N and M, the simulation is performed by creating M independent samples each containing N units. Two kinds of lattices were studied: a square lattice and a triangular lattice. In both lattices polymer samples are obtained by starting the first bead at the origin (0, 0). In the case of the square lattice, subsequent beads are placed by randomly selecting

one of four possible directions: North, South, East, or West, whereas in the case of the triangular lattice, one of the following six possible directions is chosen: Northeast, East, Southeast, Southwest, West and Northwest. In the linear case, each bead is placed one unit apart from the previously placed bead. In this study of ideal polymers, a location that has already been used by another bead is allowed to be chosen so that beads can overlap.

Each growth algorithm for the 5, 7, 8, 9, and 11 branch ideal combs utilizes the above linear polymer growth algorithm, with slight modifications. At the start of all the growth algorithms a three-branched star is grown by placing the first polymer unit at the origin (0, 0). The first branch is grown to include a pre-specified number of polymer units, N. Then, the second branch is started once again at the origin, and grown to include N additional units. The same method is employed for the third branch. In the case of the 5 branch comb, a three-branched star is grown as described. However, this time, a new origin is moved to the end of the third branch of the star and then two more branches are grown from this new origin. For the 7 branch comb, first a 5 branch comb is grown. Then, a new origin is moved to the end of the fifth branch, where two more branches are grown. The 8, 9, and 11 branch combs are grown in a similar manner.

After each polymer is completely constructed, a number of properties are calculated for that configuration. The simulated systems have values of N ranging from 1001 to 5501. The set of computed properties was then further averaged over the total number of saved samples, M = 160,000, to determine the mean and the standard deviation from the mean employing the usual equations for independent samples.

Results

All the MC simulation results are contained in Tables IA-E and IIA-E. In the results reported in the tables, the number in parenthesis denotes one standard deviation in the last displayed digits. In all cases, non-linear fits[11] of $\langle S^2 \rangle$ vs $(N-1)^{2\nu}$ gave $2\nu = 1.00 \pm 0.01$, in excellent

agreement with the well-known result of 1.00 for random walks.

The MC g-ratios in Table III have been calculated from the radius of gyration data and the errors in these quantities have been computed from the standard equation relating the error in a ratio to the error in the numerator and the error in the denominator. However, these computer results are for finite N whereas the theories are for infinite N. Infinite N g-ratio values have been obtained by fitting a scaling law as explained in Zweier and Bishop[12,13].

These extrapolated g-ratios for ideal systems are compared to other findings in Table III. The error bars on the Wei method indicate the root mean-square (RMS) of the residuals corresponding to the errors of the fitted data. Both Wei's method and the MC simulations are in excellent agreement with each other and the theoretical predictions. The g-ratios of the eight and eleven branch combs, which have a complete set of interior branches, have a relatively lower value than that found for the five, seven and eleven branch combs.

The growth MC simulation results for $\langle A \rangle$ contained in the tables display only a weak dependence on N. As was the case for the g-ratio, the data have been extrapolated to predict values for an infinite polymer. Table IV lists these extrapolated values. As expected, the results indicate that the polymers become more circular in their shape as the structure changes to higher branching and a complete set of interior branches.

The shape factor, δ_1, data have been examined in the same manner as the other properties and the extrapolated values are contained in Table V. The values for both lattices are in excellent agreement with each other and with the predictions of the Wei method. As expected, the results again indicate that the polymers become more circular in their shape (less stretched out) as the structure changes to higher branching and a complete set of interior branches.

Two dimensional ideal five branch combs were also investigated by Perrelli and Bishop[14] and Gorry and Bishop[15]. Perrelli and Bishop[14] also employed a MC growth algorithm on a square lattice but for a smaller range of N (100 to 800) and for a much smaller value of M

(10,000). They found that $g = 0.704 \pm 0.005$, $\langle A \rangle = 0.311 \pm 0.002$, and $\delta_1 = 0.785 \pm 0.005$. These values are well within two standard deviations of the mean or in the 95% confidence interval compared to the results reported in this paper.

Gorry and Bishop[15] used a pivot MC algorithm. In the pivot MC method the initial polymer configuration is constructed by linking together tangent circular units with a diameter of one. The polymer is not restricted to a fixed lattice. A random number is used to select one of the beads as a pivot and a second random number is employed to generate a random angle between 0° and 360°. All the beads further along the branch containing the pivot bead are rotated by this angle. In this MC method successive samples are not independent and it is necessary to both discard the beginning phase of the simulation and to collect data at sufficiently large intervals so as to avoid correlation effects. Gorry and Bishop[15] found that the g-ratio $= 0.713 \pm 0.002$ and $\langle A \rangle = 0.310 \pm 0.001$, in excellent agreement with the current results.

Results and discussion

Wei's method and Monte Carlo growth algorithms on both a square and triangular lattice have been used to investigate two dimensional branched comb polymers in the ideal regime. The g-ratios, the asphericities, the shape factors and their respective error bars have been determined for a wide range of N. It is found that the extrapolated values of all the techniques are in excellent agreement with each other and the available theory.

The branching of the two dimensional ideal polymer strands does not affect the universal two-dimensional ideal (non interacting) scaling behaviour. Thus e.g. the end-end distances within strands as well as for the branched structure as a whole will scale with the scaling exponent $\nu = 1/2$.

For the ideal scaling behaviour of three dimensional branched structures one will again find the same $\nu = 1/2$ exponent.

This behaviour will break however, if we take into account an environment with correlated disorder. Under the influence of such a correlated (disordered) environment the polymer strands even if they display no self-interaction will change their conformation due to the disordered background.[16]

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Table IA Effect of the Number of Beads, N, for 5-branch combs and linear chains on a square lattice.

Property	1001	1501	2001	2501
$\langle e_1 \rangle$	92.83(15)	139.14(22)	185.58(29)	232.37(36)
$\langle e_2 \rangle$	25.48(3)	38.26(5)	51.03(7)	63.84(8)
$\langle S^2 \rangle$	118.31(16)	177.39(23)	236.61(31)	296.20(39)
$\langle A \rangle$	0.310(1)	0.310(1)	0.310(1)	0.310(1)
$\langle S^2 \rangle_{\text{linear}}$	166.71(27)	249.39(40)	333.72(53)	416.95(66)

Table IB Effect of the Number of Beads, N, for 7-branch combs and linear chains on a square lattice.

Property	1401	2101	2801	3501
$\langle e_1 \rangle$	121.91(19)	182.69(29)	244.15(38)	305.17(48)
$\langle e_2 \rangle$	33.53(4)	50.33(6)	67.19(8)	84.08(10)
$\langle S^2 \rangle$	155.44(21)	233.02(31)	311.34(41)	389.26(51)
$\langle A \rangle$	0.306(1)	0.305(1)	0.306(1)	0.306(1)
$\langle S^2 \rangle_{\text{linear}}$	233.37(37)	349.77(56)	466.76(74)	584.39(93)

Table IC Effect of the Number of Beads, N, for 8-branch combs and linear chains on a square lattice.

Property	1601	2401	3201	4001
$\langle e_1 \rangle$	117.76(17)	176.49(26)	235.72(34)	294.43(43)
$\langle e_2 \rangle$	36.13(4)	54.21(6)	72.26(8)	90.55(11)
$\langle S^2 \rangle$	153.89(19)	230.71(28)	307.98(37)	384.99(46)
$\langle A \rangle$	0.274(1)	0.274(1)	0.275(1)	0.274(1)
$\langle S^2 \rangle_{\text{linear}}$	266.39(42)	400.36(64)	534.05(85)	667.03(106)

Table ID Effect of the Number of Beads, N, for 9-branch combs and linear chains on a square lattice.

Property	1801	2701	3601	4501
$\langle e_1 \rangle$	150.23(24)	224.80(36)	300.54(48)	375.90(60)
$\langle e_2 \rangle$	40.97(5)	61.45(7)	82.27(10)	102.83(12)
$\langle S^2 \rangle$	191.20(26)	286.25(38)	382.81(51)	478.72(64)
$\langle A \rangle$	0.305(1)	0.305(1)	0.304(1)	0.305(1)
$\langle S^2 \rangle_{\text{linear}}$	299.81(48)	450.31(71)	600.03(95)	750.46(119)

Table IE Effect of the Number of Beads, N, for 11-branch combs and linear chains on a square lattice.

Property	2201	3301	4401	5501
$\langle e_1 \rangle$	143.30(21)	214.72(32)	287.01(42)	358.52(52)
$\langle e_2 \rangle$	44.68(5)	67.05(7)	89.52(10)	112.02(12)
$\langle S^2 \rangle$	187.98(23)	281.77(34)	376.53(45)	470.54(57)
$\langle A \rangle$	0.265(1)	0.265(1)	0.265(1)	0.265(1)
$\langle S^2 \rangle_{\text{linear}}$	366.87(58)	550.73(87)	733.82(117)	918.03(146)

Table IIA Effect of the Number of Beads, N, for 5-branch combs and linear chains on a triangular lattice.

Property	1001	1501	2001	2501
$\langle e_1 \rangle$	92.85(14)	139.65(22)	186.13(29)	233.04(36)
$\langle e_2 \rangle$	25.58(3)	38.40(5)	51.21(7)	64.03(8)
$\langle S^2 \rangle$	118.43(15)	178.05(23)	237.34(31)	297.07(39)
$\langle A \rangle$	0.310(1)	0.310(1)	0.310(1)	0.310(1)
$\langle S^2 \rangle_{\text{linear}}$	166.81(26)	250.13(40)	334.29(53)	418.45(66)

Table IIB Effect of the Number of Beads, N, for 7-branch combs and linear chains on a triangular lattice.

Property	1401	2101	2801	3501
$\langle e_1 \rangle$	122.05(19)	183.14(29)	244.04(38)	305.42(48)
$\langle e_2 \rangle$	33.71(4)	50.52(6)	67.45(8)	84.18(10)
$\langle S^2 \rangle$	155.75(21)	233.66(31)	311.49(41)	389.60(51)
$\langle A \rangle$	0.304(1)	0.305(1)	0.305(1)	0.305(1)
$\langle S^2 \rangle_{\text{linear}}$	233.96(37)	351.00(56)	468.44(74)	584.08(93)

Table IIC Effect of the Number of Beads, N, for 8-branch combs and linear chains on a triangular lattice.

Property	1601	2401	3201	4001
$\langle e_1 \rangle$	117.74(17)	177.07(26)	235.70(34)	295.05(43)
$\langle e_2 \rangle$	36.19(4)	54.41(6)	72.64(9)	90.61(11)
$\langle S^2 \rangle$	153.93(18)	231.48(28)	308.34(37)	385.65(46)
$\langle A \rangle$	0.274(1)	0.274(1)	0.273(1)	0.274(1)
$\langle S^2 \rangle_{\text{linear}}$	267.04(42)	401.71(64)	534.70(85)	667.85(106)

Table IID Effect of the Number of Beads, N, for 9-branch combs and linear chains on a triangular lattice.

Property	1801	2701	3601	4501
$\langle e_1 \rangle$	150.16(24)	225.68(36)	300.95(48)	375.78(60)
$\langle e_2 \rangle$	41.06(5)	61.71(7)	82.29(10)	102.77(12)
$\langle S^2 \rangle$	191.22(25)	287.39(38)	383.24(51)	478.55(63)
$\langle A \rangle$	0.304(1)	0.305(1)	0.305(1)	0.305(1)
$\langle S^2 \rangle_{\text{linear}}$	300.33(48)	451.13(72)	601.47(96)	752.39(120)

Table IIE Effect of the Number of Beads, N, for 11-branch combs and linear chains on a triangular lattice.

Property	2201	3301	4401	5501
$\langle e_1 \rangle$	143.45(21)	214.80(31)	287.14(42)	358.85(53)
$\langle e_2 \rangle$	44.83(5)	67.13(7)	89.67(10)	112.24(12)
$\langle S^2 \rangle$	188.28(23)	281.93(34)	376.81(45)	471.09(57)
$\langle A \rangle$	0.265(1)	0.265(1)	0.265(1)	0.264(1)
$\langle S^2 \rangle_{\text{linear}}$	367.58(58)	550.83(88)	734.66(117)	918.83(146)

Table III Comparison of g-ratios for extrapolated Square Lattice MC, Triangular Lattice MC, and Wei method to the theoretical infinite bead values reported in the literature.

	Square Lattice MC	Triangular Lattice MC	Wei	Theory
5 branch	0.710(2)	0.712(2)	0.7120(11)	0.7120[a]
7 branch	0.666(2)	0.666(2)	0.6676(2)	0.6676[a]
8 branch	0.576(2)	0.577(2)	0.5781(7)	0.5781[b]
9 branch	0.638(2)	0.636(2)	0.6379(4)	0.6379[a]
11 branch	0.514(2)	0.514(2)	0.5131(5)	0.5131[b]

See reference a [5] b [6]

Table IV Comparison of $\langle A \rangle$ for extrapolated Square Lattice MC, Triangular Lattice MC and Wei method.

	Square Lattice MC	Triangular Lattice MC	Wei
5 branch	0.310(2)	0.310(2)	0.3095(5)
7 branch	0.306(1)	0.306(2)	0.3047(4)
8 branch	0.275(1)	0.274(2)	0.2736(3)
9 branch	0.304(2)	0.306(2)	0.3042(2)
11 branch	0.265(2)	0.265(2)	0.2640(2)

Table V Comparison of δ_1 for extrapolated Square Lattice MC, Triangular Lattice MC and Wei method.

	Square Lattice MC	Triangular Lattice MC	Wei
5 branch	0.783(1)	0.784(2)	0.7838(2)
7 branch	0.784(1)	0.783(2)	0.7835(1)
8 branch	0.765(1)	0.764(2)	0.7645(1)
9 branch	0.784(2)	0.785(2)	0.7850(1)
11 branch	0.762(2)	0.762(2)	0.7615(1)

Figures:

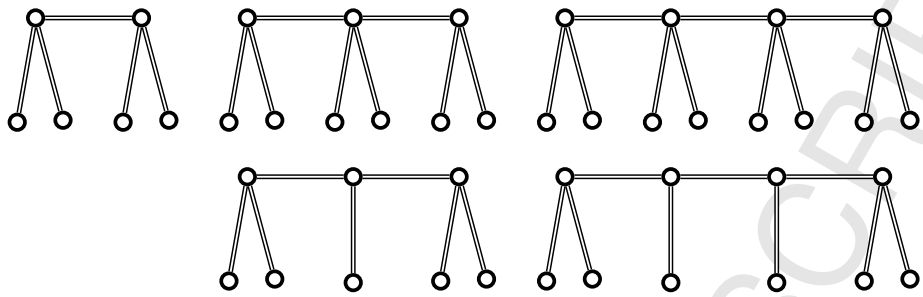

Figure 1: Sketches of the 5, 7, 8, 9, and 11 branched comb polymers discussed in this paper.

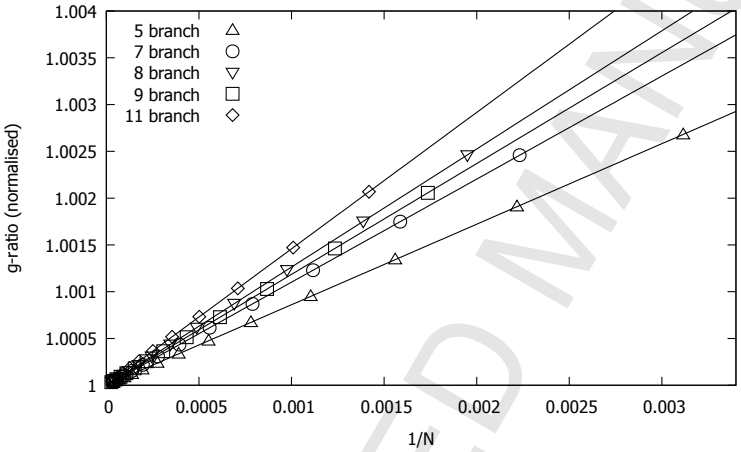

Figure 2: Extrapolation for the two dimensional g-ratio of the comb polymers discussed. Note that in order to show all the extrapolated results in a single graph the target g-ratio is normalized to 1 for all five combs.

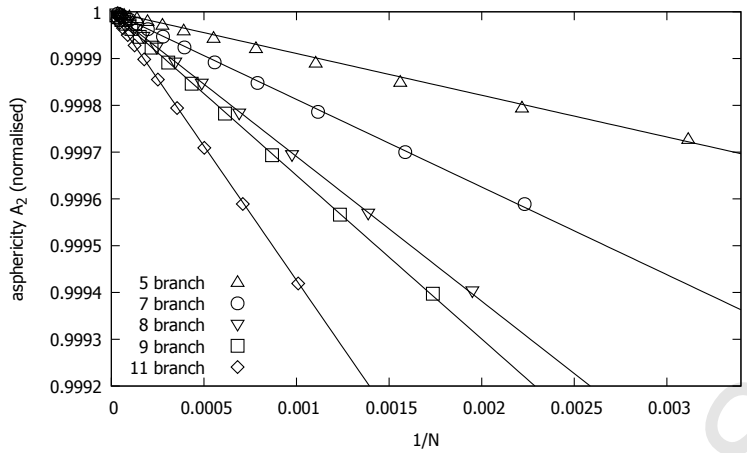

Figure 3: Extrapolation for the two dimensional asphericities of the comb polymers discussed. Note that in order to show all the extrapolated results in a single graph the target asphericity is normalized to 1 for all five combs.

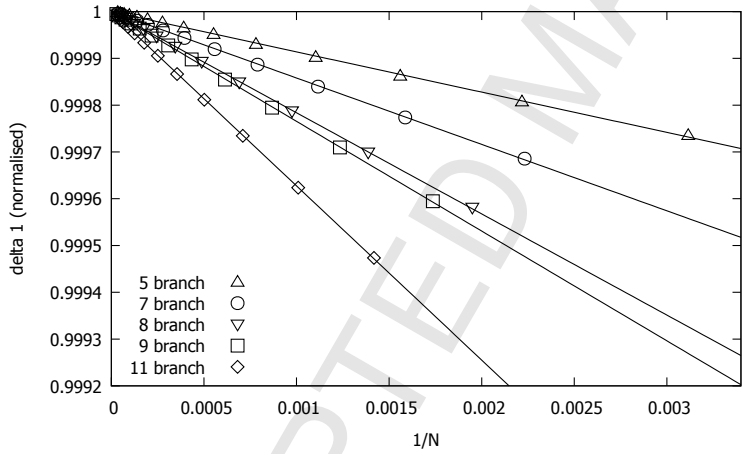

Figure 4: Extrapolation for the two dimensional δ_1 shape factors of the comb polymers discussed. Note that in order to show all the extrapolated results in a single graph the target shape factor is normalized to 1 for all five combs.