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Non-perturbative tricritical exponents of trails: I. Exact enumeration on a triangular lattice

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Abstract. As the fugacity for intersections in trails (intersecting but non-overlapping lattice walks) is increased, the configurations change from swollen ones, with the scaling exponents of self-avoiding walks, to compact ones. Separating the two regimes is a potentially new tricritical point with no perturbative renormalisation fixed point associated with it. Supporting evidence for the existence of a tricritical point, its likely location and exponents are computed for the first time from exact enumeration of all trails up to a length of fifteen lattice constants on the triangular lattice. The divergence of the specific heat indicates the location of the tricritical point. Generalised ratio and Padé methods are used to extract the scaling exponents for the number of configurations and their end-to-end distance.

1. Introduction

The statistical properties of the so-called trail configurations were first approached by Malakis [1] a few years ago. This lattice model interpolates between free random walks (RW) and the well studied self-avoiding walks (SAW) which also describe the conformations of long polymer chains. The trail problem differs from the above two in that it consists of all configurations of a random walker on a lattice which is free to intersect its path through an already visited site but is not allowed to go more than once on the same bond.

In his original work, Malakis [1] enumerated exact long trails on a square lattice and observed their scaling properties. He reached the non-trivial (and even somewhat surprising) conclusion that the trail model belongs to the SAW universality class, namely both models share the same scaling exponents. We recall that one such exponent is ν which relates the average square end-to-end distance r (or the radius of gyration) to the length of the walk l. If all lengths are measured in terms of unit lattice spacing (see, for example, [2]):

$$\langle r_l^2 \rangle \approx l^{2\nu} \tag{1.1}$$

asymptotically for very large l. If we denote the total number of configurations of length l by C_l, then the exponent γ is defined from the expected asymptotic behaviour:

$$\lim_{l\to\infty} C_l = \Gamma l^{\gamma-1}\mu^l. \tag{1.2}$$

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The amplitude Γ and the so-called growth parameter μ are not universal and are not the same in trails and in SAW. However, the exponents γ (and ν) are exactly the same in both models! We also note that the fractal dimension $\bar{d}$ of the trail is defined through

$$l \approx r^{\bar{d}} \tag{1.3}$$

with

$$\bar{d} = 1/\nu. \tag{1.4}$$

The continuum limit of the trails is intricate since in this limit there is no apparent difference between a site and a bond. However, the continuum limit was derived from the lattice Hamiltonian for the trail generating function by Shapir and Oono [3] and was found to be distinct from either of the RW or SAW ones. Basically it is a $2n$-component spin ($n \to 0$) field theory but with a new term (due to the intersections) which breaks the $O(2n)$ symmetry. This new term may be shown to be irrelevant in the RG sense (it decays away when fluctuations on larger and larger scales are integrated out), leading to similar scaling exponents for SAW and trails, as found numerically by Malakis [1]. Field theories for other generalised interacting walks (in which the rotational symmetry is unbroken) were derived by Jasnow and Fisher [4].

Another very interesting question arises, however, if the average number of intersections is controlled by assigning a fugacity $f = e^{\theta}$ with each intersection ($\theta = -\beta\varepsilon$ where ε is the corresponding energy). The trail problem defined by Malakis and discussed so far corresponds to the case $\theta = 0$. In the limit $\theta \to -\infty$, the intersections are suppressed and the SAW problem is recovered. In the other limit of very large and positive θ, the configurations with maximal number of crossings will dominate. Hence, the average form of the cluster will be compact with local disorder. In this collapsed phase, the fractal dimension is the same as the spatial one and $\nu = 1/d$ follows. So, as θ is increased from zero to positive values we expect a change from a swollen phase (with SAW scaling properties) to a collapsed compact one. A similar situation occurs in a regular polymer as a function of the monomer–monomer attraction. In this latter case, the change occurs at the so-called Θ point which is represented by a tricritical point in the critical phenomena terminology. Tricriticality of some sort is also expected in the trail model from the following general considerations. If a fugacity z per monomer (or lattice step) is introduced, the limit $l \to \infty$ corresponds to the limit $z \to z_c$ in the grand canonical ensemble [2]. The transition into the swollen phase at the critical value of the fugacity $z_c = \mu_c^{-1}$ is second order and the transition into the collapsed phase is likely to be first order. The intermediate point, hence, is expected to be a tricritical point.

The tricritical point in the trail model may be a new one characterised by its own scaling exponents. It is the main subject of our present investigation. Apart from the study of a new tricritical point *per se*, there are other important motivations to do so. The RG calculations in $d = 4 - \varepsilon$ dimensions exhibit no perturbative fixed point. Instead the RG calculations predict the SAW type of behaviour for all values of θ! This result is physically unacceptable and we are presented with one of those rare cases in which the RG is powerless in predicting the scaling exponents. We therefore have to rely on alternative approaches like the series expansions used in this paper. It is also important to note that the field theory of trails is related by an inversion symmetry in the parameter space [3] to that of the random XY model which also lacks a perturbative fixed point for the random critical transition. Only speculations can be made today on whether a random XY transition exists and what its nature may be. Although the relation between these two problems is, in all likelihood, broken by the highest-order terms, our results for the trails suggest the possibility for the existence of a non-perturbative critical random XY fixed point as well. We hope the present work will motivate more investigations of this challenging question.

Another closely related problem is that of polymers with fused loops, the results on which will be presented elsewhere [5]. In this problem only the silhouettes of the trails are considered (and each silhouette is counted once, independent of how many trail configurations have this shadow). This model describes the tricritical behaviour of dilute polymer chains with equally spaced attractive groups attached to them (self-associating polymers). This tricriticality is described by a perturbative fixed point of order $\sqrt{\varepsilon}$! In a forthcoming work [5], the behaviour of the two models will be compared.

Extensive series on triangular and other lattices for the Malakis trails were generated and analysed by Guttmann [6]. He confirmed that, when no fugacity is assigned to intersections, the scaling behaviour is SAW-like (in addition, he has found several exact results for the growth parameter). For the value of $\theta = 0$ our results agree with his and this serves as an independent check. Extensive series on fully self-avoiding walks may be found in Grassberger [7].

In this paper, the first in a series, we present (§ 2) the exact enumeration of all trails on a triangular lattice with length l up to fifteen steps. The tables give full information on the walks with a given length l, number of intersections I and end-to-end distance r. In § 3, the specific heat as a function of θ is derived in order to locate the tricritical point [8]. We then apply (§ 4) the Dlog Padé method to compute a first estimate for the tricritical couplings and exponents. A new generalised ratio method [9] is used in § 5 to yield independent estimates for the same tricritical properties to check the consistency of the results. Section 6 is devoted to conclusions.

2. The series

Throughout the work, we use the following notation: l denotes the path length (i.e. the number of monomers), I denotes the number of intersections in a given trail and r denotes its end-to-end distance. The following two series are thus generated:

$$c(l, I) = \sum_r C(l, I, r) \tag{2.1a}$$

$$d(l, I) = \sum_r r^2 C(l, I, r) \tag{2.1b}$$

where $C(l, I, r)$ is the total number of trails with length l, I intersections and end-to-end distance r. The series for $c(l, I)$ and $d(l, I)$ are tabulated in tables 1 and 2 respectively†. Our results agree exactly with those of Grassberger [7] for the $I = 0$ case.

Using the above notation, we define the average quantities:

$$U_l(\theta) = \sum_{I \geqslant 0} c(l, I)\, \mathrm{e}^{I\theta} \to l^{\gamma(\theta)-1} \mu(\theta)^l \tag{2.2a}$$

$$\langle r_l^2(\theta) \rangle = \frac{\sum_{I \geqslant 0} d(l, I)\, \mathrm{e}^{I\theta}}{\sum_{I \geqslant 0} c(l, I)\, \mathrm{e}^{I\theta}} \to l^{2\nu(\theta)}. \tag{2.2b}$$

† These were enumerated on a VAX 11/780 and took over two hundred CPU hours.

Table 1. The coefficients $c(l, I)$ (equation (2.1*a*)).

	$\frac{1}{6}c(l, I)$							
l/I	0	1	2	3	4	5	6	7
1	1							
2	5							
3	23	2						
4	103	20						
5	455	134	6					
6	1 991	766	96					
7	8 647	4 070	834	32				
8	37 355	20 672	5 706	552				
9	160 689	101 944	34 480	5 544	184			
10	688 861	491 832	194 416	42 664	3 640			
11	2 944 823	2 333 386	1 046 648	284 332	40 380	1 008		
12	12 559 201	10 925 332	5 451 522	1 736 208	336 812	24 032		
13	53 455 781	50 608 464	27 697 690	10 008 008	2 408 092	292 064	6 800	
14	227 131 875	232 356 758	137 989 466	55 378 244	15 620 432	2 654 872	162 768	
15	963 627 597	1 058 850 906	676 667 102	297 091 436	94 925 152	20 285 016	2 148 884	53 952

Table 2. The coefficients $d(l, I)$ (equation (2.1*b*)).

	$\frac{1}{6}d(l, I)$							
l/I	0	1	2	3	4	5	6	7
1	1							
2	12							
3	97							
4	654	16						
5	3 977	264	6					
6	22 624	2 688	144					
7	122 821	21 816	2 002	32				
8	644 082	154 892	20 748	936				
9	3 288 739	1 006 492	178 760	13 992	264			
10	16 440 648	6 139 944	1 360 340	153 600	7 440			
11	80 783 857	35 722 136	9 476 800	1 405 056	114 924	1 728		
12	391 310 240	200 305 480	61 812 808	11 354 704	1 303 048	54 496		
13	1 872 763 387	1 090 477 696	383 198 754	83 830 696	12 284 252	890 288	14 096	
14	8 870 963 422	5 794 647 408	2 281 480 464	577 833 912	102 407 968	10 608 592	434 304	
15	41 647 686 501	30 176 073 228	13 143 846 886	3 773 806 672	781 068 568	104 475 800	7 307 900	108 480

3. Specific heat calculations

The specific heat per link as defined in [8]:

$$h_l(\theta) = \frac{1}{l}\frac{\partial^2}{\partial\theta^2}\log U_l(\theta)$$
$$= \langle I(\theta)^2\rangle - \langle I(\theta)\rangle^2 \qquad (3.1)$$

is a measure of the relative fluctuations in the number of intersections. From the results on the Θ point [8], we expect $h_l(\theta)$ to diverge at the tricritical point, $\theta = \theta_t$. The values of $h_l(\theta)$, for $l = 11$–15, are depicted in figure 1. The plot clearly shows how the peaks

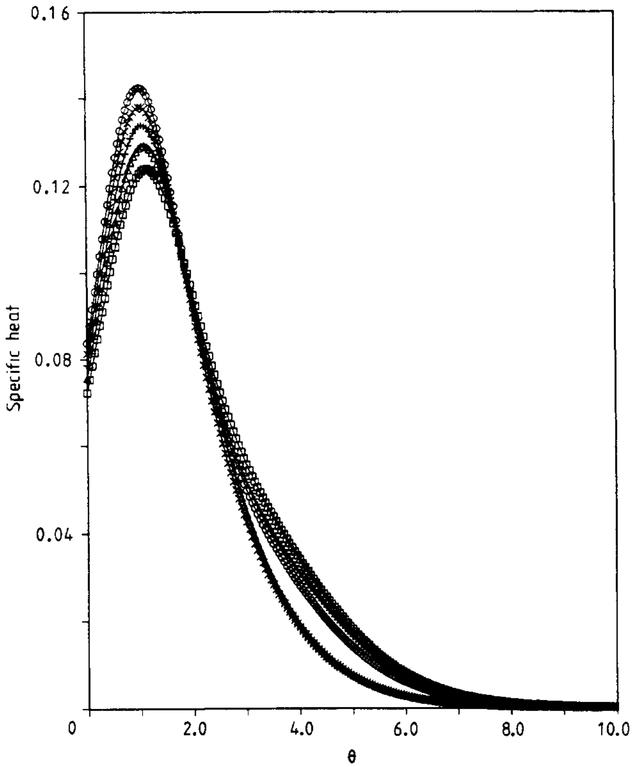

Figure 1. Specific heat plots for $l = 11$–15.

are converging to a fixed value of θ, the tricritical point. We then plot (figure 2) $\theta_{max}(l)$ against $1/l$. Using linear regression, we find the θ_{max} intercept (corresponding to $l = \infty$) which gives us our estimate θ_t: $\theta_t = 0.60 \pm 0.05$. Non-linear terms may somewhat increase or decrease this value. Note that this range is substantially smaller than the last maxima obtained for $l = 15$, which is $\theta = 1.0$.

4. Padé analysis

To find the tricritical values of the growth parameter μ and the exponent γ, we apply the standard Dlog Padé method to the series of $U_l(\theta)$. In figure 3 we show how μ changes as a function of θ for different Padé approximants $[L/M]$. The effective exponents $\gamma(\theta)$ are depicted in figure 4. In table 3, values of γ_t and μ_t for $0.6 \leqslant \theta \leqslant 1.0$ are quoted. Our best estimate for the value θ_t is 0.6. The approximants [6/7] and [7/7] suffer from interference of non-physical poles which cause anomalous deviations. From the best approximants, we estimate

$$\mu_t = 5.00 \pm 0.02$$

$$\gamma_t = 1.18 \pm 0.04.$$

The other rows, from $\theta = 0.7$ to $\theta = 1.0$ (the latter being the maximum of the specific heat for $l = 15$), are given in order to facilitate comparison with results obtained using the generalised ratio method (see § 5) and in order to highlight the crucial importance

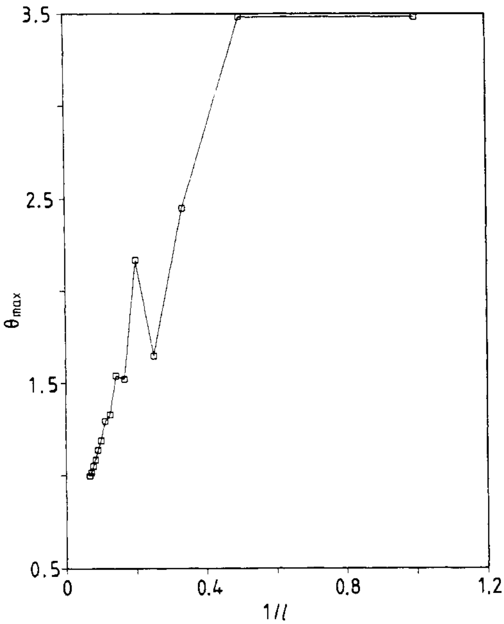

Figure 2. The specific heat maxima, θ_{max}, plotted against $1/l$.

of the linear extrapolation to obtain the right values of θ_t (and also γ_t and ν_t which strongly depend on the determination of θ_t).

The exponent ν_t is extracted from the series for $\langle r_l^2(\theta)\rangle$ (equation (2.2*b*)). In figure 5, we depict $\nu(\theta)$ for various approximants (the location of the tricritical point is $\bar{\mu}_t = 1.0$ since $\langle r_l^2(\theta)\rangle$ is a ratio of two series which diverge at the same point). In table 4, the values of ν_t and $\bar{\mu}_t$ are quoted in the same range ($0.6 \leqslant \theta \leqslant 1.0$). Again, the right values should be in the range determined by the first two rows. Our best estimate at $\theta_t = 0.6$ is

$$\nu_t = 0.52 \pm 0.02.$$

Values of ν_t at $0.7 \leqslant \theta \leqslant 1.0$ are given for later comparison with the generalised ratio method.

5. Generalised ratio method

In a recent analysis of the Θ point [9], Privman suggested an extension of the ratio method which gives both the location of the tricritical point and the tricritical value of ν with improved accuracy. They are extracted from recursive estimates:

$$\nu_l = \frac{1}{2}\log\left(\frac{r_l^2}{r_{l-1}^2}\right)\left[\log\left(\frac{l}{l-1}\right)\right]^{-1} \tag{5.1}$$

and the deviations from the average ν:

$$\delta\nu_l = \nu_l - \frac{1}{m}\sum_{k=n+1}^{n+m} \nu_k. \tag{5.2}$$

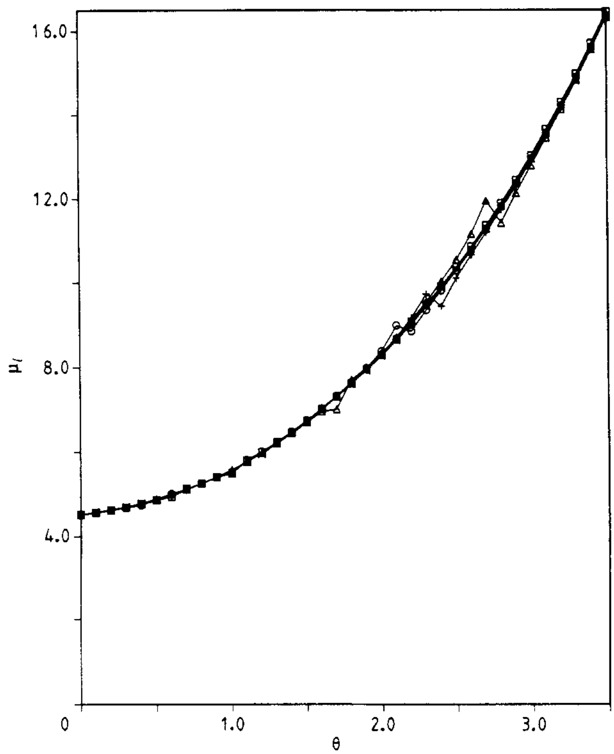

Figure 3. The growth constant $\mu_l(\theta)$ for approximants [5/6] ($\times$), [6/6] ($\bigcirc$), [6/7] ($\square$), [7/6] ($\triangle$) and [7/7] (+).

In figures 6 and 7, we plot ν_l and $\delta\nu_l$ respectively for $l = 11$-15 ($n = 10$, $m = 5$). The tricritical point is at the point of minimal spread in $\delta\nu$ and from it, we get

$$\theta_t = 1.0 \pm 0.3$$

$$\nu_t = 0.46 \pm 0.04.$$

If we compare these values with those of tables 3 and 4, we arrive at the following conclusion: the ratio method gives both for θ_t and the exponent the corresponding Padé values but at $\theta = 1.0$, which is the location of the last maximum of the specific heat ($l = 15$) without the extrapolation to lower values of θ. From the way the locations of the maxima are varying with increasing l, we conclude this extrapolation to be necessary. We therefore also anticipate that, if higher-order results were available, the point of minimal spread in $\delta\nu_l$ (equation (5.2)) will also shift towards smaller values of θ. (At present we do not have enough terms to estimate the shift and to confirm our estimate of the extrapolation (made using linear regression on θ_{max}) given in § 3.) This, of course, raises doubts as to the accuracy of the generalised ratio method in predicting the location and exponent at the tricritical Θ point made in [9]. One property which may influence this inaccuracy is the value of the crossover exponent. We have attempted to compute the crossover exponent ϕ from the θ derivatives of the series but our error bars are too large to yield a credible estimate.

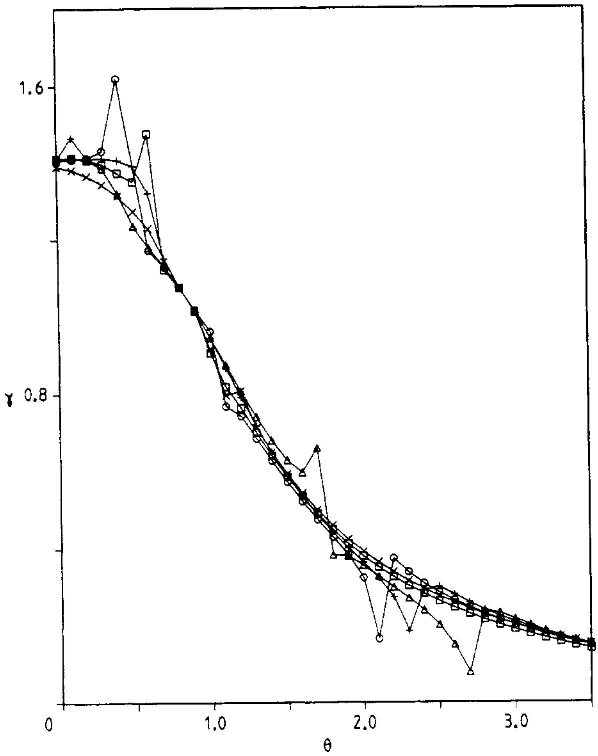

Figure 4. The effective exponent $\gamma(\theta)$ for approximants [5/6], [6/6], [6/7], [7/6] and [7/7] (notation as in figure 3).

Table 3. $\gamma_t(\mu_t)$ against θ between $\theta_{max}(l=15)=1.0$ and θ_{max} (extrapolated) = 0.6. ×, defective poles.

	$\gamma_t(\mu_t)$				
$[L/M]/\theta$	0.6	0.7	0.8	0.9	1.0
[5/4]	1.186 (5.002)	1.133 (5.123)	1.076 (5.258)	1.016 (5.408)	0.955 (5.573)
[5/5]	1.192 (4.999)	1.134 (5.122)	1.076 (5.258)	1.021 (5.403)	× (×)
[5/6]	1.229 (4.986)	× (×)	1.076 (5.258)	1.014 (5.409)	0.916 (5.506)
[6/5]	1.178 (5.008)	1.132 (5.124)	1.076 (5.258)	1.010 (5.412)	0.921 (5.593)
[6/6]	1.173 (5.019)	1.129 (5.126)	1.075 (5.258)	1.018 (5.407)	0.962 (5.532)
[6/7]	1.476 (4.946)	1.122 (5.137)	1.076 (5.258)	1.016 (5.408)	0.907 (5.502)
[7/6]	1.180 (5.006)	1.132 (5.123)	1.076 (5.258)	1.014 (5.409)	0.946 (5.580)
[7/7]	1.321 (4.965)	1.151 (5.114)	1.074 (5.259)	1.016 (5.408)	0.946 (5.580)

6. Conclusions

In this paper, we have tabulated the triangular lattice series for the number of configurations and end-to-end distances for trails according to their length and number of intersections.

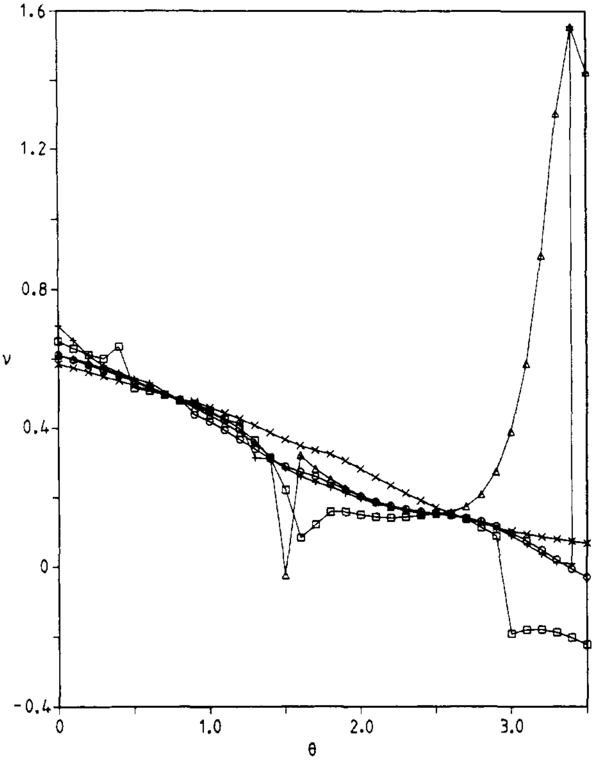

Figure 5. The effective exponent $2\nu(\theta)$ for approximants [5/6], [6/6], [6/7], [7/6] and [7/7] (notations as in figure 3).

Table 4. $\nu_t(\bar{\mu}_t)$ against θ between $\theta_{max}(l=15)=1.0$ and θ_{max} (extrapolated) $=0.6$. ×, defective poles.

	$\nu_t(\bar{\mu}_t)$				
$[L/M]/\theta$	0.6	0.7	0.8	0.9	1.0
[5/4]	0.789 (0.965)	0.761 (0.966)	0.734 (0.966)	0.710 (0.966)	0.688 (0.965)
[5/5]	0.497 (1.009)	0.488 (1.007)	0.482 (1.004)	0.476 (1.000)	0.469 (0.997)
[5/6]	0.510 (1.007)	0.496 (1.005)	0.480 (1.004)	0.477 (1.000)	0.460 (0.999)
[6/5]	0.520 (1.006)	0.500 (1.005)	0.480 (1.004)	0.460 (1.003)	0.440 (1.002)
[6/6]	0.516 (1.006)	0.496 (1.005)	0.482 (1.004)	0.439 (1.005)	0.420 (1.004)
[6/7]	0.508 (1.007)	0.496 (1.005)	0.479 (1.004)	0.472 (1.001)	0.450 (1.000)
[7/6]	0.519 (1.006)	0.499 (1.005)	0.479 (1.004)	0.459 (1.003)	0.437 (1.002)
[7/7]	0.530 (1.005)	× (×)	0.481 (1.004)	0.465 (1.002)	0.445 (1.001)

We have also computed the 'specific heat' (mean square fluctuations in the number of intersections) and showed the potential existence of a novel tricritical point as the fugacity for crossing is increased.

The maxima in the specific heat exhibit a regular trend towards lower values of θ as the order l in the series increases. We therefore have to extrapolate the value of θ_t and deduce the best bounds on the tricritical exponents. The generalised ratio method

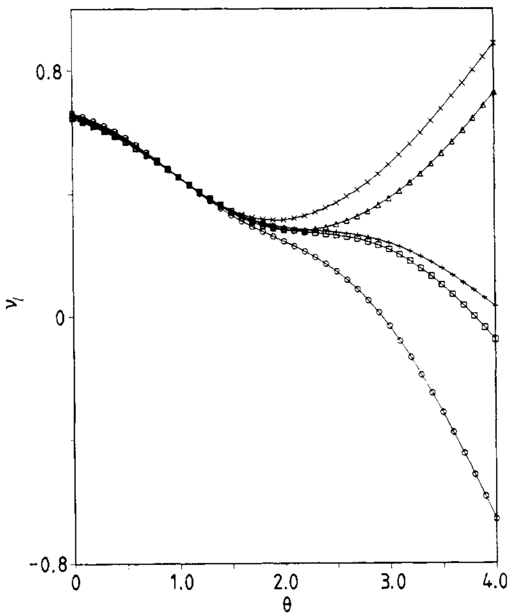

Figure 6. $\nu_l(\theta)$ (equation (5.1)) for $l = 11$–15.

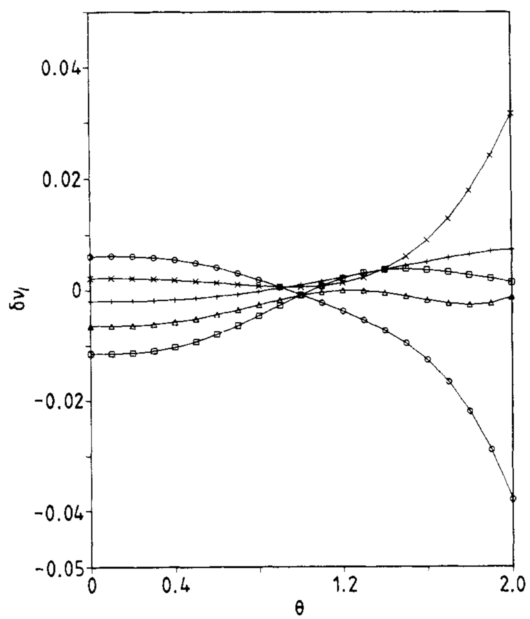

Figure 7. $\delta\nu_l(\theta)$ (equation (5.2)) for $l = 11$–15.

does not account for this trend and therefore yields values which are only consistent with the largest order ($l = 15$) available. Longer series or alternative methods like Monte Carlo or finite-size scaling will be necessary to extract more precise exponents. We note, for example, that our estimates yield a relation $\gamma_t > 2\nu_t$. This implies an unexpected negative value for the exponent η. It can be negative in the collapsed phase [10] but is expected to be non-negative at the tricritical point. But $\eta = 0$ was recently conjectured for the Θ point [11]. Despite the supporting evidence for a new tricritical behaviour, other possibilities, such as a fast crossover with rapid variation in various quantities (but no singularities) or a tricritical behaviour analogous to standard tricritical polymers (see, however, the above comment on the symmetry difference in their respective field theories), cannot be completely ruled out. We hope that the open questions will stimulate a more accurate determination of the tricritical properties for this special point which is inaccessible by renormalisation group and is not described by a perturbative fixed point in $4-\varepsilon$ dimensions. Finally, an identification of the tricritical point within the classification implied by conformal invariance may yield exact values for the tricritical exponents [10, 11].

Acknowledgments

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