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Oriented self-avoiding walks with orientation-dependent interactions

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Abstract. We consider oriented self-avoiding walks on the square lattice with different energies between steps that are oriented parallel or antiparallel across a face of the lattice. Rigorous bounds on the free energy and exact enumeration data are used to study the statistical mechanics of this model. We conjecture a phase diagram in the parallel–antiparallel interaction plane, and discuss the order of the associated phase transitions. The question, raised by previous field theoretical considerations, of the existence of an exponent that varies continuously with the energy of interaction is discussed at length. In connection with this we have also studied two oriented walks fixed at a common origin; this being the simplest model of branched oriented polymers in two dimensions. The evidence, although not conclusive, tends to support the field theoretic prediction.

1. Introduction

The statistics of flexible long-chain polymers in dilute solution is a subject of continuing theoretical interest, and the consideration of models that describe a situation where the effective forces between different (asymmetric) monomers depends on their relative orientation in space has received recent attention [1]. Oriented self-avoiding walks (these are self-avoiding walks (SAW) with a direction attached to the whole walk, which in turn is associated with each step of the walk) without interactions [2] have been studied previously in connection with a model of oriented polymers (such as A–B polyester). Miller [2] identified these walks with a *complex* $O(n \to 0)$ field theory, in an extension of the self-avoiding walk/$O(n \to 0)$ field theory correspondence of de Gennes [3].

An exciting set of predictions has arisen from conformal field theory in two dimensions [1]. These results flow partly from the work of Chaudhuri and Schwartz [4]. The most intriguing result is the prediction that if one considers the problem of oriented self-avoiding walks with a short-range interaction between sections of the walk that are oriented parallel to each other, the exponent associated with the partition function (usually denoted γ) depends continuously on the temperature (at least for a repulsive energy), while the exponent associated with the radius of gyration (or size) of the walk (usually denoted ν) is constant in the same range of temperatures.

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In this paper we consider a lattice model of oriented polymers in two dimensions which have two types of monomer–monomer interaction depending on their relative orientation in space. We consider the monomers as situated *on the bonds* of a SAW constructed on a square lattice, and simply add a direction to the walk to give each step an orientation. Interactions are considered between bonds of a walk that lie on the opposite edges of any face of the lattice. An oriented walk with the two types of interaction (IOSAW) is shown in figure 1. An energy $-\varepsilon_p$ is associated with parallel pairs of bonds which are indicated by the wavy lines on figure 1, while an energy $-\varepsilon_a$ is associated with antiparallel pairs of bonds which are indicated by the crosshatched lines. We will also consider two IOSAW fixed from the same origin: these are called interacting oriented two-legged stars (IO2S) and an example is shown in figure 2 (also with the interactions illustrated).

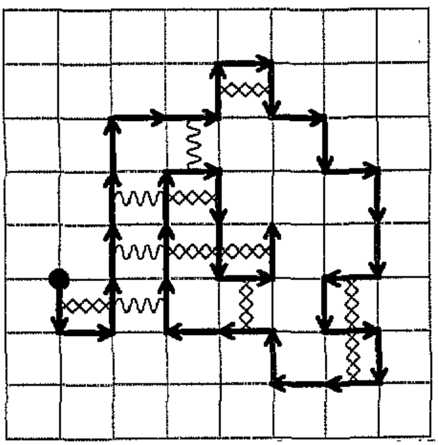

Figure 1. An oriented self-avoiding walk on the square lattice with parallel (wavy lines) and antiparallel (cross hatched lines) interactions identified. An energy $-\varepsilon_p$ ($-\varepsilon_a$) is associated with each pair of parallel (antiparallel) bonds.

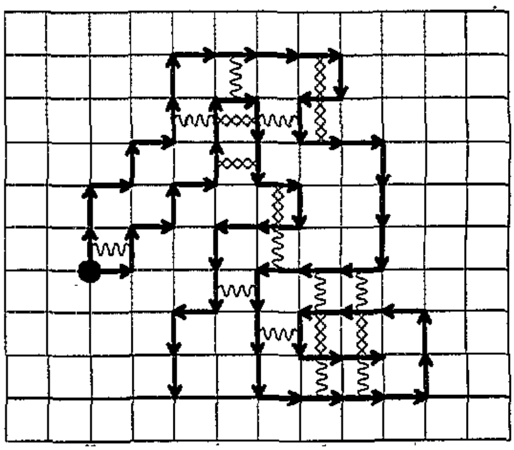

Figure 2. An oriented two-legged star with the parallel (wavy lines) and antiparallel (cross hatched lines) interactions highlighted. The origin is clearly identified.

We will prove some rigorous results, develop some heuristic arguments and analyse various exact enumerations in an attempt to map out the phase diagram of the model described above, as well as investigating the field theoretic predictions.

The paper is set out as follows. In the next section we define the partition function and other quantities of interest in the IOSAW model and state various predictions about their behaviour. We then prove some rigorous (and semi-rigorous) results concerning the free energy of IOSAW in section 3. Section 4 is a technical one explaining the exact enumeration of various quantities we have calculated for IOSAW and IO2S. The analysis of these enumerations in relation to the exponent γ is discussed in some detail in the following section (section 5). The qualitative phase diagram is mapped out by calculating the specific heat from the enumerations while various heuristic and exact results are used to conjecture an exact phase diagram in section 6. We end with a summary and cautionary statements about our results.

2. The model

The partition function of any of these interacting oriented problems is given by

$$Z_n(\beta_p, \beta_a) = \sum_{m_p, m_a} g_n(m_p, m_a)\, e^{\beta_p m_p + \beta_a m_a} \tag{1}$$

where the sum is over all allowed values of the number of parallel interactions, m_p, and the number of antiparallel interactions, m_a, and $g_n(m_p, m_a)$ is the number of configurations of length n with m_p and m_a parallel and antiparallel interactions respectively. For a two-legged star n is the total length of the two 'arms', and interactions are considered both between different steps within an arm and between steps in different arms equally. The convenient parameters β_p and β_a are given by $\beta_p = \beta\varepsilon_p$ and $\beta_a = \beta\varepsilon_a$ where $-\varepsilon_p$ and $-\varepsilon_a$ are the energies of a single parallel and antiparallel interaction respectively and β is the inverse temperature. The average energy is given by

$$\langle E\rangle = -\langle \varepsilon_p m_p + \varepsilon_a m_a\rangle \tag{2}$$

and the specific heat per step by

$$C_n = \frac{\langle E^2\rangle - \langle E\rangle^2}{n}. \tag{3}$$

The reduced free energy per step in the thermodynamic limit is

$$\kappa(\beta_p, \beta_a) = \lim_{n\to\infty} \frac{1}{n} \log[Z_n(\beta_p, \beta_a)]. \tag{4}$$

Another quantity we shall be interested in is the mean-square end-to-end displacement $\langle R_n^2\rangle$ which is a function of β_p and β_a also. We will consider these quantities for three cases: open walks; closed walks (or loops); and two-legged stars. Where necessary for clarity we shall denote walks, loops and stars by the superscripts w, l or s respectively (e.g. κ^w is the free energy for open walks).

We will examine the case where $\varepsilon_a = 0$ in some detail, which we call the parallel interaction model (note that this does not mean that antiparallel interactions are forbidden, only that their energy is zero). For this restriction the average energy is simply $\langle E\rangle = -\varepsilon_p\langle m_p\rangle$. The case of $\varepsilon_a = \varepsilon_p$ is a minor variation of the usual interacting self-avoiding walk problem (interactions are between bonds rather than sites).

It is expected that for some region around the origin of the (β_p, β_a) plane the partition function behaves like

$$Z_n(\beta_p, \beta_a) \sim A\mu^n n^{\gamma-1} \tag{5}$$

as $n \to \infty$. This should be true throughout the quadrant $(\beta_p \leqslant 0, \beta_a \leqslant 0)$. When $\beta_a = \beta_p$ it is assumed the A and μ (the connective constant) depend on the temperature while γ does not. At the free SAW point $\beta_a = \beta_p = 0$ we shall denote the connective constant μ by μ_s. However, the work of Cardy [1] predicts that $\gamma = \gamma(\beta_p)$ is a non-constant function of β_p when $\beta_a = 0$ (at least for negative values of β_p). For negative values of β_p it is rather μ that is constant, as we shall prove below. The change $\gamma(0) - \gamma(\beta_p)$ is expected to be positive as $\gamma(\beta_p)$ is expected to increase monotonically with β_p. Hence, $\gamma(0) - \gamma(-\infty)$ is greater than $\gamma(0) - \gamma(\beta_p)$ for $-\infty < \beta_p \leqslant 0$. The accepted value of $\gamma(0)$ is 43/32 [5].

More precisely, for $\beta_a = 0$, Cardy [1] predicts that the scaling dimensions x_q of 'charge' q associated with the vertices of an oriented star polymer are given by

$$x_q(\beta_p) = (\tfrac{9}{48} + 2\pi\lambda(\beta_p))q^2 - \tfrac{1}{12} \tag{6}$$

where $\lambda(\beta_p)$ is a function of β_p having the opposite sign to its argument (therefore being 0 at 0 argument) and probably monotonic. Further, the partition function exponent γ_L of a L-legged star polymer of oriented arms is given by

$$\gamma_L(\beta_p) = \nu(2L - x_L(\beta_p) - Lx_1(\beta_p)). \tag{7}$$

For a single oriented polymer the exponent γ is $\gamma(\beta_p) = \nu(2 - 2x_1(\beta_p))$. Let us define the change in $\gamma_L(\beta_p)$ as $\Delta\gamma_L = \gamma_L(0) - \gamma_L(\beta_p)$ then from (6) we have

$$\Delta\gamma_1 = 4\pi\nu(\lambda(0) - \lambda(\beta_p)) \tag{8}$$

and

$$\Delta\gamma_2 = 12\pi\nu(\lambda(0) - \lambda(\beta_p)) \tag{9}$$

hence

$$\frac{\Delta\gamma_2}{\Delta\gamma_1} = 3. \tag{10}$$

This result allows a finer check on any confirming results we might produce to support the predicted change in γ for walks, since (10) predicts that the change in γ for two-legged stars should be exactly three times larger than for walks.

A related prediction concerns the number of parallel contacts. Restricting ourselves to the parallel interaction problem ($\beta_a = 0$) and, assuming the necessary Tauberian theorem, differentiating equation (5), and normalizing with the partition function, we obtain

$$\langle m_p \rangle \sim \frac{\mathrm{d}\log A}{\mathrm{d}\beta_p} + \frac{\mathrm{d}\gamma}{\mathrm{d}\beta_p}\log n + \frac{\mathrm{d}\log\mu}{\mathrm{d}\beta_p}n \tag{11}$$

as $n \to \infty$. Now, if μ is a constant then

$$\langle m_p \rangle \sim \gamma'(\beta_p)\log n \tag{12}$$

for $\beta_p \leqslant 0$ (the prime denoting differentiation). Hence, one test of the Cardy predictions is to calculate $\langle m_p \rangle$ at the free SAW point $\beta_p = \beta_a = 0$ as this should grow logarithmically in n and the amplitude should give the change in γ near the origin. This second observation serves as a check on any values of γ calculated directly for the partition function.

Simultaneously, it is expected that the mean-square end-to-end distance of the IOSAW scales like

$$\langle R_n^2 \rangle \sim Bn^{2\nu} \tag{13}$$

as $n \to \infty$, with ν a constant in some region around the origin including the quadrant ($\beta_p \leqslant 0, \beta_a \leqslant 0$). This value of ν can then be inferred from its value at the point $\beta_p = \beta_a = 0$, given by Nienhuis [5] as $\nu = 3/4$. In particular, this should be true for the whole of the line $\beta_p \leqslant 0, \beta_a = 0$. We then have a situation where for the negative axis one exponent, ν, is a constant while another, γ, varies continuously.

One question that we shall tackle in this paper is whether this scenario is true for $\beta_a = 0$, or more simply whether $\gamma(-\infty) \neq \gamma(0)$? The other topic discussed will be a general elucidation of the phase diagram in the (β_p, β_a) plane. If $\beta_a = \beta_p$ one obtains a model of the θ-point collapse transition which should occur at some attractive value of the interactions. On the other hand a large value of β_p at fixed β_a favours *compact, spiral* configurations. Hence on the line $\beta_a = 0$ there should be a transition at some positive value of β_p to a phase dominated by such configurations. In fact, we will show in the next section that there must be at least one point of non-analyticity in the free energy on this line.

3. Free energy bounds

We begin by noting that oriented loops do not contain any parallel pairs of bonds and so all quantities calculated from only loop configurations are independent of β_p. Hence $Z_n^l(\beta_p, \beta_a) \equiv Z_n^l(\beta_a)$.

Let us consider the reduced free energy per step, $\kappa(\beta_a, \beta_p)$. The limit (4) is known to exist at the free SAW point for open walks and loops (a reformulation of these proofs, originally by Hammersley, is given in the book by Madras and Slade [6] with references). It is also known to be the same positive value, which is given by $\log \mu_s$. We begin by restricting ourselves to the 'parallel problem' $\beta_a = 0$.

Let $\beta_p < 0$ and $\hat{g}_n(m_p) = \sum_{m_a} g_n(m_p, m_a)$ then

$$Z_n^w(\beta_p, 0) = \sum_{m_p} \hat{g}_n(m_p)\, e^{\beta_p m_p} < \sum_{m_p} \hat{g}_n(m_p) = Z_n^w(0,0) \tag{14}$$

provided at least one $m_p > 0$. Also, the set of oriented loops (oriented rooted polygons) of length $n+1$ is in one-to-one correspondence with oriented open walks of length n whose starting and ending points are one lattice spacing apart (just remove the last step of the polygon to make a walk and *vice versa*. These walks clearly do not possess any parallel interactions, and so they form a proper subset of the number of open walks without any parallel interactions (a rod configuration is also in this set). Hence,

$$\begin{aligned} Z_n^w(\beta_p, 0) &= \sum_{m_p, m_a} g_n^w(m_p, m_a)\, e^{\beta_p m_p} > \sum_{m_p, m_a} g_{n+1}^l(m_p, m_a)\, e^{\beta_p m_p} \\ &= \sum_{m_a} g_{n+1}^l(0, m_a) = Z_{n+1}^l(0). \end{aligned} \tag{15}$$

Considering both the above inequalities and then taking logarithms gives

$$\log(Z_{n+1}^l(0)) < \log(Z_n^w(\beta_p, 0)) < \log(Z_n^w(0,0)). \tag{16}$$

Taking the limit $n \to \infty$ proves that the free energy $\kappa(\beta_p, 0)$ exists and is equal to

$$\kappa(\beta_p, 0) = \log \mu_s \qquad \text{for } -\infty < \beta_p \leqslant 0. \tag{17}$$

For $\beta_p > 0$ it is true that

$$Z_n^w(\beta_p, 0) > Z_n^w(0,0) \tag{18}$$

and so if one *assumes* that the free energy exists in this range one has

$$\kappa(\beta_p, 0) \geqslant \log \mu_s \qquad \text{for } 0 < \beta_p < \infty. \tag{19}$$

However, there are other bounds one can find *assuming* that the walk free energy exists. These are predicated on the fact that the maximum number of parallel interactions $m_p^{\max}(n) \sim n$ as $n \to \infty$. For any n, let k be the largest integer such that $k^2 \leqslant n$. Now consider oriented walk configurations of length k^2. There is one configuration which is a tightly bound square spiral that has $k^2 - 4k + 4$ parallel contacts. This is constructed from the origin by a single step in some direction followed by a step to the left followed by two steps to the left of that, and then again, then three steps for the next two left turns, etc (one could equally well choose all right turns). By extending this configuration to length n in such a manner that it keeps its spiral shape, we see that

$$n - 6n^{1/2} \leqslant k^2 - 4k + 4 \leqslant m_p^{\max}(n). \tag{20}$$

It is clear that $m_p^{\max}(n) < n$ and so

$$\lim_{n\to\infty} \frac{m_p^{\max}(n)}{n} = 1. \tag{21}$$

Now,

$$Z_n^{\rm w}(\beta_{\rm p},0)=\sum_{m_{\rm p}}\hat g_n(m_{\rm p})\,{\rm e}^{\beta_{\rm p}m_{\rm p}} > \hat g_n(m_{\rm p}^{\rm max})\,{\rm e}^{\beta_{\rm p}m_{\rm p}^{\rm max}} \tag{22}$$

as the partition function is a sum of positive terms, so

$$\kappa(\beta_{\rm p},0)\geqslant\beta_{\rm p}. \tag{23}$$

Also, defining $g_n=\sum_{m_{\rm p}}\hat g_n(m_{\rm p})$,

$$Z_n^{\rm w}(\beta_{\rm p},0)=\sum_{m_{\rm p}}\hat g_n(m_{\rm p})\,{\rm e}^{\beta_{\rm p}m_{\rm p}} < g_n\sum_{m_{\rm p}=0}^{m_{\rm p}^{\rm max}}{\rm e}^{\beta_{\rm p}m_{\rm p}} < Z_n^{\rm w}(0,0)\left(\frac{{\rm e}^{n\beta_{\rm p}}-1}{{\rm e}^{\beta_{\rm p}}-1}\right) \tag{24}$$

since $g_n>\hat g_n(m_{\rm p})$, and hence

$$\kappa(\beta_{\rm p},0)\leqslant\beta_{\rm p}+\log\mu_s \qquad \text{for } 0<\beta_{\rm p}<\infty. \tag{25}$$

These bounds are illustrated in figure 3.

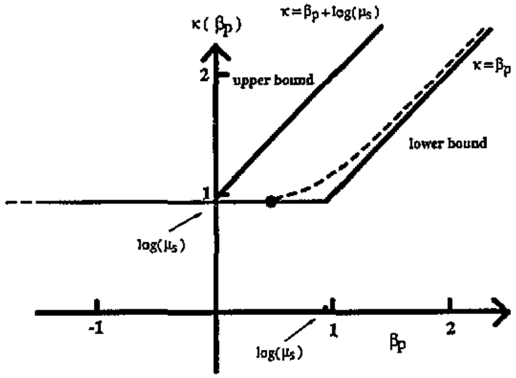

Figure 3. This figure illustrates the bounds on the (reduced) free energy $\kappa(\beta_{\rm p})$ of the parallel interaction model ($\beta_{\rm a}=0$) plotted against $\beta_{\rm p}$ (bold lines). It also gives a general scenario (broken line) for the behaviour of $\kappa(\beta_{\rm p})$ where it has one singularity (the point indicated)—it must have one non-analytic point but may have more than one. For negative values of $\beta_{\rm p}$ the value of $\kappa(\beta_{\rm p})$ is constrained to be $\log\mu_s$.

For $\beta_{\rm a}\neq 0$, and fixed, the above bounds on the free energy as a function of $\beta_{\rm p}$ still hold with the point $\beta_{\rm p}=\beta_{\rm a}$ taking the place of $\beta_{\rm p}=\beta_{\rm a}=0$. However, we no longer know that the free energy exists at this point, although it would be commonly accepted among physicists that it does! The following can be deduced assuming that the free energy exists. First, for all $\beta_{\rm a}$

$$\kappa(\beta_{\rm p},\beta_{\rm a})=\kappa(\beta_{\rm a},\beta_{\rm a}) \qquad \text{for } -\infty<\beta_{\rm p}\leqslant\beta_{\rm a}. \tag{26}$$

This can be proved using a simple generalization of the argument given above for the case with $\beta_{\rm a}=0$ and uses the fact that removing a bond from a loop removes a maximum of two antiparallel contacts. In fact, this result is implied if one accepts that the free energy of walks and loops are equal since the free energy of loops is independent of $\beta_{\rm p}$. However, for $\beta_{\rm p}>0$ it can be shown in a manner similar to above that

$$\kappa(\beta_{\rm p},\beta_{\rm a})\geqslant\beta_{\rm p} \tag{27}$$

and this implies that the walk and loop free energies must differ for $\beta_{\rm p}$ large enough. Also, for all $\beta_{\rm p}$ and $\beta_{\rm a}$,

$$\kappa(\beta_{\rm p},\beta_{\rm a})\geqslant\kappa(\beta_{\rm a},\beta_{\rm a}). \tag{28}$$

These results imply that for any fixed value of $\beta_{\rm a}$ the free energy $\kappa(\beta_{\rm p},\beta_{\rm a})$ has at least one non-analytic point as a function of $\beta_{\rm p}$. The simplest scenario imaginable is that there is only one such point and further that this point is given by the equation

$$\beta_{\rm p}^{\rm t}(\beta_{\rm a})=\kappa(\beta_{\rm a},\beta_{\rm a}) \tag{29}$$

where β_p^t denotes that single transition value of the interaction parameter β_p. We will argue later that this is a likely scenario! Other, more complicated, possibilities are as follows. There could be a single non-analyticity of κ at a positive value of β_p smaller than that given by the above. This must therefore correspond to the spiral collapse transition, and it could be of first or second order. However, we shall argue that this possibility is unlikely since it would require the spiral phase to have a non-zero $O(n)$ (total) entropy in addition to its energy per unit length. Alternatively, there could be more than one point of non-analyticity, with the one at the smallest value of β_p not corresponding to the collapse transition. In that case the latter could occur at a value of β_p larger than that given by (29), and it could be first or second order. This possibility is unattractive because there appears to be no physical reason for any non-analyticity arising apart from at the collapse transition.

4. Exact enumerations

4.1. Calculation of series

We have enumerated oriented walks, and oriented stars with two arms, on the square lattice. The basic algorithm is the simple backtracking method [7]. However, as all our enumerations have been carried out on a multiprocessor Intel Paragon supercomputer we were able to significantly enhance the speed of the algorithm by dividing up the enumerations among the available processors. When all possible symmetries on the square lattice for walks are exploited, the total number of distinct configurations of length 5 is 36 (as opposed to 284 without exploiting symmetry). For each particular five-step walk we programmed its configuration into the code running on a different processor. We did this so that each (of 36) processor used counted only those configurations containing a particular five-step pattern at the beginning of the walk. Except for some final additions that required communication among the processors the algorithm was nearly fully parallelized. We obtained a parallelization of about 86%.

Our algorithm counted the number of walks and stars, $g_n(m_p, m_a)$, with m_p parallel and m_a antiparallel interactions along with a calculation of the sum of their square end-to-end displacements $r_n^2(m_p, m_a)$. We were able to obtain all walks of length $n = 29$ and stars of total length $n = 27$. These enumerations took 116 and 151 h of CPU time respectively for walks and stars. These results were checked completely independently for walks up to $n = 24$, using a backtracking algorithm on a Sun workstation.

The sum over m_a can be performed if one is interested only in $\beta_a = 0$ and these series are given in tables 1 and 2†. These coefficients can be used in the following way to obtain the quantities of interest. For both walks and stars, the partition function for $\beta_a = 0$ is given by

$$\hat{Z}_n(\beta_p) = Z_n(\beta_p, 0) = \sum_{m_p} \hat{g}_n(m_p)\, e^{\beta_p m_p} \tag{30}$$

while the mean-square end-to-end distance for $\beta_a = 0$ is given as

$$\langle R_n^2 \rangle = \frac{\sum_{m_p} \hat{r}_n^2(m_p)\, e^{\beta_p m_p}}{\hat{Z}_n(\beta_p)}. \tag{31}$$

† The full series can be obtained via e-mail to tonyg@mundoe.maths.mu.oz.au

Table 1. The enumerations for open oriented walks of lengths $n = 1$ to 29 in the case of the parallel interaction problem. One quarter of the number of walks $\hat{g}_n(m_p)/4$ of length n with m_p parallel interactions and one quarter of the total square end-to-end distance of walks $\hat{r}_n^2(m_p)/4$ of length n with m_p parallel interactions are given.

		IOSAW				IOSAW	
n	m_p	$\hat{g}_n(m_p)/4$	$\hat{r}_n^2(m_p)/4$	n	m_p	$\hat{g}_n(m_p)/4$	$\hat{r}_n^2(m_p)/4$
1	0	1	1	2	0	3	8
3	0	9	41	4	0	25	176
5	0	71	679	6	0	195	2452
7	0	543	8447	8	0	1475	28 112
					1	4	8
9	0	4059	91 107	10	0	10 969	289 084
	1	8	40		1	56	240
11	0	29 945	901 729	12	0	80 665	2 772 904
	1	120	952		1	552	4064
	2	8	40		2	16	144
13	0	218 959	8 425 599	14	0	588 473	25 340 572
	1	1288	14 760		1	4848	54 528
	2	128	960		2	270	3240
					3	20	160
15	0	1 590 803	75 542 739	16	0	4 267 549	223 467 640
	1	11 960	186 600		1	40 316	637 400
	2	1346	14 458		2	3136	48 280
	3	36	484		3	324	3592
	4	4	20		4	8	72
17	0	11 501 007	656 574 599	18	0	30 806 097	1 917 488 084
	1	102 488	2 087 160		1	324 100	6 793 752
	2	12 382	181 950		2	30 682	595 104
	3	692	11 092		3	3588	52 288
	4	100	980		4	196	2960
					5	20	136
19	0	82 824 995	5 569 812 347	20	0	221 570 087	16 100 667 256
	1	837 204	21 529 156		1	2 542 572	67 798 696
	2	106 986	2 054 706		2	273 664	6 558 000
	3	8648	166 040		3	34 672	644 600
	4	1282	18 170		4	2924	55 584
	5	32	400		5	356	4304
	6	8	40		6	16	144
21	0	594 580 341	46 338 890 829	22	0	1 588 892 227	132 837 329 628
	1	6 630 148	209 613 636		1	19 587 076	644 303 064
	2	887 978	21 490 010		2	2 310 642	67 101 896
	3	88 712	2 047 720		3	311 984	7 194 912
	4	13 400	247 664		4	33 404	771 224
	5	768	12 800		5	4428	74 296
	6	160	1424		6	324	4480
					7	36	240

Table 1. (Continued)

	IOSAW				IOSAW		
n	m_{p}	$\hat{g}_n(m_{\mathrm{p}})/4$	$\hat{r}_n^2(m_{\mathrm{p}})/4$	n	m_{p}	$\hat{g}_n(m_{\mathrm{p}})/4$	$\hat{r}_n^2(m_{\mathrm{p}})/4$
23	0	4 257 153 519	379 418 996 743	24	0	11 365 906 867	1 080 126 940 904
	1	51 379 748	1 954 239 492		1	148 817 252	5 896 747 672
	2	7 159 090	212 333 074		2	18 815 380	650 879 520
	3	820 700	22 577 372		3	2 675 412	74 804 088
	4	127 336	2 929 944		4	332 200	9 135 048
	5	10 996	227 412		5	46 848	997 352
	6	1992	27 912		6	4762	86 776
	7	56	696		7	576	6472
	8	16	80		8	28	256
					9	4	32
25	0	30 413 572 867	3 065 516 572 683	26	0	81 134 673 811	8 675 779 763 380
	1	391 860 612	17 615 053 412		1	1 118 471 472	52 382 283 568
	2	56 483 202	2 008 548 714		2	149 323 228	6 062 674 824
	3	7 133 984	231 238 944		3	22 168 440	737 346 552
	4	1 141 204	31 765 052		4	3 043 658	98 205 200
	5	123 804	3 100 588		5	452 576	11 736 512
	6	21 430	409 630		6	55 378	1 273 968
	7	1328	20 192		7	7256	116 816
	8	288	2512		8	628	8312
	9	8	104		9	108	968
27	0	216 867 806 851	24 489 537 270 883	28	0	578 138 389 481	68 960 647 337 768
	1	2 952 534 332	154 553 727 500		1	8 333 319 312	454 210 850 712
	2	438 258 816	18 357 949 744		2	1 162 706 168	54 701 002 072
	3	59 500 600	2 246 701 928		3	179 025 656	6 973 388 848
	4	9 808 858	323 464 450		4	26 432 542	988 534 848
	5	1 229 096	36 493 368		5	4 113 356	126 922 432
	6	211 412	5 098 244		6	568 528	15 863 280
	7	19 116	368 620		7	79 776	1 670 376
	8	3582	47 598		8	9242	156 408
	9	208	3104		9	1428	18 392
	10	36	228		10	56	624
					11	16	136
29	0	1 543 880 629 933	193 750 855 625 205				
	1	22 035 454 044	1 326 500 048 108				
	2	335 579 3648	163 197 192 464				
	3	481 959 556	20 975 284 964				
	4	81 693 978	3 140 425 418				
	5	11 297 676	391 447 100				
	6	1 964 474	57 355 802				
	7	220 416	5 264 576				
	8	39 372	716 612				
	9	3640	61 224				
	10	564	5396				
	11	24	328				
	12	8	104				

4.2. Analysis

After construction of the partition function (mean-square end-to-end distance) at some value of the interaction parameters, the corresponding exponent γ (2ν) was investigated utilizing

Table 2. The enumerations for (open) oriented two-legged stars of lengths $n = 1$ to 27 in the case of the parallel interaction problem. One quarter of the number of stars $\hat{g}_n(m_p)/4$ of (total) length n with m_p parallel interactions and one quarter of the total square end-to-end distance of stars $\hat{r}_n^2(m_p)/4$ of length n with m_p parallel interactions are given.

		IO2S				IO2S	
n	m_p	$\hat{g}_n(m_p)/4$	$\hat{r}_n^2(m_p)/4$	n	m_p	$\hat{g}_n(m_p)/4$	$\hat{r}_n^2(m_p)/4$
1	0	2	2	2	0	9	22
3	0	32	136	4	0	109	692
	1	4	12		1	16	88
5	0	358	3094	6	0	1133	12 722
	1	64	472		1	216	2152
	2	4	36		2	16	200
7	0	3528	49 184	8	0	10 709	181 480
	1	740	9092		1	2332	35 496
	2	72	1016		2	254	4240
	3	4	76		3	16	376
9	0	32 266	646 154	10	0	95 487	2 233 170
	1	7412	133 156		1	22 528	477 104
	2	908	17 364		2	2964	65 040
	3	80	1944		3	280	7688
	4	4	132		4	16	616
11	0	281 332	7 539 916	12	0	818 181	24 936 756
	1	68 672	1 668 136		1	203 916	5 662 144
	2	9692	239 692		2	30 080	839 032
	3	1088	31 664		3	3524	114 632
	4	88	3320		4	312	12 824
	5	4	204		5	16	920
13	0	2 372 066	81 125 738	14	0	6 811 357	259 953 914
	1	605 680	18 896 240		1	1 767 972	61 762 992
	2	93 964	2 906 180		2	282 444	9 723 496
	3	12 176	422 480		3	37 788	1 446 160
	4	1264	53 760		4	4244	192 584
	5	96	5208		5	344	19 880
	6	4	292		6	16	1288
15	0	19 511 564	822 836 156	16	0	55 482 625	2 574 520 744
	1	5 159 792	199 396 528		1	14 866 224	633 818 392
	2	856 404	32 288 844		2	2 521 324	104 575 176
	3	122 060	4 999 852		3	369 360	16 487 168
	4	14 952	714 688		4	47 712	2 428 008
	5	1504	86 264		5	5024	306 272
	6	104	7672		6	376	29 112
	7	4	396		7	16	1720

differential approximants [8]. This method involves fitting the available series coefficients sequentially to linear, quadratic and higher-order recurrence relations of a specific form which can then be solved, giving linear homogeneous differential equations with polynomial coefficients. The solution of these equations allows us to estimate the critical point (which

Table 2. (Continued)

		IO2S				IO2S	
n	m_p	$\hat{g}_n(m_p)/4$	$\hat{r}^2_n(m_p)/4$	n	m_p	$\hat{g}_n(m_p)/4$	$\hat{r}^2_n(m_p)/4$
17	0	157 466 362	7 979 393 866	18	0	444 313 587	24 505 683 562
	1	42 830 048	1 995 912 944		1	122 161 464	6 209 885 320
	2	7 481 440	336 721 760		2	21 707 340	1 064 065 048
	3	1 144 440	54 635 112		3	3 397 164	175 208 000
	4	157 032	8 429 896		4	483 078	27 615 652
	5	18 884	1 164 812		5	59 948	3 929 440
	6	1720	130 488		6	5972	465 040
	7	112	10 776		7	408	40 776
	8	4	516		8	16	2216
19	0	1 251 745 156	74 695 658 044	20	0	3 509 847 821	225 997 101 028
	1	348 452 556	19 179 211 604		1	985 932 348	58 666 824 000
	2	63 383 944	3 346 568 312		2	181 882 272	10 372 945 776
	3	10 244 772	563 293 156		3	29 952 024	1 767 614 056
	4	1 525 636	91 821 956		4	4 577 618	292 866 008
	5	206 012	13 865 308		5	635 440	45 226 944
	6	22 864	1 803 312		6	75 144	6 113 400
	7	2036	190 660		7	6988	678 232
	8	120	14 584		8	440	55 128
	9	4	652		9	16	2776
21	0	9 828 842 750	679 593 229 246	22	0	27 416 700 147	2 031 108 027 406
	1	2 789 973 524	178 393 992 692		1	7 842 733 220	538 198 519 240
	2	524 606 968	32 024 938 488		2	1 492 230 550	97 726 183 660
	3	88 613 584	5 554 247 272		3	256 005 572	17 129 182 904
	4	14 039 136	944 112 728		4	41 393 562	2 950 240 772
	5	2 063 364	151 977 100		5	6 229 020	483 465 816
	6	262 608	21 876 008		6	828 246	71 585 412
	7	28 812	2 719 988		7	93 708	9 207 424
	8	2276	266 732		8	8270	959 180
	9	128	19 160		9	472	72 424
	10	4	804		10	16	3400
23	0	76 393 936 468	6 039 599 531 780	24	0	212 163 044 863	17 866 761 710 728
	1	22 049 670 504	1 615 798 341 344		1	61 647 532 900	4 819 202 200 448
	2	4 262 685 728	297 226 995 592		2	12 039 089 638	895 407 169 216
	3	746 564 464	52 862 012 088		3	2 136 429 452	160 725 211 776
	4	124 218 080	9 290 761 824		4	361 446 000	28 562 113 904
	5	19 487 852	1 570 169 684		5	57 840 228	4 898 028 968
	6	2 738 440	243 298 120		6	8 388 392	775 409 184
	7	344 124	33 768 580		7	1 084 700	110 533 688
	8	34 336	3 931 920		8	116 838	13 460 664
	9	2736	367 504		9	9656	1 319 088
	10	136	24 568		10	542	93 792
	11	4	972		11	16	4088

gives the growth constant of the series) and its corresponding critical exponent.

For each length N, a number of approximants were found, with any defective approximants being ignored in the subsequent analysis. Any approximant was considered defective if there was a singularity on the positive real axis closer to the origin or if there was a singularity beyond but close to the physical singularity. In our analysis we have taken

Table 2. (Continued)

	IO2S				IO2S		
n m_p		$\hat{g}_n(m_p)/4$	$\hat{r}_n^2(m_p)/4$	n m_p		$\hat{g}_n(m_p)/4$	$\hat{r}_n^2(m_p)/4$
25	0	588 682 707 150	52 628 502 262 702	26	0	1 628 804 584 207	154 343 794 929 098
	1	172 388 128 812	14 314 983 158 164		1	479 774 019 936	42 285 075 888 720
	2	34 123 384 304	2 689 802 910 376		2	95 807 788 074	8 016 110 246 356
	3	6 160 580 012	488 817 785 572		3	17 493 573 012	1 468 723 280 368
	4	1 066 842 440	88 311 219 792		4	3 072 124 056	267 874 866 528
	5	176 292 148	15 511 352 276		5	516 195 828	47 627 183 536
	6	26 687 132	2 541 894 340		6	80 064 018	7 939 041 756
	7	3 703 508	382 363 892		7	11 390 324	1 220 242 496
	8	434 376	50 230 536		8	1 408 482	165 814 436
	9	43 788	5 625 076		9	146 412	19 245 920
	10	3084	490 212		10	12 060	1 796 704
	11	144	30 872		11	560	117 744
	12	4	1156		12	16	4840
27	0	4 503 113 843 288	450 988 762 706 944				
	1	1 335 517 920 776	124 473 960 244 504				
	2	269 815 586 320	23 831 141 297 856				
	3	49 990 905 792	4 413 168 205 768				
	4	8 950 830 880	816 067 121 248				
	5	1 543 132 656	147 914 590 640				
	6	247 633 380	25 334 694 404				
	7	37 072 832	4 053 152 856				
	8	4 884 144	582 100 736				
	9	574 076	73 948 772				
	10	53 188	7 799 540				
	11	3908	65 412				
	12	152	38 136				
	13	4	1356				

approximants to be defective if they are within a factor of 1.3 of the physical singularity. More precisely, approximants with singularities in the complex plane found within a strip bounded by $\pm 0.05i$ and $[0, 1.3x_c]$, where x_c is the estimate of the physical singularity's position, are considered defective. The non-defective approximants were then averaged, with the error given as two standard deviations. As N increases, the values of the exponent and critical point are expected to become more accurate, and a weighted average of the most accurate values of the exponent with at least four non-defective approximants were taken to give an estimate of the exponent for large N. These values, and a discussion on their significance, are given in section 5.

As discussed in section 6, the specific heat per step $C_n(\beta_p)$ has been used to probe the possible onset of any phase transitions. We initially set $\beta_a = d_1\beta_p$ (since for a system with (non-zero) fixed energies ε_p and ε_a one has $d_1 = \varepsilon_a/\varepsilon_p$), but such rays emanating from the origin are close to tangential to part of a phase boundary. Accordingly, we have also set $\beta_a = d_1\beta_p + d_2$, and for particular values of d_1 and d_2 made simple plots of $C_n(\beta_p)$ against β_p so as to find the maximum of $C_n(\beta_p)$ along a line in the (β_p, β_a) plane. This allows us to gain a full two-dimensional representation of the specific heat behaviour (see figure 7) by choosing different values of d_2. Figure 7 has been produced from the choice $d_1 = -1$ and $d_1 = 4$, and varying d_2 over a range of values, in order to cover the plane.

5. The exponent γ

We will only consider the parallel interaction model with $\beta_a = 0$. Although a variation in γ is predicted to occur for other values of β_a it is at $\beta_a = 0$ that the value of the connective constant is most accurately known, and this will help with the analysis.

We utilized unbiased second-order differential approximants of the generating function $G(x) = \sum_n Z_n x^n$ of the (walk) series $\hat{Z}_n^w(\beta_p)$ in order to determine the critical point $x_c(\beta_p) = 1/\mu(\beta_p)$ and associated exponent $\gamma(\beta_p)$ for various values of β_p. Initially we found that for $\beta_p = 0$ (the free SAW point) $x_c(0) = 0.379\,0520(4)$, which may be compared with the best numerical estimate available of 0.379 0524(5) [9], and $\gamma(0) = 1.343\,58(22)$ which may be compared to the exact value of $\gamma^{\text{exact,w}}(0) = 43/32 = 1.343\,75$ (a difference of 0.000 17(22)). In figure 4 we show a plot of $\gamma^{\text{exact,w}}(0) - \gamma(\beta_p)$ against β_p for walks, and $\frac{1}{3}[\gamma^{\text{exact,s}}(0) - \gamma(\beta_p)]$ for stars, obtained from this type of analysis, where for stars $\gamma^{\text{exact,s}}(0) = 75/32 = 2.343\,75$ (see equations (6) and (7)). As one can see $\gamma(\beta_p)$ seems to be monotonic so we shall concentrate our discussion on the case $\beta_p = -\infty$. Our estimate for $\gamma(-\infty)$ is 1.3347(33) which implies that $\gamma^{\text{exact,w}}(0) - \gamma(-\infty)$ is 0.0091(33). This is not particularly large! Moreover, there is a small apparent shift in the estimated critical point to $x_c(0) - x_c(-\infty) = 0.000\,017(13)$ which gives one some apprehension about attaching significance to the shift in the exponent.

We also analysed the series with the coefficients $\hat{Z}_n(0)/\hat{Z}_n(-\infty)$. This series was estimated to have a critical point at 1.000 063(19) (by theory it should be exactly 1) and an exponent (which should be identified with $\gamma(0) - \gamma(-\infty)$) of 0.0115(15). Hence this gives a slightly larger result for the change in γ than does the Z_n series alone, though with overlapping error bars and a slightly worse critical point estimate. It appears that, without the knowledge of Cardy's prediction, such an analysis of IOSAW is unlikely to prompt one to suggest that γ is varying with β_p. However, given the prediction, neither does it rule it out, and we feel that the further considerations (below) tip the balance in the positive direction for such a prediction.

One can compare the behaviour of these results to a corresponding analysis of the end-to-end distance series $\langle R_n^2 \rangle$. The exponent ν is usually less well behaved, and so it is not surprising that we estimate $\nu(0) = 0.7458(6)$ and $\nu(-\infty) = 0.7335(11)$ with critical points at 0.999 936(16) and 0.999 757(34) respectively. While the exponent values do not necessarily inspire confidence that our perceived change in γ reflects the real situation, it does hint that the critical point change is small enough to be considered insignificant. We also mention that we attempted to use biased approximants for many of these analyses but were hindered by the fact that this consistently gave rather few non-defective approximants. Worryingly, however, these approximants that did survive gave a change in γ that was even smaller than given above from the unbiased results.

Our first consistency check (for walks) was to estimate $\gamma'(0)$ from our plot of $\gamma(\beta_p)$ and also from the local slope of the graph of $\langle m_p \rangle$ against $\log(n)$ for the largest values of n available. The first gave $\gamma'(0) = 0.014(4)$ while the second gave 0.013(5). The errors quoted are simple statistical errors: the first deduced from the errors in the values of $\gamma(\beta_p)$ and the second from linear regression on the largest four values of n. They should not be invested with too much authority! One can, for example, change the value of the slope obtained (within the errors quoted) by plotting $\langle m_p \rangle$ against $\log(n - a)$ for some constant a in the (reasonable) range -4 to 7. However, the values give some confidence that the theory developed in section 2 is consistently (if only weakly) confirmed by our walk enumerations. On the other hand it would be surprising if there were not significant corrections to scaling even for moderate values of n in the $\langle m_p \rangle$ plot and so the value of the slope estimated without extrapolation is likely to contain systematic error. Figure 5 is a plot of $\langle m_p \rangle$ against $\log(n)$ for walks and stars. Of course, the divergence in $\langle m_p \rangle$ as n becomes large indicates that γ should change (assuming the form (5)). More generally, if m_p grows without bound in any fashion, it indicates that the asymptotic form (5) for the weighted number of walks (with γ independent of β_p) cannot be correct.

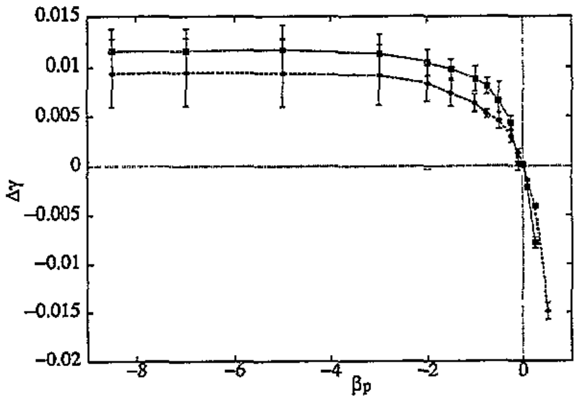

Figure 4. A plot of $(43/32-\gamma^{w}(\beta_p))$ against β_p for walks (diamonds) and $\frac{1}{3}(75/32 - \gamma^{s}(\beta_p))$ against β_p for stars (squares) obtained from analysis of the series for $\hat{Z}_n(\beta_p)$. The factor of $\frac{1}{3}$ highlights the field theoretic prediction that the ratio of the changes in γ^w and γ^s should be $\frac{1}{3}$.

We then repeated this exercise for the two-legged star enumeration data. This perhaps provides the strongest evidence that the theory is correct. We obtained a change in the exponent γ^s that gave the estimate $\frac{1}{3}[\gamma^{\text{exact},s}(0) - \gamma^s(-\infty)] = 0.0116(24)$ using the $\hat{Z}_n^s$ series, and $\frac{1}{3}[\gamma^s(0) - \gamma^s(-\infty)] = 0.0113(23)$ using the ratio $\hat{Z}_n^s(0)/\hat{Z}_n^s(-\infty)$. These compare favourably, within error bars (see also figure 4 which uses the $\hat{Z}_n^s$ series over a range of β_p), with the changes given above for $\gamma^{\text{exact},w}(0) - \gamma^w(-\infty)$ from $\hat{Z}_n^w$ and $\gamma^w(0) - \gamma^w(-\infty)$ from the ratio $\hat{Z}_n^w(0)/\hat{Z}_n^w(-\infty)$ (that is, 0.0091(33) and 0.0115(15) respectively). The value of $\gamma^s(0)$ was estimated to be 2.343 38(89) compared to the exact value $\gamma^{\text{exact},s}(0)$ of $75/32 = 2.343\,75$, while $x_c^s(0) = 0.379\,0511(39)$ which should be the same as for walks. The critical point $x_c^s(-\infty)$ was estimated to be $x_c(0) - x_c(-\infty) = 0.000\,061(44)$; a slightly larger change than for walks. The values of $\nu^s(0) = 0.7485(18)$ and $\nu^s(-\infty) = 0.7647(12)$ differ from the exact 0.75 by about similar (absolute) amounts to those obtained in the walk case (see above), which indicates that the factor of three found in the changes in γ between walks and two-legged stars is not simply due to less accurate estimation for stars.

Again we considered the value of $\gamma'^{,s}(0)$ estimated from the plot in figure 4 and compared this to the slope of $\langle m_p^s \rangle$ against $\log(n)$ (see figure 5). This gave 0.07(2) for the first compared to 0.08(2) for the second method. As for walks the errors should not be invested with too much significance. This is less convincing than in the walk case but there is a clear curvature left in the plot of $\langle m_p^s \rangle$ against $\log(n)$ and so this could be due to the corrections to scaling being stronger here. On the negative side these estimates are quite far from three times their walk cousins (which require values closer to 0.04 to 0.05) but as noted there is curvature in the plots, which is in the direction required to bring the numerical results into registration with the theory. Once again, we note that while biased approximants were attempted, the results suffered from a lack of acceptable approximants.

In summary, we conclude that while a small change in γ has been found from a differential approximant analysis of partition function series, the modest length of the series precludes any conclusive statements. Supportive evidence for a small change in γ arises from the analysis of the expected value of the number of parallel contacts and the partition

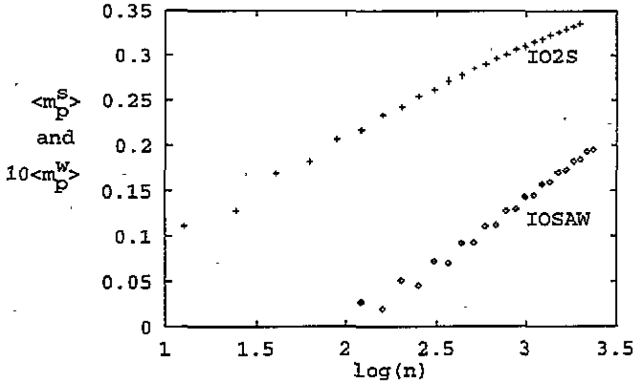

Figure 5. A plot of $\langle m_p \rangle$ against $\log(n)$ obtained from exact enumeration for walks ($n \leqslant 29$) and stars ($n \leqslant 27$) at the free SAW point ($\beta_p = \beta_a = 0$). The walk data are multiplied by a factor of 10 to place them on the same scale.

function series of two-legged stars. However, we do point out that the change in γ is numerically small.

6. Phase diagram

6.1. Parallel interaction model

We begin by considering the parallel interaction model with $\beta_a = 0$. Assuming that the free energy exists the rigorous results of section 3 imply that there must be at least one point of non-analyticity in the free energy. Of course, whatever transition does take place is an unusual one since the free energy of loops is constant in β_p (there are no parallel bonds in loops) and hence for β_p greater than the value of the first transition the loop and walk free energies are not the same!

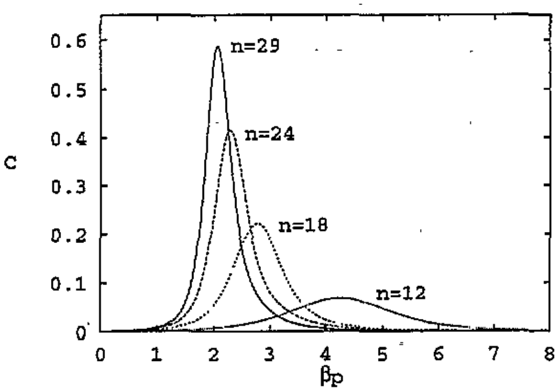

Figure 6. A plot of the specific heat $C_n(\beta_p)$ against β_p for four values of length ($n = 12, 18, 24, 29$).

In an attempt to find any phase transitions we have tabulated the specific heat per step $C_n(\beta_p)$ as a function of β_p for IOSAW at lengths $n = 1$ to 29. The specific heat for a selection of four lengths is plotted against β_p in figure 6. There is a single marked peak in the specific heat which is moving closer to the origin as n is increased. Usually it is possible to obtain a rough estimate of the specific heat exponent α from data such as this and an estimate of the critical temperature [10]. Any such attempt here has proved futile and values of the exponent α thus obtained have been bigger than one. This is because the height and position of the peak are changing very rapidly (and erratically) and this is an indication that the series are far from the asymptotic regime. However, this strong movement of the heights of the specific heat is consistent with a *first-order* transition at about $\beta_p \approx 1$. Harking back to the discussion in section 3, the simplest scenario possible for the behaviour of the free energy is $\kappa(\beta_p, 0) = \log \mu_s \equiv \kappa(0, 0)$ for $\beta_p \leqslant \log \mu_s$ and $\kappa(\beta_p, 0) = \beta_p$ for $\beta_p \geqslant \log \mu_s$. This would give a first-order phase transition at $\beta_p = \log \mu_s$ with a jump in the parallel interaction density $\lim_{n\to\infty}\langle m_p \rangle / n$ from 0 to 1 as β_p is varied from below $\log \mu_s$ to above it. The enumeration data are consistent with this scenario but a more cautious conclusion is the following: there is one transition with a diverging specific heat, and it occurs somewhere in the range (0, 2.1), probably near $\beta_p = 1$ (this conclusion is arrived at from the observation that the specific heat peaks are generally moving towards lower values of β_p as n is increased and for $n = 29$ the peak occurs approximately at $\beta_p = 2.1$).

On the other hand there is a heuristic argument as to why the usual collapse transition is second order, but the spiral transition may not be. Suppose the usual collapse transition were first order, so that close to the critical point there are two coexisting phases, of free energies f_1 and f_2 per unit length (where of course $f_1 = f_2$ at the critical point, but their derivatives are not equal.) Then we can imagine a long walk as having some parts in one phase and some parts in the other. If we ignore the self-avoidance restriction between these different parts, the total partition function is that of a one-dimensional Ising model, so that the actual free energy is $f = -\ln(e^{-f_1} + e^{-f_2})$. It is easy to check that this has a continuous derivative at the critical point, and so it is a second-order transition. *Reductio ad absurdum.* If such an argument applies to the spiral collapse, it is not so straightforward because the topological constraints make it difficult for spiral sections to occur in the middle of a walk. Indeed, for the chain sizes we have considered in the enumerations, nearly all the parallel contacts are close to the ends. This suggests that the spiral transition should be first order and rather strong.

This transition, whatever its order, is between the free SAW phase characterized by $\nu = \frac{3}{4}$ and a phase dominated by tightly bound spirals (at least for sufficiently large β_p). Since tightly bound spirals are compact this phase should have $\nu = \frac{1}{2}$. Given that the number of such tightly bound spirals is small (connective constant 1) the ground state will have zero entropy per step in the thermodynamic limit. The walk density is an order parameter for this transition as is the parallel interaction density. However, more useful may be the average winding number per step as an order parameter. This would enable one to clearly distinguish between a spiral compact phase and the normal compact phase of the collapse transition ($\beta_p = \beta_a > \beta^\theta$). Further work may be able to utilize this observation.

6.2. Full model: parallel–antiparallel interaction plane

In figure 7 we have plotted the loci of maxima of the specific heat for length $n = 29$. This shows that the possible free-to-spiral transition extends along a line essentially parallel (though not exactly so) to the β_a axis, while the θ-point peak (a weak singularity) extends parallel to the β_p axis. We shall argue below that this second phase transition line does indeed lie parallel to the β_p axis exactly. The free-to-spiral transition line curves away from the β_a axis when meeting the θ-line and continues in a direction away from the origin so as to separate the normal collapsed phase (large β_a) and the compact spiral phase (large β_p). The size of the specific heat peak for the collapse-to-spiral and free-to-spiral transitions is much larger than the free-to-collapsed θ-point peak.

This enumeration evidence along with some heuristic arguments and the free energy bounds allows us to predict a phase diagram with some confidence. The enumerations suggest that the simple scenario of one transition on varying β_p at fixed β_a is likely.

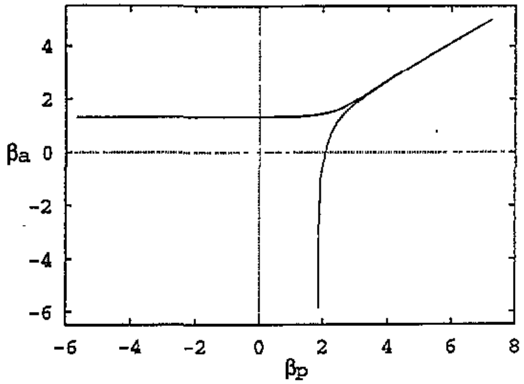

Figure 7. A plot of the position of the maximum of the specific heat for $n = 29$ in the full (β_p, β_a) plane for IOSAW.

Moreover, this transition may well be first order. The collapse-to-spiral transition would seem to be first order since for large β_a the transition takes place at large β_p. Under these conditions the spiral phase and the collapse phase should be close to their respective ground states. Now, the (thermodynamic limit) entropy per step of these two states is different (it should be 0 for the compact spirals) and so the transition should be first order with a jump in the entropy (per step) at the transition. As argued above, the free-to-spiral transition should also be first order. The θ-point is second order and there is no reason not to assume that this extends along the length of the free-to-collapsed line.

Figure 8 illustrates the conjectured phase diagram we believe provides the most likely scenario for this model. There are three phases: free, collapsed and compact-spiral. The free-to-collapsed is exactly parallel to the β_p axis and occurs at $\beta_a = \beta^\theta$. This should be so for the following reason. We know that on the line $\beta_a = \beta_p$ there exists the θ-point at some β^θ. The free energy at this point is $\kappa(\beta^\theta, \beta^\theta)$. By the result (26) we have that the free energy along the line $\beta_a = \beta^\theta$ for $\beta_p < \beta^\theta$ should also be given by $\kappa(\beta^\theta, \beta^\theta)$. Similarly, for lines of fixed β_a near $\beta_a = \beta^\theta$ the free energy is constant and equal to $\kappa(\beta_a, \beta_a)$ for $\beta_p \leqslant \beta_a$. This means that for a fixed value of $\beta_p < \beta^\theta$ the free energy on varying β_a is given by $\kappa(\beta_a, \beta_a)$ for β_a near β^θ (at least). The free energy then displays a transition at $\beta_a = \beta^\theta$ and is independent of β_p. Hence the transition line is parallel to the β_p axis for $\beta_p \leqslant \beta^\theta$, at least. The equation of the transition line should be analytic (otherwise one must introduce a new singularity) until it meets the spiral transition line (at some finite angle) and so is always parallel to the β_p axis. This result is clear if one accepts that loops and walks have the same free energy in the free and standard collapsed phases.

The spiral transition seems to be a single first-order transition. It is then a simple extension to conjecture that this transition takes place at the point of the largest possible value of β_p for any fixed β_a, as this would necessarily be first order. This is equivalent to the assumption that the compact spiral phase always has $o(n)$ (total) entropy and the transition, when it takes place, does so directly to the set of states whose energy differs from that of the ground state by an amount O(1) (which we assume, but certainly have not proved, are $e^{o(n)}$ in number). This rather strong and unusual assumption is consistent with the enumeration data. It is, however, the weakest of our conjectures and it certainly may be the case that the transition takes place close to but not exactly at the limiting value of β_p. Such a weaker scenario is sketched in figure 3 for the case of $\beta_a = 0$. Making this assumption however implies that the spiral transition line is given by (29), that is $\beta_p^t(\beta_a) = \kappa(\beta_a, \beta_a)$. Hence for $\beta_a = 0$ we have $\beta_p^t(0) = \log \mu_s$ while for $\beta_a = -\infty$ we have $\beta_p^t(-\infty) = \log \mu_{naw}$ where μ_{naw} is the connective constant for (bond) neighbour

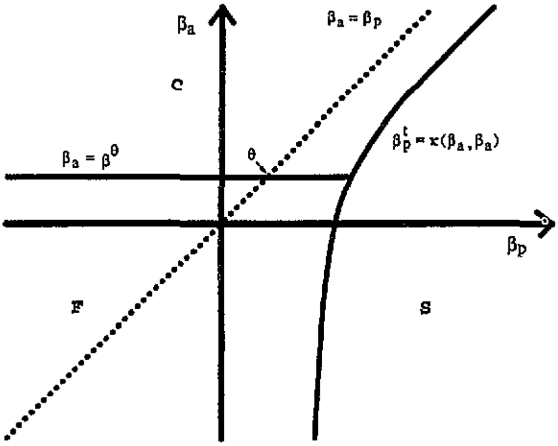

Figure 8. A schematic illustration of a conjectured phase diagram in the (β_p, β_a) plane showing the three phases: free (F); collapsed (C); and spiral collapsed (S). The dotted line is the normal collapse problem with $\beta_a = \beta_p$ and contains the θ-point.

avoiding walks. The neighbour-avoiding walk connective constant will be different (for site neighbour-avoiding walks the connective constant is 2.315 92(1) [11] as opposed to that for free SAW which is 2.638 16(1)), though not much so, to the connective constant for free SAW. This explains why the free-to-spiral transition line runs almost but not quite parallel to the β_a axis, for β_a negative.

For large positive β_a on the other hand $\kappa(\beta_a, \beta_a)$ is the (reduced) free energy of the normal collapsed phase at very low temperatures. This should be given (approximately) by $\kappa(\beta_a, \beta_a) = \beta_a + \log \mu_c$ where μ_c is the connective constant for compact walks. The equation of the transition line is then $\beta_a = \beta_p - \log \mu_c$. This explains why the transition line is moving away from the origin and does not cross the line $\beta_a = \beta_p$.

7. Conclusions

We have considered the statistical mechanics of IOSAW in the plane of parallel–antiparallel interaction. For this model we have given several rigorous results and several semi-rigorous results (rigorous contingent on the existence of the free energy). These results and exact enumerations have allowed us to map out a phase diagram. Our main conclusion is that there are three phases in this plane: the free SAW phase; the normal collapsed phase; and a phase dominated by tightly bound, compact, spirals. The transition to this last phase may well be first order from either of the other two.

The question of the continuously varying exponent γ is more controversial. Our analysis of the exact enumeration data is not unambiguous. It may simply be the case that due to the sparsity of parallel interactions in typical SAW configurations of modest length our exponent estimates are tainted by large corrections to scaling. In this case maybe our sequence of estimates has a turning point at some larger value of n. If that is not the case, and assuming that there is a change in γ on varying β_p, our enumerations show that it is very small: less than 1%. If this variation is real, a theoretical puzzle is presented as to why $\gamma'(0)$ is so small. The field theory quantitatively predicts only the dependence of γ on $\lambda(\beta_p)$ (see (6)), and not the non-universal form of $\lambda(\beta_p)$ itself. Nonetheless, it is possible to estimate this with various assumptions concerning the continuum limit of the interaction on the square lattice, with the result that $\gamma'(0)$ is expected to be about $1/(2\pi)$, to within factors of order unity. This is much larger than the observed variation. This analytic result is supported by an exact calculation for ordinary (non-self-avoiding) random walks with interactions β_a and

β_p (see the appendix). In this model, if $\beta_a = -\beta_p$ then $\gamma'(0) = 1/(2\pi)$ exactly.

However, for IOSAW, given that we have rigorously shown that the connective constant is unchanging for $\beta_p < 0$ when $\beta_a = 0$, assuming the form (5) (which includes the existence of the exponent γ), and acknowledging that the exact enumeration results at least show that the average number of parallel contacts $\langle m_p \rangle$ diverges, then γ must change with β_p (and the divergence of $\langle m_p \rangle$ be logarithmic). Conversely, if γ exists but does not vary, then $\langle m_p \rangle$ should not diverge, or perhaps the form (5) is incomplete and must be modified with a factor like $\rho(\beta_p)^{\sqrt{\log(n)}}$. The first is not supported by the evidence to date, although certainly not ruled out and the second is simply too difficult to test. (It could also be that in the ordinary collapsed and free phases $\langle m_p \rangle$ approaches a constant as n diverges but with logarithmic corrections; this constant diverging on approach to the spiral transition line.)

There is a close analogy that gives an argument which sheds light on this question. Another oriented SAW problem is that of interacting walks on the Manhattan lattice. On this lattice SAW are oriented by default but in the interacting case there are no parallel interactions. This is like the restriction $\beta_p = -\infty$ although the connective constant is not the same as the square lattice SAW value since further types of configurations are disallowed (parallel steps across 3, 5, etc faces are also disallowed). This problem has been recently mapped to an exactly solvable model at the collapse point [12]. The exponent ν is equal to the value at the normal θ point being 4/7 [13]. However, the exponent $\gamma = 6/7$ in opposition to the accepted θ exact value of 8/7. This is then an example of a closely analogous problem where the general flavour of the field theoretic predictions for IOSAW seems to hold at the collapse point. One may, of course, ask about the high temperature case and it is here that previous series work [14] has given values of γ close to the SAW value, 43/32, similar to our $\beta_a = 0$. This early work was based on rather short enumerations, which would not be sensitive enough to recognize a change in γ (from the square lattice value) of the magnitude observed here. Indeed, we [15] are currently extending the Manhattan enumerations to check this point.

The avenue is clearly open for some long Monte Carlo simulations to tackle this problem further [16]. These simulations are also being currently undertaken [16]. On the other hand, this paper has produced a consistent picture of several of the salient properties of IOSAW.

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Appendix. Mean numbers of parallel and antiparallel contacts for ordinary random walks

The problem studied in the body of the paper for self-avoiding walks may be solved exactly if the self-avoiding constraint is removed. In this case $Z_n(0,0) = \mu^n$ exactly, where $\mu = 4$ for the square lattice. The mean number of antiparallel (parallel) contacts is given by the $O(\beta_a)$ (respectively $O(\beta_p)$) term in the expansion of $Z_n(\beta_p, \beta_a)$. Consider first the former. This comes from all walks with at least one antiparallel contact, that is a square in which a pair of opposite sides is occupied by antiparallel bonds. There are four possible orientations for such a contact on the square lattice. An oriented random walk possessing such a contact may be connected up to it in two possible ways, and consists of three independent pieces: a section from the beginning of the walk to the first corner of the chosen square; an intermediate section connecting the second corner with the third; and a final section from the last corner to the end of the walk. Let the number of steps in each of these sections be n_1, n_2 and n_3 respectively. The $O(\beta_a)$ term is then

$$8\beta_a \sum_{n_1+n_2+n_3=n-2} \mu^{n_1} c_{n_2}(1)\mu^{n_3} \tag{32}$$

where $c_n(r)$ is the number of n-step walks whose ends are a distance r apart. For ordinary walks, this satisfies a simple recurrence relation, whose asymptotic solution for $r^2 \ll n$ is

$$c_n(r) \sim \frac{\mu^{n+1}}{4\pi n} e^{-\mu r^2/4n} \sim \frac{\mu^{n+1}}{4\pi n}\left(1 - \frac{\mu r^2}{4n} + \cdots\right). \tag{33}$$

Substituting this into (32) gives

$$\frac{2}{\pi}\beta_a \mu^{n-1} \sum_{n_2=1}^{n-2} \frac{(n-2-n_2)}{n_2}\left(1 - \frac{\mu}{4n_2} + \cdots\right). \tag{34}$$

The $O(\beta_p)$ term is similar, except that the central portion of the walk has to connect two sites which are a distance $\sqrt{2}$ apart. The leading term is therefore identical, but the correction is greater by a factor of two. In either case, the leading terms behave like $n \ln n$ for large n. This indicates that, for ordinary walks, the mean numbers of parallel and antiparallel contacts both grow in this manner. In order to compare more closely with the case of self-avoiding walks, it is necessary to choose $\beta_a = -\beta_p$ so as to cancel this leading term. The non-leading term is then

$$\frac{1}{2\pi}\beta_p \mu^n \sum_{n_2} \frac{n-2-n_2}{n_2^2}. \tag{35}$$

This is still $O(n)$, indicating that the free energy per unit length is still dependent on β_p, in contrast to the self-avoiding case. To compare with the field-theoretic predictions for the shift in γ, however, we should look at the $O(\ln n)$ term in (35). This then gives the result $\gamma'(0) = 1/(2\pi)$, quoted in the text.

It is possible to study this problem using the continuum approach. For ordinary walks, the current–current correlation function $\langle J(r)J(0)\rangle$ studied in [1] behaves as $\ln r/r^2$ rather than being a pure $1/r^2$ power as it is in the interacting theory. This additional logarithm is responsible for the $n \ln n$ terms found above. However, the field-theoretic calculation of the $O(\ln n)$ term, at least to first order in β_p, appears to be identical in both the ordinary and self-avoiding walk models. Since the mappings between the lattice and the continuum limit should be similar for both problems, this suggests that the result $\gamma'(0) = 1/(2\pi)$ should hold approximately even for self-avoiding walks.

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