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Exact enumeration study of free energies of interacting polygons and walks in two dimensions

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Abstract. We present analyses of substantially extended series for both interacting self-avoiding walks (ISAW) and polygons (ISAP) on the square lattice. We argue that these provide good evidence that the free energies of both linear and ring polymers are equal above the θ-temperature, thus extending the application of a theorem of Tesi *et al* to two dimensions. Below the θ-temperature the conditions of this theorem break down, in contradistinction to three dimensions, but an analysis of the ratio of the partition functions for ISAP and ISAW indicates that the free energies are in fact equal at all temperatures within 1% at least. Any perceived difference can be interpreted as the difference in the size of corrections to scaling in both problems. This may be used to explain the vastly different values of the crossover exponent previously estimated for ISAP to that predicted theoretically, and numerically confirmed, for ISAW. An analysis of newly extended neighbour-avoiding self-avoiding walk series is also given.

1. Introduction

Long linear polymers in dilute solution are expanded objects under good solvent conditions but if the solvent quality is decreased or, equivalently, the temperature lowered below the θ-temperature, the polymers appear to undergo a sudden collapse transition from an expanded coil to a compact globule. This phenomenon has been studied experimentally by light scattering [2, 3] and by viscosity measurements [4]. In addition, it has been modelled [5] by interacting self-avoiding walks (ISAW) on a lattice with an interaction energy proportional to the number of nearest-neighbour contacts. Considerable progress in the study of this model occurred following the work of de Gennes [6], especially in two dimensions where many critical properties have been determined using Coulomb gas [7] and conformal invariance [8] methods. The model has also been studied numerically using a wide variety of techniques including transfer matrices [9, 10], exact enumeration [11–16], $1/d$-expansions [18, 19] and Monte Carlo [19–28]. As a result, for ISAW in $d = 2$ at the θ-point, the critical exponents are believed to take on the values predicted by Duplantier and Saleur [30], in particular the crossover exponent $\phi = \frac{3}{7} = 0.428\ldots$. In addition, the value

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of the temperature parameter β at the collapse transition has been estimated numerically (see [28]) and has a value around $\beta_c = 0.66$ for the square lattice.

A similar collapse transition is believed to occur in randomly branched polymers modelled by lattice animals or lattice trees [31, 32]. For lattice animals, the crossover exponent and certainly the location of the transition seem to depend on the details of the model. For example, for the k-model, a contact model which is a natural generalization of the ISAW model, $\phi = 0.60 \pm 0.03$, $\beta_c = 0.38 \pm 0.05$ on the square lattice [33], while for the C-model, a cycle model, one finds [34] on the same lattice $\phi = 0.657 \pm 0.025$, $\beta_c = 1.87 \pm 0.02$. Both pairs of values are quite different from the corresponding pair for ISAW quoted above.

On the other hand, there is a growing belief [35, 36, 1, 37] that all models with a given architecture (e.g. polygons, uniform f-stars, combs, brushes, ...) not only have the same collapse temperature and crossover exponent as ISAW but their limiting reduced free energies have the same dependence on the value of the temperature parameter β as do ISAW. Let us review the evidence.

First, we define the partition functions for ISAW, interacting self-avoiding polygons (ISAP) and uniform f-stars (ISAS-f) by

$$Z_n(\beta) = \sum_k c_n(k) e^{\beta k} \tag{1.1}$$

$$Z_n^0(\beta) = \sum_k p_n(k) e^{\beta k} \tag{1.2}$$

and

$$Z_n(\beta; f) = \sum_k s_n(k; f) e^{\beta k}. \tag{1.3}$$

Here, $c_n(k)$ and $p_n(k)$ are the number of self-avoiding walks (SAW) and polygons (SAP), respectively, with n edges and k contacts, and $s_n(k; f)$ is the number of uniform stars with f branches, n edges in each branch and k contacts. Clearly, $s_n(k; 1) = c_n(k)$. It has been proved rigorously [1, 37] that on a d-dimensional simple hypercubic lattice the corresponding limiting reduced free energies

$$\kappa(\beta) = \lim_{n\to\infty} \frac{1}{n} \ln Z_n(\beta) \tag{1.4}$$

$$\kappa^0(\beta) = \lim_{n\to\infty} \frac{1}{n} \ln Z_n^0(\beta) \tag{1.5}$$

and

$$\kappa_f(\beta) = \lim_{n\to\infty} \frac{1}{nf} \ln Z_n(\beta; f) \tag{1.6}$$

exist, and are equal to one another for all $\beta \leqslant 0$. (More precisely, the proofs by Tesi *et al* [1] for walks and polygons are for $d = 3$ but similar arguments should work for general d.) Yu *et al* [37] also reported, but without proof, that this result extends to uniform combs and brushes.

For $\beta > 0$, the existence of the limiting value $\kappa^0(\beta)$ has been proved rigorously, as has the fact that the limiting function is monotonic and convex [14]. Otherwise, little else has been proved rigorously. However, there is mounting evidence in support of the conjecture

$$\kappa(\beta) = \kappa^0(\beta) = \kappa_f(\beta) \qquad \forall\beta \text{ and } d. \tag{1.7}$$

More specifically, Yu *et al* [37] have derived and analysed exact enumeration data for ISAW through orders $n = 25, 18$ and 17, for ISAP through $n = 26, 18$ and 16, for ISAS-3 through $n = 9, 5$ and 6, and for ISAS-4 through $n = 7, 5$ and 4, for the square (SQ), triangular (T) and simple cubic (SC) lattices, respectively. For ISAS-5, the data extend through $n = 4$ (T, SC) and for ISAS-6 through $n = 4$ (T) and 3 (SC). (For f-stars, the maximum values of n may seem quite small, but it should be remembered that it is the total number of edges, obtained by multiplying the above values by f, that is comparable with the n values for walks and polygons.) The numerical plots of Yu *et al* (see figures 2–4 of [37]) suggest that all these limiting free energies are identical at least up to $\beta = 2$ ($d = 2$) and $\beta = 1.3$ ($d = 3$), both corresponding to temperatures well into the collapsed regions.

Support for $\kappa(\beta) = \kappa_f(\beta)$ for all values of β and d comes from their $1/d$-expansions, which Yu *et al* [37] derived through order $1/d$ for general f, and through order $1/d^2$ for $f = 3$. The terms in the expansions are β-dependent but turn out to be independent of f and agree term-by-term with the $1/d$-expansion for ISAW, which is known through order $1/d^5$ [19]. However, it has been speculated [36], in the context of the collapse transition for lattice animals, that the range of validity of $1/d$-expansions is limited by the collapse transition at $\beta_c(d)$. If the same happens for ISAW and ISAS-f, then the above argument concerning the term-by-term equality of their $1/d$-expansions would have nothing to say when $\beta > \beta_c$.

Support for $\kappa(\beta) = \kappa^0(\beta)$ in $d = 3$ comes from the Monte Carlo results presented by Tesi *et al* [1]. They show (see figure 4 of [1]) that, for the SC lattice, the difference in the relative free energies of ISAW and ISAP, at least up to $\beta = 0.5$ (still well into the collapsed region—see (1.9) below), decreases as n increases (at least up to $n = 1200$), consistent with the limiting free energies being equal for all values of β. Further confirmation is obtained by using theorem 2.8 of [1], which we shall refer to as the *contact theorem*. This proves that if the mean number, $\langle k\rangle_n^0$, of contacts for ISAP is at least as large as the mean number, $\langle k\rangle_n$, for ISAW, at all $\beta > 0$, for n sufficiently large, then the limiting free energies are equal. Tesi *et al* studied the behaviour of $\langle k\rangle_n^0/\langle k\rangle_n$ as a function of β for several values of $n \leqslant 1200$ and their Monte Carlo results (see figures 5 and 6 of [1]) clearly support the equality of the limiting free energies in three dimensions, well into the collapsed region.

We have reviewed the evidence in support of the conjecture (1.7). Assuming now that the conjecture is true implies that the location β_c of the collapse transition and the value of the crossover exponent ϕ (using the relation, $\phi = 2 - \alpha$, between ϕ and the exponent α characterizing the singularity in the free energy at β_c), are the same for interacting walks, polygons and f-stars, as well as, possibly, for other polymer architectures modelled by uniform embeddings of graphs of fixed homeomorphism type. Indeed, there are some direct numerical estimates which are consistent with ISAW and ISAP collapsing at the same value of β. Thus, in $d = 2$, recent results for ISAW [21–23, 25, 15, 16, 26, 27] and for ISAP [13, 14] are consistent with a common value around

$$\beta_c = 0.663 \pm 0.016 \qquad \text{(SQ)} \tag{1.8}$$

while in $d = 3$ a common value around

$$\beta_c = 0.277 \pm 0.009 \qquad \text{(SC)} \tag{1.9}$$

is indicated [1, 38].

As for the crossover exponent ϕ, there is the conjecture that $\phi = \frac{3}{7}$ in $d = 2$ [30], while in $d = 3$—the upper-critical dimension for tricritical walks—ϕ is believed to take on its mean-field value $\phi = \frac{1}{2}$ with a leading correction term which is logarithmic [39, 40], for both ISAW and ISAP. As emphasised by Brak *et al* [41], crossover exponents are notoriously difficult to determine numerically. Thus, over the past few years, there has been considerable controversy [9, 11, 21–23, 25] concerning the value of ϕ for ISAW in $d = 2$, with direct numerical estimates ranging from $\phi = 0.48 \pm 0.07$ [9] to $\phi = 0.66 \pm 0.02$ [23]. However, in more recent Monte Carlo work, first on the Manhattan lattice, Prellberg and Owczarek [42] found an estimate of $\phi = 0.430 \pm 0.006$ utilizing walks of length, n, up to 10^6 and then, with good statistics for $n \leqslant 2048$, Grassberger and Hegger [27] gave $\phi = 0.435 \pm 0.006$ for the square lattice, both of which seem to confirm the theoretical value of $\phi = \frac{3}{7}$. Grassberger and Hegger argue that the neglect of extremely large correction-to-scaling terms may have been the cause of the earlier difficulties.

In the case of ISAP in $d = 2$, the best numerical estimate seems to be $\phi = 0.90 \pm 0.02$ [13] which is a long way from $\phi = \frac{3}{7}$, but is based upon exact enumerations only up to $n = 28$ (i.e. 13 terms).

When $d = 3$, most workers [1, 38] have simply accepted the expected theoretical value of $\phi = \frac{1}{2}$ and we know of no recent direct estimates for either ISAW or ISAP.

In this paper, our aim is to provide additional support for one part of the conjecture (1.7), namely, $\kappa(\beta) = \kappa^0(\beta)$ for $\beta > 0$ and $d = 2$. We do this by first deriving new exact enumeration data for ISAW and ISAP on the square lattice through orders $n = 29$ and $n = 42$, respectively. These new data extend the published data for walks and polygons [43, 13] by nine and seven terms and the unpublished data used by Yu *et al* [37] by four and eight terms, respectively.

The new data are used, most importantly, for comparing $\langle k \rangle_n$ with $\langle k \rangle_n^0$ for a range of temperatures to determine whether the conditions of the contact theorem [1] are satisfied. This evidence, and that mentioned below, strongly suggests that the free energies of ISAW and ISAP are equal above the θ-temperature ($\beta \leqslant \beta_c$). Intriguingly however, it seems that the conditions of the contact theorem are *not* satisfied at any temperature below the θ-temperature, using any reasonable extrapolation technique. This coincides with the region where we suggested that the $1/d$-expansions may break down and so are unable to provide an argument for the equality of the ISAW and ISAS-f free energies (the other part of conjecture (1.7)). However, we have directly estimated the difference in the limiting free energies of ISAP and ISAW,

$$\Delta\kappa \equiv \kappa^0(\beta) - \kappa(\beta) \tag{1.10}$$

as a function of β, and found that for a wide range deep into the collapsed phase this difference is 0.00 ± 0.01 (where κ and κ^0 are of the order 1.0). At most high temperatures the error is considerably smaller (about 0.001). We have supplemented the exact enumeration data by simulating ISAP using a Monte Carlo algorithm which we argue only provides reliable information for n well below 1000 at the temperatures required, at, and below, the collapse temperature. The analysis of the data illustrates the near impossibility of extracting reliable direct estimates of the critical parameters from data of this order of n. Hence we propose that radically new algorithms are needed to simulate ISAP near, and especially below, the θ-temperature in $d = 2$. Umbrella sampling and multiple Markov chain methods ([29] and references therein) have proved to be successful in $d = 3$ and these are promising techniques for future work in $d = 2$.

The paper is organized as follows. In section 2 we describe the exact enumeration and Monte Carlo techniques utilized. In section 3 we present our analyses and discuss their meaning, concluding with a short summary of our results in section 4.

2. Data derivation

This section describes the methods that we have used to extend the exact enumeration data for ISAP and ISAW on the square lattice, and the details of the Monte Carlo algorithm used to simulate ISAP.

2.1. Finite-lattice method

Exact enumeration results, giving the complete polynomials in $w = e^{\beta}$, were obtained for all square lattice polygons with perimeter up to $n = 28$ by Maes and Vanderzande [13]. We have used the finite-lattice method to extend these data by seven terms up to $n = 42$. (Only terms with perimeters of even length contribute, of course.) We take the opportunity to correct a small error in table I of [13]; the number $C(26, 9)$ should be 679 848, rather than 679 484 as printed.

The finite-lattice method of enumerating SAPs on the square lattice was first introduced by Enting [44]—the enumeration extending to polygons with $n = 38$—increasing the number of terms known at that time by over 50%. Later work extended this enumeration to $n = 56$ [45, 46], and currently stands at $n = 70$ [47]. It has also been possible to augment these enumerations with calculations of other geometrical properties of the polygons. Thus, calliper moments up to $n = 54$ were obtained by Guttmann and Enting [46] and the enumeration of polygons by both perimeter and area was given by Enting and Guttmann [48].

The technique has also been applied to other planar lattices. Series for the L and Manhattan lattices were obtained up to $n = 48$ [45] and recently extended to $n = 84$ [49], for the honeycomb lattice up to $n = 82$ [50], and for the triangular lattice up to $n = 25$ [51] classified by both perimeter and area.

The quantity that we wish to determine is $p_n(k)$ in (1.2), the number of square lattice unrooted polygons with n edges and k nearest-neighbour contacts. For convenience in this section, we write $p_{n,k} \equiv p_n(k)$, so that (1.2) becomes

$$Z_n^0(w) = \sum_k p_{n,k} w^k. \tag{2.1}$$

For any fixed n, the $p_{n,k}$ are all zero for $k > k_{\max}(n)$ since the sum on the right-hand side of (2.1) is a polynomial in w. Since each site of the polygon can be involved in at most two near-neighbour contacts and since each near-neighbour contact involves two sites, we must have $k_{\max}(n) \leqslant n$. In practice, we can set $k_{\max}$ empirically and use the total n-edge polygon count to ensure that we have used a sufficiently large value. Finally, we define the generating function

$$C(x, w) = \sum_n Z_n^0(w) x^n = \sum_{k,n} p_{n,k} w^k x^n. \tag{2.2}$$

The finite-lattice method of enumerating polygons involves two steps. First, we need to enumerate polygons constrained to lie within various finite rectangles. The second step is that such enumerations for finite rectangles are combined to give a truncated approximation of the infinite-lattice polygon generating function. If the factors used in the linear combination of the finite-lattice generating functions are chosen correctly, then the first incorrect term in the infinite-lattice generating function will correspond to the largest polygon that cannot be embedded in any of the rectangles that are used.

When enumerating polygons constrained to lie within various finite rectangles one needs to classify the polygons according to some quantity such as perimeter or area that grows as the size of the rectangles increases. Such a quantity forms the expansion variable of the generating function. There is, however, no need to confine the classification to just one quantity; apart from the (non-trivial) overhead of working with series in two variables, the finite-lattice method applies to polygon enumerations involving several variables, as (for example) in the enumeration of polygons by perimeter and area [50, 48].

The weights $a_{\ell,m}$ used to combine the finite-lattice generating functions are used in the expression

$$C(x, w) \approx \sum_{\ell,m} a_{\ell,m} G_{\ell,m} \tag{2.3}$$

where $G_{\ell,m}$ is the generating function for polygons that can be embedded in a rectangle of width ℓ and length m so as to span the length of the rectangle. The lattice symmetry gives some degree of choice in the weights. Enting and Guttmann (see equations (2.8*a*–*e*) in [45]) give the weights used in most of the polygon enumerations. However, in this calculation, we use a slightly different formulation given by Guttmann and Enting [46] when enumerating calliper moments, even though we do not retain the calliper moments in this calculation.

Let $p_{n,k;q}$ be the number of n-edge polygons with k contacts which span a distance q in the horizontal direction, i.e. the difference between the maximum and minimum values of the horizontal coordinates is q lattice units. Then, the jth calliper moment is

$$C^{[j]}(x, w) = \sum_{n,k,q} q^j p_{n,k;q} w^k x^n. \tag{2.4}$$

We define

$$S_q(x, w) = \sum_{n,k} p_{n,k;q} w^k x^n \tag{2.5}$$

whence

$$C^{[j]}(x, w) = \sum_{q} q^j S_q(x, w). \tag{2.6}$$

The finite-lattice approximations for the S_q are

$$S_q(x, w) = \sum_{j=1}^{2N+1-q} (G_{q,j} - 2G_{q-1,j} + G_{q-2,j}) \qquad q \leqslant N \tag{2.7}$$

and

$$S_q(x, w) = G_{2N+1-q,q} - G_{2N-q,q}. \tag{2.8}$$

(This last expression also corrects a minor typographical error in equation (6) of Guttmann and Enting [46].) These expressions give the correct enumeration of polygons of up to $4N + 2$ edges (and their calliper moments).

The enumeration of the generating functions, $G_{\ell,m}$, for polygons in rectangles uses a transfer-matrix technique. The basic technique is as described by Enting [44] with the formalism extended to take account of nearest-neighbour contacts. The transfer-matrix technique works with the generating functions for sets of loops in partly constructed lattices (shown by full points in figure 1). The boundary of the partly constructed lattice is defined by a transect line drawn on the dual lattice, as shown by the broken line in figure 1. Each step of the construction involves moving the transect line (from the broken position to the dotted position) so as to add one site (shown as circled) and two new edges (shown as ++++++) to the partially completed lattice. The construction of self-avoiding polygons only requires a knowledge of how the bonds of the polygon intersect the transect line. As

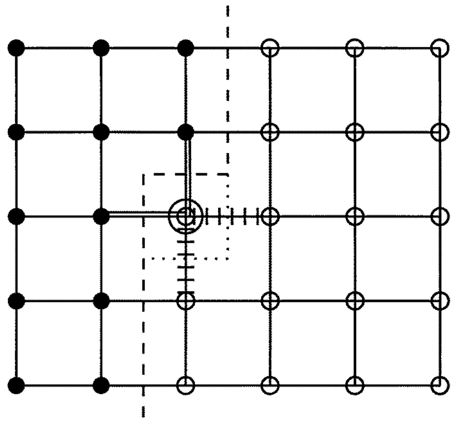

Figure 1. The way in which a transect line (broken) is drawn through the square lattice, cutting $W + 2$ edges for a rectangle of width W. The dotted line shows the new position of the transect line after the elementary step of adding one new site (circled) and two new outgoing edges $+\!\!+\!\!+\!\!+\!\!+$ to replace two old incoming edges (double).

described by Enting [44], it is sufficient to distinguish between edges with no bond of the polygon (denoted '0'), edges with a bond of the polygon that is the uppermost arm of a loop (denoted '1') and edges with a bond that is the lower arm of a loop (denoted '2'). This '1','2' notation uniquely specifies the connectivity of the loops of the partly constructed polygon. For this study, we need to add a new edge state ('3') to denote edges along which a nearest-neighbour contact occurs or, more precisely, edges along which a nearest-neighbour contact may occur if an occupied site is added at the end of a type '3' bond, as the lattice is constructed.

The process of adding a site (shown as a double circle in figure 1) consists of linking the two incoming edges (shown with double lines in figure 1) that occur at the kink in the transect line and assigning states to the two new edges (shown as $+\!\!+\!\!+\!\!+\!\!+$ in figure 1) leaving the site. Enting [44] lists the allowed outputs for all allowed combinations of '0', '1', '2' on the input edges, where '0' corresponds to no step, '1' and '2' to the uppermost (lowermost) end of a loop, respectively. The rules for the present case are the same with the following re-interpretations. For the purposes of classifying input states, type '3' is equivalent to type '0'. An output state of '0' in the tabulation of Enting [44] is replaced by '3' except for the case when a $(0, 0)$ pair is transformed to a new $(0, 0)$ pair. A factor of $w^{n(3)}$, where $n(3)$ is the number of incoming type '3' edges, is included except when the output is $(0, 0)$. A summary of these rules is given in table 1.

The use of '1' and '2' to denote upper and lower ends of loops constrains the relative arrangements of such edges, but the '0' and '3' can be interspersed freely amongst them. (The same situation applies on the triangular lattice where we classify sites according to four states.) The number of configurations needed to enumerate polygons with nearest-neighbour contacts on a rectangle of width W is the same as the number of configurations used when enumerating triangular-lattice polygons on a strip of width $W + 1$.

The maximum width that we have used is ten and so we have been able to enumerate polygons of up to 42 steps, with a complete specification of the distribution of nearest-neighbour contacts. This limit is imposed by storage requirements rather than time limitations. Our results are given in appendix A.

Table 1. Rules for allowed states of outgoing edges (x, y) for all possible states of incoming edges. The new partial generating function incorporates a factor of $x^{n(1)+n(2)}$, where $n(j)$ is the number of outgoing edges of type j, and a factor of $w^{k(3)}$, where $k(3)$ is the number of incoming edges of type '3', except in the case '*' where no bonds pass through the site. In the cases marked†, other edges must be relabelled as specified by Enting [44]. In the case marked‡ there is no new state, but the partial generating function is included in the running total for $C(x, w)$ with the appropriate $a_{\ell,m}$ factor.

Inputs	(0, 1)	(0, 2)	(0, 0)	(1, 2)	(2, 1)	(1, 1)
	(3, 1)	(3, 2)	(0, 3)			(2, 2)
	(1, 0)	(2, 0)	(3, 0)			
	(3, 0)	(2, 3)	(3, 3)			
Outputs	(1, 3)	(2, 3)	(0, 0)*	‡	(3, 3)	(3, 3)†
	(3, 1)	(3, 2)	(1, 2)			

2.2. Direct enumeration

The direct enumeration of ISAW on the square lattice, giving the complete polynomials in w, were given by Ishinabe [43] through $n = 20$ (see table 1 of [43]). Five more terms were derived, but not published, by Yu *et al* (1997) in their study of the free energies of ISAW, ISAP and ISAS-f. We have used a 52 processor Intel Paragon supercomputer to extend the direct enumeration of ISAW up to $n = 29$. All the terms, Z_1 through Z_{29}, are given in appendix B. The calculation took about 100 h.

Recently, a 1024 processor Intel Paragon supercomputer was used by Conway and Guttmann [52] to implement a finite-lattice method which extended the enumeration of square lattice SAW from $n = 39$ to $n = 51$. Unfortunately, the parallelized algorithm, which is challenging to implement efficiently, has not so far been generalized to enumerate ISAW.

As the temperature parameter β approaches $-\infty$, the walks become neighbour avoiding. In this special case we have extended the series to 32 terms. The coefficients are also given in appendix B, as they are the coefficients $c_n(0)$.

2.3. Monte Carlo algorithm

Monte Carlo estimates of thermodynamic properties, including the energy and heat capacity, were obtained at a series of temperatures and lengths of polygons. The algorithm was a basic Metropolis algorithm involving sampling along a realisation of a Markov chain whose unique limit distribution was the Boltzmann distribution at the required temperature. The underlying symmetric Markov chain was first defined for walks by a set of pivot moves [53, 54] combined with local moves to improve the 'slow mode' problem associated with near-neighbour contacts. For polygons we hence used the corresponding 'cut-and-paste' algorithm invented by Madras *et al* [55]. This algorithm works well, in the sense that the autocorrelation times of the various observables are short, for high temperatures, but less well at lower temperatures. However, for values of n less than 200 we were able to sample effectively at temperatures just below that corresponding to the maximum in the heat capacity, so that the polygon was just inside the collapsed regime.

3. Free energy and contact number analysis

The exact enumeration data given in appendices A and B for ISAP and ISAW respectively, were first used to calculate the expected number of contacts for each model at a range of values of β. For $\beta \leqslant 0.663$, we plotted the contact densities for ISAW and ISAP, $m_n(\beta) = \langle k \rangle_n / n$ and $m_n^0(\beta) = \langle k \rangle_n^0 / n$, respectively, against $1/n$ on the same graph, while for $\beta > 0.663$ we plotted these against $1/\sqrt{n}$—six of these plots are given in figure 2. We have used these scales since these corrections are expected from the partition function scaling forms most likely in each regime [56].

For small $\beta < 0.6$ the polygon data, m_n^0, are larger than the walk data, m_n, at the largest values of n: there is a crossing point at low n which moves to larger n as β increases. Using linear and quadratic fits, and adding in $n^{-3/2}$ corrections allowed us to estimate the thermodynamic limit for $m_n(\beta)$ and $m_n^0(\beta)$ which we denote $m(\beta)$ and $m^0(\beta)$ respectively. If the thermodynamic limit free energies are the same so should these limiting contact densities, and for $\beta < 0.663$ this is true within 0.5%. It is also true, that if anything, the extrapolations would infer that $m^0 \geqslant m$, but the contact theorem then implies that the free energies and hence these average contact densities are equal. Near and above the estimated θ-temperature our extrapolations lead us to believe that $m_n^0(\beta) \geqslant m_n(\beta)$ for n large enough (that is, there is at least a crossover point beyond the extent of the series), which would again allow the use of the contact theorem. Hence we deduce that $m(\beta) = m^0(\beta)$ for all $\beta < 0.663$

For temperatures below the critical temperature ($\beta \geqslant 0.663$), the crossing point of the walk and polygon data disappears (see figure 2). It is unclear whether there may be one at large n or whether the θ-temperature marks a point where the crossing point moves off to ∞, thereby marking the beginning of a regime where, for all n, $m_n > m_n^0$. The conditions of the contact theorem would no longer apply, admitting the *possibility* that the ISAW and ISAP free energies may be different. In addition, our extrapolations were now far more sensitive to the number of terms used, and to small variations of the extrapolation function, especially for the walk data. The values of $m(\beta)$ and $m^0(\beta)$ may reasonably differ by up to 5% if any fairly conservative extrapolation is taken seriously.

For finite n, the curves of the contact densities are substantially different for ISAW and ISAP, and further differentiation, giving specific heats and third cumulants (the contact density curve is the first derivative of the free energy in the variable β), produce radically different graphs. Moreover, extrapolations seem to need different extrapolation functions to obtain results consistent with the equality of the free energies at all β. It is no wonder that past use of the ISAP data has produced vastly different results to the ISAW data. We have also previously simulated SAPs with a cut-and-join algorithm (see section 2.3) essentially in an attempt to find the θ-temperature and crossover exponent for ISAP, without great success. While we were able to simulate lengths up to 1000, long autocorrelation times restricted the use of the data to around maximum lengths of 100 to 200. The size of the corrections-to-scaling in ISAP and their clear difference in magnitude, manifested in the contact data described above, rendered that analysis less useful than we had hoped. We do point out that using the third cumulant, which is expected to diverge at β_c we estimated ϕ to be around 0.5. (Although had we chosen higher derivatives, different values would have ensued.) We do not give error bars since we do not believe that convergence has been achieved. While this cannot be used to confirm the theoretical value of $\frac{3}{7}$ for ISAP, it does throw considerable doubt on the value of 0.90 ± 0.02, previously quoted [13]. We remark that to reconcile the ISAW and ISAP results near and below the θ-temperature with Monte Carlo data will require the simulation of ISAP of lengths over 1000 with good statistics:

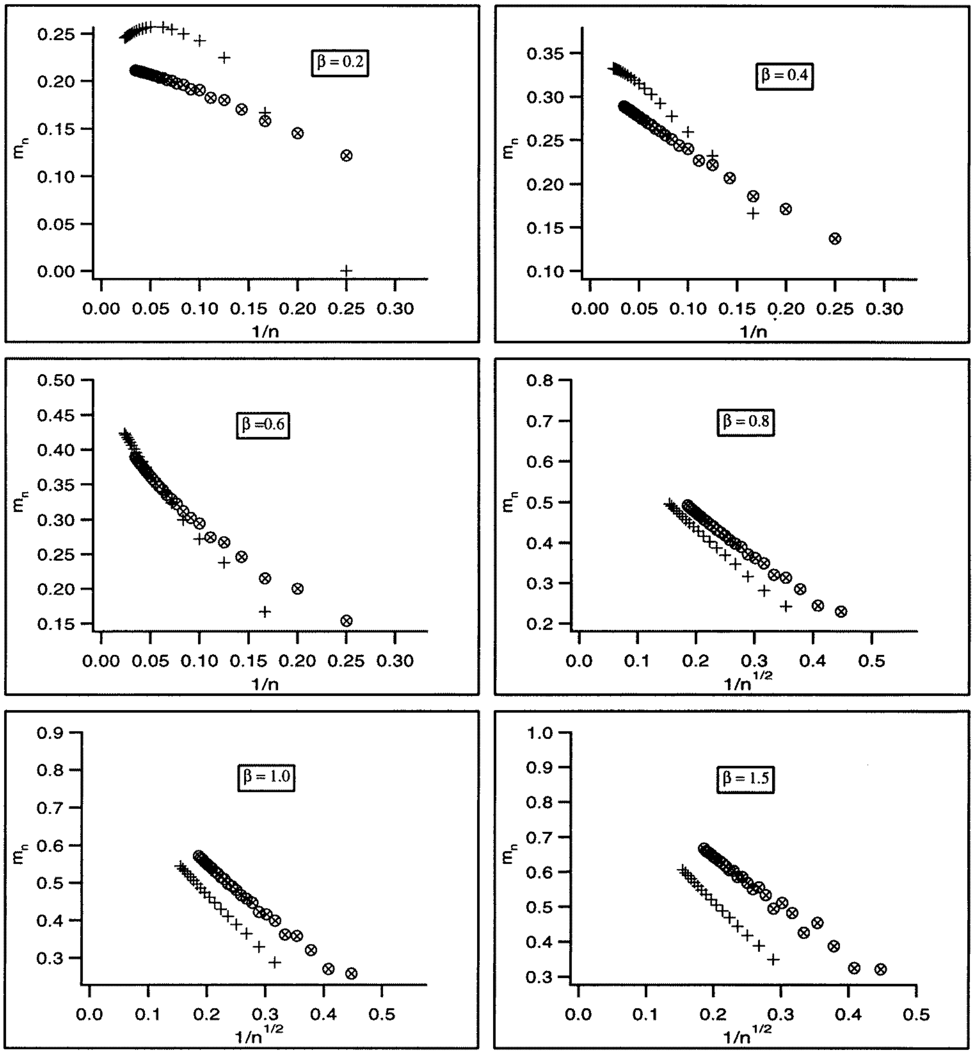

Figure 2. The six graphs are plots of the expected number of contacts $m_n(\beta)$ and $m_n^0(\beta)$ for ISAW (circles with crosses) and ISAP (crosses) respectively at six different (fixed) values of β. For $\beta = 0.2$, 0.4, and 0.6, which are expected to lie in the expanded phase we have plotted the two sequences m_n against $1/n$, while for $\beta = 0.8$, 1.0, and 1.5, which are expected to lie in the collapsed regime, we have used $1/\sqrt{n}$. These scales were chosen to reflect the expected corrections-to-scaling in those regimes, which in turn reflect the expected asymptotic forms of the partition function scaling.

this is something the cut-and-join algorithm and current computing power seem unable to achieve. However, we were able to use our Monte Carlo data to reinforce our conclusions concerning the extrapolations of the expected density of contacts mentioned above, in each regime.

To clarify the low-temperature situation and provide additional support for the conclusions at higher temperatures, we have analysed the series formed by the ratio of the polygon partition function to the walk partition function over the same range of temperature

Table 2. A list of estimates of the reduced free energy of ISAP from a differential approximant analysis. The value for $\beta = -\infty$ is obtained from walk data.

β	κ^0
$-\infty$	0.839 810(7)
−2.0	0.854 2(3)
−1.0	0.881 6(2)
−0.5	0.911 94(6)
−0.25	0.936 344(3)
0	0.970 081 1(1)
0.2	1.007(1)
0.4	1.060(2)
0.6	1.141(5)
0.663	1.170(4)
0.8	1.254(5)
1.0	1.40(2)
1.2	1.55(3)
1.5	1.79(5)

considered above. The standard method of differential approximants was used [57], with a statistical averaging procedure over a wide range of inhomogeneous approximants applied. To use even and odd n, we in fact analysed the series $Q_n(\beta)$, where

$$Q_n = \begin{cases} \dfrac{\sqrt{Z^0_{n+1} Z^0_{n-1}}}{Z_n} & \text{for } n \text{ odd} \\[2ex] \dfrac{Z^0_n}{Z_n} & \text{for } n \text{ even.} \end{cases} \tag{3.1}$$

If the expected asymptotic behaviour occurs for the partition functions (including the equality of the ISAW and ISAP free energies), the quantity Q_n [16] should behave as a power law with connective constant 1: the exponent of the power law will be different below, at, and above the θ-temperature. Here we are not interested in identifying this power law or the value of its exponent, only in verifying that the connective constant is indeed 1, since it is this fact that implies the equality of the ISAW and ISAP free energies. The difference in free energy is given by

$$\Delta\kappa = \ln\left(\lim_{n\to\infty} (Q_n)^{1/n}\right). \tag{3.2}$$

We examined a range of β from 0 to 1.5 and the value of $\Delta\kappa$ was 0.0000 within the errors found. The errors for the following β, that is 0, 0.2, 0.4, 0.6, 0.663, 0.8, 1.0, 1.2, and 1.5, were 0.0004, 0.0004, 0.0006, 0.002, 0.002, 0.002, 0.006, 0.008, and 0.01, respectively. These data would seem to imply that the conjecture (1.7) holds for ISAW and ISAP at all temperatures despite the conditions of the contact theorem probably failing and the possible breakdown in the $1/d$-expansions.

While several authors in the past have plotted $\kappa(\beta)$ for ISAW, we give above a table of values of $\kappa^0(\beta)$ found from a differential approximant analysis of the Z^0_n series: see table 2. We note that the values for $\beta < 1.0$ fall within graphical accuracy on the curve drawn by Nidras [28] following his analysis of Monte Carlo data for ISAW.

For $\beta = -\infty$ we have neighbouring-avoiding walks and polygons. This is an interesting problem in its own right. We have analysed the series given in appendix B by the standard

Table A1. The coefficients $p_n(k)$ for $n \leqslant 42$.

n	k	$p_n(k)$	n	k	$p_n(k)$	n	k	$p_n(k)$	n	k	$p_n(k)$
4	0	1	6	0	0	8	0	1	10	0	2
			6	1	2	8	1	0	10	1	8
						8	2	6	10	2	0
									10	3	18
12	0	9	14	0	36	16	0	154	18	0	668
12	1	20	14	1	96	16	1	408	18	1	1 832
12	2	40	14	2	110	16	2	562	18	2	2 564
12	3	0	14	3	156	16	3	488	18	3	2 704
12	4	51	14	4	16	16	4	584	18	4	2 218
12	5	4	14	5	138	16	5	176	18	5	2 292
			14	6	36	16	6	372	18	6	1 074
						16	7	188	18	7	1 076
						16	8	6	18	8	740
									18	9	100
20	0	2 932	22	0	13 016	24	0	58 364	26	0	264 208
20	1	8 372	22	1	38 876	24	1	183 044	26	1	871 596
20	2	12 388	22	2	60 918	24	2	304 010	26	2	1 533 190
20	3	13 464	22	3	70 350	24	3	370 780	26	3	1 971 494
20	4	12 983	22	4	69 208	24	4	382 224	26	4	2 118 120
20	5	10 368	22	5	62 212	24	5	348 888	26	5	2 010 196
20	6	9 194	22	6	47 482	24	6	292 470	26	6	1 718 270
20	7	5 120	22	7	37 628	24	7	214 628	26	7	1 360 788
20	8	3 679	22	8	22 364	24	8	158 126	26	8	969 218
20	9	2 532	22	9	14 490	24	9	95 828	26	9	679 848
20	10	766	22	10	8 604	24	10	59 986	26	10	414 052
20	11	28	22	11	3 924	24	11	32 256	26	11	250 622
			22	12	500	24	12	16 232	26	12	132 908
						24	13	4 280	26	13	63 386
						24	14	154	26	14	24 452
									26	15	3 028
28	0	1 206 818	30	0	5 558 724	32	0	25 803 509	34	0	120 638 466
28	1	4 189 420	30	1	20 297 228	32	1	99 008 272	34	1	485 808 492
28	2	7 791 274	30	2	39 822 158	32	2	204 447 542	34	2	1 053 436 400
28	3	10 541 380	30	3	56 574 708	32	3	304 436 224	34	3	1 641 203 412
28	4	11 805 811	30	4	66 024 666	32	4	369 974 212	34	4	2 075 439 970
28	5	11 601 068	30	5	67 216 160	32	5	390 203 512	34	5	2 266 884 096
28	6	10 285 214	30	6	61 558 578	32	6	369 111 558	34	6	2 214 114 652
28	7	8 337 688	30	7	51 656 214	32	7	319 477 936	34	7	1 975 494 948
28	8	6 320 269	30	8	40 178 374	32	8	256 686 755	34	8	1 634 546 818
28	9	4 399 656	30	9	29 443 298	32	9	193 161 096	34	9	1 267 837 116
28	10	2 975 016	30	10	20 083 644	32	10	137 613 088	34	10	927 667 754
28	11	1 808 576	30	11	13 178 456	32	11	92 079 812	34	11	645 059 158
28	12	1 057 622	30	12	7 968 438	32	12	59 007 648	34	12	424 295 022
28	13	567 540	30	13	4 551 574	32	13	35 428 684	34	13	266 938 184
28	14	262 116	30	14	2 446 186	32	14	19 977 836	34	14	158 957 976
28	15	112 192	30	15	1 153 074	32	15	10 655 808	34	15	89 006 190
28	16	27 560	30	16	483 900	32	16	5 163 928	34	16	47 110 136
28	17	1 204	30	17	166 728	32	17	2 163 628	34	17	23 154 978
			30	18	22 112	32	18	818 630	34	18	10 030 816
			30	19	308	32	19	199 836	34	19	3 814 080
						32	20	13146	34	20	1 238 968
									34	21	191 868
									34	22	4 864

Table A2. (Continued)

n	k	$p_n(k)$	n	k	$p_n(k)$	n	k	$p_n(k)$	n	k	$p_n(k)$
36	0	567 732 133	38	0	2 687 937 916	40	0	12 796 823 923	42	0	61 235 363 802
36	1	2 396 065 580	38	1	11 871 631 876	40	1	59 058 603 772	42	1	294 873 317 972
36	2	5 444 273 148	38	2	28 208 568 050	40	2	146 480 771 246	42	2	762 110 650 372
36	3	8 859 088 348	38	3	47 864 522 384	40	3	258 774 823 792	42	3	1 399 688 241 956
36	4	11 647 025 630	38	4	65 356 204 120	40	4	366 598 059 998	42	4	2 055 118 460 378
36	5	13 169 303 200	38	5	76 458 854 924	40	5	443 457 246 668	42	5	2 568 728 314 030
36	6	13 275 125 086	38	6	79 511 992 592	40	6	475 535 061 978	42	6	2 838 932 155 072
36	7	12 202 175 232	38	7	75 247 286 342	40	7	463 109 497 364	42	7	2 843 720 976 824
36	8	10 388 601 811	38	8	65 868 482 586	40	8	416 535 589 099	42	8	2 626 666 404 320
36	9	8 284 253 876	38	9	53 955 153 548	40	9	350 206 578 292	42	9	2 265 228 537 960
36	10	6 237 262 394	38	10	41 706 504 166	40	10	277 676 883 848	42	10	1 840 844 618 944
36	11	4 454 547 472	38	11	30 609 613 076	40	11	208 991 818 212	42	11	1 419 474 224 078
36	12	3 034 098 341	38	12	21 408 550 092	40	12	150 036 552 328	42	12	1 043 977 291 720
36	13	1 965 904 908	38	13	14 324 532 228	40	13	103 039 789 644	42	13	735 151 740 056
36	14	1 218 682 494	38	14	9 157 864 514	40	14	67 883 242 114	42	14	496 824 634 882
36	15	719 371 560	38	15	5 608 439 482	40	15	42 879 298 560	42	15	322 875 667 652
36	16	401 071 891	38	16	3 282 544 430	40	16	25 992 755 022	42	16	201 753 866 414
36	17	211 258 692	38	17	1 824 153 318	40	17	15 097 553 036	42	17	121 230 197 502
36	18	104 443 870	38	18	958 806 512	40	18	8 363 957 186	42	18	69 955 721 188
36	19	46753216	38	19	475774598	40	19	4 395 853 816	42	19	38 635 944 222
36	20	18225676	38	20	217437824	40	20	2 187 904 502	42	20	20 323 389 508
36	21	6406616	38	21	88559862	40	21	1 014 394 516	42	21	10 146 432 880
36	22	1 615 006	38	22	31 817 912	40	22	428 257 958	42	22	4 758 325 428
36	23	139 760	38	23	9 956 348	40	23	159 976 584	42	23	2 059 822 102
36	24	1072	38	24	1 733 664	40	24	53 453 638	42	24	805 102 310
			38	25	81 020	40	25	13 638 392	42	25	279 144 480
						40	26	1 582 186	42	26	83 753 436
						40	27	34 972	42	27	16 591 468
									42	28	1 212 792
									42	29	10 640

method of differential approximants and find for walks

$$\text{unbiased } x_c = 0.431\,80(2) \qquad \gamma = 1.344(1) \tag{3.3}$$

$$\text{biased } x_c = 0.431\,792\,5(1) \tag{3.4}$$

where the biased value has imposed $\gamma = \frac{43}{32}$ on the approximants, and x_c (from which the free energy can be calculated) is the closest singularity to the origin of the generating function of partition functions. For polygons (noting that x_c for polygons should be equal to the square of x_c for walks since only even length polygons exist) we obtain

$$\text{unbiased } x_c = 0.186\,7(6) \qquad 2 - \alpha = 1.5(2) \tag{3.5}$$

$$\text{biased } 2 - \alpha = 1.43(16) \text{ (first order)} \qquad 1.47(11) \text{ (second order)} \tag{3.6}$$

where the biased exponent estimates have been obtained using the value given in (3.4) for the critical point. The exponent estimates are consistent with the expected value of $\alpha = \frac{1}{2}$.

4. Summary

We have presented and analysed substantially extended series for both ISAW and ISAP on the square lattice. Our analysis provides good evidence that the free energies of both

Table B1. The coefficients $c_n(k)/4$ for $n \leqslant 29$ and all k, and for $k = 0$ with $n \leqslant 32$.

n	k	$c_n(k)/4$	n	k	$c_n(k)/4$	n	k	$c_n(k)/4$	n	k	$c_n(k)/4$
1	0	1	2	0	3	3	0	7	4	0	17
						3	1	2	4	1	8
5	0	41	6	0	99	7	0	235	8	0	561
5	1	22	6	1	64	7	1	184	8	1	508
5	2	8	6	2	32	7	2	86	8	2	268
						7	3	38	8	3	132
									8	4	10
9	0	1 331	10	0	3 167	11	0	7 485	12	0	17 753
9	1	1 344	10	1	3 556	11	1	9 244	12	1	23 876
9	2	850	10	2	2 458	11	2	6 900	12	2	19 250
9	3	346	10	3	1 152	11	3	3 888	12	3	11 436
9	4	196	10	4	596	11	4	1 606	12	4	5 660
				5	96	11	5	888	12	5	2 524
						11	6	62	12	6	734
13	0	41 867	14	0	99 043	15	0	233 157	16	0	550 409
13	1	60 884	14	1	154 792	15	1	389 792	16	1	979 240
13	2	52 934	14	2	143 140	15	2	383 628	16	2	1 018 166
13	3	33 472	14	3	96 904	15	3	276 892	16	3	774 040
13	4	19 076	14	4	56 594	15	4	169 214	16	4	500 926
13	5	7 444	14	5	27 300	15	5	91 128	16	5	275 232
13	6	3 978	14	6	11 310	15	6	37 466	16	6	134 610
13	7	720	14	7	4 244	15	7	17 324	16	7	53 040
			14	8	284	15	8	5 410	16	8	21 890
						15	9	138	16	9	3 780
17	0	1 293 817	18	0	3 048 915						
17	1	2 442 268	18	1	6 080 388						
17	2	2 681 356	18	2	7 008 782						
17	3	2 149 774	18	3	5 894 524						
17	4	1 459 644	18	4	4 168 254						
17	5	841 890	18	5	2 537 728						
17	6	444 576	18	6	1 362 950						
17	7	189 650	18	7	658 576						
17	8	79 632	18	8	267 858						
17	9	30 716	18	9	105 212						
17	10	3 346	18	10	30 408						
			18	11	1 088						
19	0	7 158 201	20	0	16 843 573	21	0	39 504 435			
19	1	15 049 866	20	1	37 200 956	21	1	91 512 966			
19	2	18 207 818	20	2	47 034 904	21	2	120 863 206			
19	3	16 046 364	20	3	43 256 096	21	3	115 919 582			
19	4	11 829 258	20	4	33 149 118	21	4	92 235 318			
19	5	7 530 130	20	5	21 896 316	21	5	63 319 470			
19	6	4 240 496	20	6	12 912 128	21	6	38 842 204			
19	7	2 170 710	20	7	6 763 244	21	7	21 312 058			
19	8	968 778	20	8	3 274 210	21	8	10 792 706			
19	9	387 378	20	9	1 369 416	21	9	4 893 520			
19	10	154 960	20	10	518 706	21	10	1 986 952			
19	11	34 190	20	11	183 172	21	11	756 634			
19	12	1 006	20	12	22 452	21	12	239 288			
						21	13	23 168			
22	0	92 838 503	23	0	217 549 387	24	0	510 702 499			
22	1	224 889 896	23	1	550 409 212	24	1	1 346 063 500			
22	2	309 216 494	23	2	787 511 174	24	2	1 998 666 370			
22	3	308 316 464	23	3	815 771 144	24	3	2 145 565 908			

Table B1. (Continued)

n	k	$c_n(k)/4$	n	k	$c_n(k)/4$	n	k	$c_n(k)/4$	n	k	$c_n(k)/4$
22	4	254 062 502	23	4	695 840 182	24	4	1 890 521 138			
22	5	180 643 016	23	5	511 950 948	24	5	1 435 323 712			
22	6	114 457 820	23	6	335 858 110	24	6	971 353 634			
22	7	65 452 948	23	7	199 169 112	24	7	593 724 016			
22	8	34 023 448	23	8	108 005 076	24	8	333 701 296			
22	9	16 342 620	23	9	54 030 120	24	9	171 821 676			
22	10	7 029 848	23	10	24 789 036	24	10	82 408 644			
22	11	2 663 104	23	11	10 292 240	24	11	35 940 268			
22	12	974 308	23	12	3 847 090	24	12	14 044 418			
22	13	219 996	23	13	1 358 836	24	13	5 056 504			
22	14	9 154	23	14	263 792	24	14	1 523 664			
			23	15	7 994	24	15	179 920			
						24	16	2 162			
25	0	1 195 823 247	26	0	2 804 575 869	27	0	6 562 607 385			
25	1	3 280 337 168	26	1	7 989 432 672	27	1	19 398 952 628			
25	2	5 052 329 956	26	2	12 735 745 520	27	2	31 990 605 456			
25	3	5 617 273 282	26	3	14 635 149 660	27	3	37 975 439 858			
25	4	5 110 374 048	26	4	13 723 257 002	27	4	36 687 855 574			
25	5	4 002 750 354	26	5	11 066 113 256	27	5	30 446 746 918			
25	6	2 793 373 142	26	6	7 942 250 944	27	6	22 474 908 138			
25	7	1 763 705 626	26	7	5 160 559 796	27	7	15 025 151 052			
25	8	1 023 991 992	26	8	3 080 396 086	27	8	9 237 967 176			
25	9	548 429 998	26	9	1 703 470 136	27	9	5 264 647 012			
25	10	273 099 178	26	10	873 273 892	27	10	2 797 593 720			
25	11	125 831 856	26	11	417 566 464	27	11	1 387 134 186			
25	12	53 364 032	26	12	184 559 436	27	12	642 687 898			
25	13	20 253 608	26	13	74 060 220	27	13	276 027 632			
25	14	7 197 122	26	14	26 965 768	27	14	107 944 142			
25	15	2 002 618	26	15	8 860 896	27	15	38 397 784			
25	16	201 500	26	16	1 853 750	27	16	12 289 666			
25			26	17	105 188	27	17	2 326 206			
25						27	18	90 476			
28	0	15 378 643 401	29	0	35 964 253 315	30	0	84 216 378 195			
28	1	47 081 130 896	29	1	113 955 364 388	31	0	196 843 613 381			
28	2	80 171 819 670	29	2	200 285 841 574	32	0	460 644 961 545			
28	3	98 143 110 328	29	3	252 719 748 694						
28	4	97 542 797 720	29	4	258 304 841 600						
28	5	83 171 958 968	29	5	226 229 739 140						
28	6	63 017 743 614	29	6	175 916 739 126						
28	7	43 234 422 648	29	7	123 873 896 460						
28	8	27 284 382 172	29	8	80 239 865 186						
28	9	15 960 029 252	29	9	48 245 510 340						
28	10	8 725 745 632	29	10	27 125 641 348						
28	11	4 452 294 048	29	11	14 304 265 858						
28	12	2 130 127 362	29	12	7 085 279 050						
28	13	950 315 284	29	13	3 293 828 278						
28	14	389 858 002	29	14	1 432 023 556						
28	15	145 741 920	29	15	573 273 466						
28	16	49 190 166	29	16	209 372 954						
28	17	13 502 664	29	17	69 353 438						
28	18	1 799 226	29	18	18 180 612						
28	19	32 588	29	19	2 011 954						
			29	20	26 996						

linear and ring polymers are equal above the θ-temperature; this result is consistent with an extension of a theorem of Tesi *et al* [1], but below the θ-temperature the conditions of this theorem break down. However, an analysis of the ratio of the partition functions for ISAP and ISAW indicate that the free energies are in fact equal at all temperatures to at least within 1%. Any perceived difference can be interpreted as the difference in the size of corrections-to-scaling in both problems. This may explain the vastly different values of the crossover exponent previously estimated for ISAP to that predicted theoretically, and numerically confirmed, for ISAW. We also present newly extended neighbour-avoiding SAW series and analyse them. We develop a Monte Carlo approach to this problem, and discuss its application to ISAPs.

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Appendix A. Interacting self-avoiding polygon enumerations

Table A1 shows the coefficients $p_n(k)$ for the numbers of SAPs of length n with k nearest-neighbour contacts up to $n = 42$.

Appendix B. Interacting self-avoiding walk enumerations

Table B1 shows the coefficients $c_n(k)$ (actually we give $c_n(k)/4$) the numbers of SAWs of length n with k nearest-neighbour contacts up to $n = 29$. When $k = 0$ neighbour-avoiding walks are realized and the numbers, $c_n(0)$, in table B1 gives the numbers of neighbour-avoiding walks up to $n = 32$.

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