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A study of uniform stars using $1/d$-expansions and numerical methods

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Abstract. We study a lattice model of an interacting uniform self-avoiding star polymer with f branches. A $1/d$-expansion for the limiting reduced free energy is derived through order $1/d$ for general f and, for $f = 3$, to order $1/d^2$. The terms in the expansion are independent of f and agree term by term with the corresponding expansion for interacting self-avoiding walks. We also present a miscellany of numerical results obtained by more conventional series and Monte Carlo techniques. All our results, both past and present, support the conjecture that the limiting reduced free energies of f-stars, walks and polygons are identical for all values of the interaction parameter β.

1. Introduction

We consider a lattice model of a uniform f-star polymer with nearest-neighbour contact interactions. An *f-star* is a connected subgraph of the lattice with one vertex of degree f and f vertices of degree one. A *branch* is the sequence of edges connecting the vertex of degree f to a vertex of degree 1. A star is *uniform* if each of the f branches has the same number of edges. A nearest-neighbour *contact* is a pair of vertices of the star which are one lattice space apart but not joined by an edge of the star.

Let the number of uniform f-stars on a d-dimensional simple hypercubic lattice with n edges in each branch and with k contacts be $s_n(k; f)$. Clearly, $s_n(k; 1) \equiv c_n(k)$, the number of self-avoiding walks with n edges and k contacts. Let $p_n(k)$ be the corresponding number of self-avoiding polygons. We define the partition functions for interacting self-avoiding polygons (ISAP), interacting self-avoiding walks (ISAW) and interacting uniform f-stars (ISAS-f) by

$$Z_n^o(\beta) = \sum_k p_n(k)\mathrm{e}^{\beta k} \tag{1.1}$$

$$Z_n(\beta) = \sum_k c_n(k)\mathrm{e}^{\beta k} \tag{1.2}$$

and

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

respectively. The corresponding limiting reduced free energies (per edge) are then given by

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

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

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and

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

It has been proven rigorously (Tesi *et al* 1996a) that $\kappa^o(\beta)$ exists for all values of the interaction parameter $\beta < \infty$, and that the limiting free energies for polygons and walks are identical for $\beta \leqslant 0$. In a previous paper (Yu *et al* 1997), we proved rigorously that, for values of $\beta \leqslant 0$, $\kappa_f(\beta)$ exists and $\kappa_f(\beta) = \kappa(\beta)$, independent of f. Although Yu *et al* (1997) were unable to construct rigorous proofs of the corresponding results for $\beta > 0$, they presented some numerical results for the triangular, square and simple cubic lattices which suggested that the limiting free energies of ISAP, ISAW and ISAS-f are identical for *all* values of β, i.e.

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

If true, this result would imply that the heat capacity (essentially the second derivative of the free energy), the location β_c of the collapse transition and the value of the corresponding crossover exponent ϕ, were the same for all three polymer architectures. Indeed, it has been speculated (Yu *et al* 1997, Bennett-Wood *et al* 1998) that these results extend to uniform embeddings of graphs of every fixed homeomorphism type.

In this paper, we present some non-numerical evidence based upon $1/d$-expansions (Fisher and Gaunt 1964) that the limiting reduced free energy (per edge) of interacting uniform f-stars is the same as for self-avoiding walks *for all values of* β. We also derive exact enumeration and Monte Carlo data which are used to estimate numerically β_c and ϕ for f-stars. These estimates are compared with extant results for walks and polygons.

2. $1/d$-expansions

The algebraic techniques we use in this section are similar to those described previously by Peard and Gaunt (1995) for self-interacting (weakly embeddable) lattice animals.

We consider a d-dimensional simple hypercubic lattice with coordination number $q (= \sigma + 1)$ given by

$$q = 2d = \sigma + 1. \tag{2.1}$$

The partition function (1.3) is rewritten as

$$Z_n^{(d)}(x; f) = \sum_{\ell=1}^{fn} \sum_{k\geqslant 0} s_{k,\ell}^{(n)}(f) x^k \binom{d}{\ell} \tag{2.2}$$

in which $s_{k,\ell}^{(n)}(f)$ is the number of uniform f-stars with k-contacts and n steps in each branch, spanning an ℓ-dimensional subspace. The Boltzmann factor in (1.3) is given by

$$x = e^{\beta}. \tag{2.3}$$

With the aid of computer enumeration data, we have derived the $Z_n^{(d)}(x; f)$ through orders $n = 4, 3, 2$ and 2 for $f = 3, 4, 5$ and 6, respectively. The results which, it should be emphasized, hold *for arbitrary* d are presented in appendix A. Of course, for small values of d and f, more extensive data can be derived and these are given in appendix B. We also give data for the triangular lattice through orders $n = 5, 5, 4$ and 4 for $f = 3, 4, 5$ and 6, respectively. On putting $x = 1$, these data check and extend by up to two terms the exact enumeration data of Wilkinson *et al* (1986) for the *total* number of uniform f-stars.

Using combinatorics, we now calculate the general form of the coefficient $s_{k,\ell}^{(n)}(f)$ occurring in (2.2), at least for sufficiently large ℓ-dimensional subspaces. The largest value of

ℓ is clearly $\ell = fn$, which occurs when each of the n steps in every one of the f branches is in a new dimension not visited by other steps. It is not difficult to see that for all such embeddings $k = 0$. Hence, all the $s^{(n)}_{k,fn}(f)$ are zero except

$$s^{(n)}_{0,fn}(f) = \frac{(fn)!2^{fn}}{f!}. \tag{2.4}$$

The $(fn)!$ factor appears because the fn dimensions may be chosen in any order while the factor 2^{fn} arises because when a step enters a new dimension, there are two possible directions. The $f!$ factor arises from the indistinguishability of the f branches.

When an f-star is embedded in $\ell = fn-1$ dimensions, it simply means that two of the fn steps are parallel or antiparallel to each other, but each of the remaining steps is directed into a new dimension. All such distinct embeddings fall into one of the following three categories:

(1) Choose any two of the f branches, say the pth and qth. Let the sth step ($1 \leqslant s \leqslant n$) of the pth branch be parallel or antiparallel to the sth step of the qth branch, with the remaining steps spanning an $(fn-2)$-dimensional subspace. Two different cases must be considered.

(i) $s = 1$. In this case, the first step of the pth branch must be antiparallel to the first step of the qth branch (i.e. they lie on the same axis) and there are no contact interactions. This contributes an amount

$$K_{1a} = (fn-1) \times (fn-2)!2^{fn-2} \times \frac{1}{(f-2)!} = \frac{(fn-1)!2^{fn-1}}{2!(f-2)!}. \tag{2.5}$$

The factor $(fn-1)$ is the number of possible axes the antiparallel pair can lie on. The remaining $(fn-2)$ steps can be embedded in $(fn-2)!2^{fn-2}$ different ways. The $(f-2)!$ factor arises from the indistinguishability of the remaining branches.

(ii) $s = 2, 3, \ldots, n$. Similar arguments to those above can be used with the difference that the chosen pair of steps can now be parallel or antiparallel to each other. Hence, the total contribution of these $(n-1)$ types is

$$K_{1b} = (n-1) \times 2 \times \frac{(fn-1)!2^{fn-1}}{2!(f-2)!}. \tag{2.6}$$

(2) Choose any one of the f branches. Let the sth step and the tth step be parallel or antiparallel to each other with the remaining steps, on the chosen branch and the other unchosen branches, being directed into different unvisited dimensions. The following cases have to be considered.

(i) $t = s + 1$, i.e. the sth step is immediately followed by the tth step. As these two steps are parallel to each other, there can be no contact interactions. Since $1 \leqslant s \leqslant (n-1)$, such embeddings contribute a total of

$$K_{2a} = (n-1) \times \frac{(fn-1)!2^{fn-1}}{(f-1)!}. \tag{2.7}$$

(ii) $t = s + 2$ with $1 \leqslant s \leqslant (n-2)$. If the sth and tth steps are parallel to each other, there is no contact interaction. If, on the other hand, the sth and tth steps are antiparallel, there will be one contact. The contribution from configurations of each type is

$$K_{2b} = \frac{1}{2} \times (n-2) \times \frac{(fn-1)!2^{fn-1}}{(f-1)!} \times 2. \tag{2.8}$$

(iii) $t = s + i$ with $i > 2$ and $1 \leqslant s \leqslant (n-i)$. In this case, there are no contact interactions whether the sth and tth steps are parallel or antiparallel to each other. For each i, the contribution is

$$(n-i) \times \frac{(fn-1)!2^{fn-1}}{(f-1)!} \times 2.$$

Since $3 \leqslant i \leqslant (n-1)$, the total contribution is

$$K_{2c} = [(n-3) + (n-4) + \cdots + 2 + 1] \times \frac{(fn-1)!2^{fn-1}}{(f-1)!} \times 2$$
$$= \frac{1}{2}(n-2)(n-3) \times \frac{(fn-1)!2^{fn-1}}{(f-1)!} \times 2. \tag{2.9}$$

(3) Finally, choose any two branches and let the sth step of one branch be parallel or antiparallel with the $(s+k)$th step of the other branch, where $1 \leqslant s < (s+k) \leqslant n$. Let all the remaining steps be directed into different unvisited dimensions. The following cases arise.

(i) $k = 1; s = 1$. Configurations with one contact contribute

$$K_{3a} = \frac{(fn-1)!2^{fn-1}}{(f-2)!} \tag{2.10}$$

and the same amount with no contacts.

(ii) $k = 1; s = 2, 3, \ldots, (n-1)$. For all values of s, the configurations are free of contacts and contribute

$$\frac{(fn-1)!2^{fn-1}}{(f-2)!} \times 2.$$

Since s can take $(n-2)$ different values, the total contribution is

$$K_{3b} = (n-2) \times \frac{(fn-1)!2^{fn-1}}{(f-2)!} \times 2. \tag{2.11}$$

(iii) $k = 2, 3, \ldots, (n-1); s = 1, 2, \ldots, (n-k)$. These configurations contribute an amount

$$(n-k) \times \frac{(fn-1)!2^{fn-1}}{(f-2)!} \times 2$$

for each value of k, giving a total contribution of

$$K_{3c} = [(n-2) + (n-3) + \cdots + 2 + 1] \times \frac{(fn-1)!2^{fn-1}}{(f-2)!} \times 2$$
$$= \frac{1}{2}(n-1)(n-2) \times \frac{(fn-1)!2^{fn-1}}{(f-2)!} \times 2. \tag{2.12}$$

Summing all the contributions discussed above yields the rigorous result

$$\sum_{k\geqslant 0} s^{(n)}_{k,fn-1}(f)x^k = (K_{1a} + K_{1b} + K_{2a} + K_{2b} + K_{2c} + K_{3a} + K_{3b} + K_{3c}) + (K_{2b} + K_{3a})x$$
$$= \left[\frac{n^2 - \frac{3}{2}}{(f-2)!} + \frac{n^2 - 3n + 3}{(f-1)!}\right] \times (fn-1)!2^{fn-1}$$
$$+ \left[\frac{n-2}{(f-1)!} + \frac{1}{(f-2)!}\right] x \times (fn-1)!2^{fn-1}. \tag{2.13}$$

Substituting the results in (2.4) and (2.13) into (2.2) one obtains, following some manipulation,

$$Z_n^{(d)}(x; f) = \frac{(fn)!2^{fn}}{f!}\binom{d}{fn}$$
$$+\{[f^2n^2 - 3fn - \tfrac{3}{2}f(f-3)] + [fn + f(f-3)]x\}$$
$$\times \frac{(fn-1)!2^{fn-1}}{f!}\binom{d}{fn-1} + \cdots. \tag{2.14}$$

Unfortunately, we have been unable to derive higher-order terms in this expansion owing to the complexity of the combinatorics. The equation is valid for self-interacting f-stars with

$f \geqslant 3$ and for all $n \geqslant 2$, as can be confirmed numerically using appendix A. It is also true for ISAW obtained by setting either $f = 1$ or (barring a trivial factor of 2) $f = 2$.

Expanding the binomial coefficients in (2.14) in inverse powers of σ—see, for example, Peard and Gaunt (1995), equation (2.17)—gives

$$Z_n^{(d)}(x; f) = \frac{\sigma^{fn}}{f!}\left\{1 + \left[-\frac{3}{2}f^2 + \left(\frac{9}{2} - n\right)f + [fn + f(f-3)]x\right]\sigma^{-1} + \cdots\right\}. \tag{2.15}$$

Then formally taking the logarithm of $Z_n^{(d)}(x; f)$, dividing by nf and letting $n \to \infty$, as in (1.6), we obtain the $1/\sigma$-expansion for the limiting free energy per edge through first order, namely

$$\kappa_f^{(d)}(x) = \log\sigma + (x-1)\sigma^{-1} + \cdots. \tag{2.16}$$

This expansion, which is independent of f, agrees exactly through order $1/\sigma$ with the corresponding expansion (see Nemirovsky *et al* (1992), equation (19)) for ISAW. This result supports our conjecture that interacting uniform f-stars and interacting walks have the same limiting free energy over the entire range of β (or x) on a d-dimensional hypercubic lattice.

Although we have been unable to derive the next term in the expansion (2.14) for arbitrary f, we do have sufficient information to derive the next term for the case of $f = 3$. One finds

$$\begin{aligned} Z_n^{(d)}(x; 3) = {} & \frac{(3n)!2^{3n}}{3!}\binom{d}{3n} + [9n(n-1) + 3nx]\frac{(3n-1)!2^{3n-1}}{3!}\binom{d}{3n-1} \\ & +[(\tfrac{81}{2}n^4 - 117n^3 + \tfrac{207}{2}n^2 - 23n - 4) + (27n^3 - 45n^2 + 3n + 6)x \\ & +(\tfrac{9}{2}n^2 + \tfrac{9}{2}n - 3)x^2]\frac{(3n-2)!2^{3n-2}}{3!}\binom{d}{3n-2} + \cdots \end{aligned} \tag{2.17}$$

where the first two terms are obtained by setting $f = 3$ in (2.14). As may be confirmed from appendix A, this expansion is correct for $n = 4$ and is expected to be valid for all $n \geqslant 4$. It follows from (2.17) that, through second order in $1/\sigma$,

$$\kappa_3^{(d)}(x) = \log\sigma + (x-1)\sigma^{-1} + [-1 + (x-1) + \tfrac{3}{2}(x-1)^2]\sigma^{-2} + \cdots \tag{2.18}$$

which is in precise agreement with equation (19) in Nemirovsky *et al* (1992) for ISAW. This further supports the notion that interacting 3-stars and walks have the same limiting free energy for all values of β.

Finally, it is interesting to define a two-variable model for interacting uniform-star polymers in which one distinguishes contact interactions between monomers on the same branch (interaction parameter β_x) and between monomers on different branches (interaction parameter β_y). The partition function for such a polymer is the two-variable generalization of (2.2), namely

$$Z_n^{(d)}(x, y; f) = \sum_{\ell=1}^{fn}\sum_{k\geqslant 0}\sum_{h\geqslant 0} s_{k,h,\ell}^{(n)}(f)x^k y^h \binom{d}{\ell}. \tag{2.19}$$

Here $x = e^{\beta_x}$, $y = e^{\beta_y}$ and $s_{k,h,\ell}^{(n)}(f)$ is the number of f-stars with n steps in each branch, k β_x-interactions and h β_y-interactions spanning an ℓ-dimensional subspace.

By using similar arguments to those used in the derivation of (2.4), one can readily see that all $s_{k,h,fn}^{(n)}(f)$ are zero unless $k = h = 0$ in which case

$$s_{0,0,fn}^{(n)}(f) = \frac{(fn)!2^{fn}}{f!}. \tag{2.20}$$

We also saw that K_{2b} in (2.8) is the contribution from stars with one β_x-interaction, while K_{3a} in (2.10) is from stars with one β_y-interaction. Thus,

$$\begin{aligned}\sum_{k\geqslant 0}\sum_{h\geqslant 0} s^{(n)}_{k,h,fn-1}(f)x^k y^h &= (K_{1a}+K_{1b}+K_{2a}+K_{2b}+K_{2c}+K_{3a}+K_{3b}+K_{3c})\\ &\quad +K_{2b}x+K_{3a}y\\ &= \left[\frac{n^2-\frac{3}{2}}{(f-2)!}+\frac{n^2-3n+3}{(f-1)!}\right]\times(fn-1)!2^{fn-1}\\ &\quad +\left[\frac{n-2}{(f-1)!}x+\frac{1}{(f-2)!}y\right]\times(fn-1)!2^{fn-1}\end{aligned}\tag{2.21}$$

is the correct generalization of (2.13). Substituting (2.20) and (2.21) into (2.19) leads to

$$\begin{aligned}Z_n^{(d)}(x,y;f) &= \frac{(fn)!2^{fn}}{f!}\binom{d}{fn}\\ &\quad +\{[f^2n^2-3fn-\tfrac{3}{2}f(f-3)]+[(fn-2f)x+f(f-1)y]\}\\ &\quad \times\frac{(fn-1)!2^{fn-1}}{f!}\binom{d}{fn-1}+\cdots\end{aligned}\tag{2.22}$$

which reproduces (2.14) when $y=x$. Like that equation, (2.22) is valid for all $f\geqslant 1$ and $n\geqslant 2$.

Expanding the binomial coefficients in (2.22) in powers of $1/\sigma$, taking the logarithm of the partition function, dividing by nf and letting $n\to\infty$ gives the limiting reduced free energy as

$$\kappa_f^{(d)}(x,y)=\log\sigma+(x-1)\sigma^{-1}+\cdots.\tag{2.23}$$

We note that the coefficients in this expansion are independent of y through leading order in $1/\sigma$ and that the expansion is identical to that in (2.16). This implies that the limiting free energy is dominated by the self-interactions within each branch, at least for large d.

3. Numerical results

In a previous paper (Yu *et al* 1997), we estimated limiting reduced free energies from the sequence of partition functions Z_n for sizes $n=1,2,3,\ldots$. The limiting free energy has been proved to exist for ISAP for all $\beta<\infty$ and for ISAW and ISAS-f for $\beta\leqslant 0$. These suggest that asymptotically

$$Z_n(\beta)\sim n^{\gamma(\beta)-1}\mu(\beta)^n \qquad (\text{ISAW, ISAS}-f)\tag{3.1}$$

and

$$Z_n(\beta)\equiv 2nZ_n^o(\beta)\sim n^{\gamma(\beta)-1}\mu(\beta)^n \qquad (\text{ISAP})\tag{3.2}$$

where the modification for ISAP maintains consistency with the definition of Duplantier (1989), who has predicted theoretical values for the exponent $\gamma(0)$. Suppose $\mathcal{L}$ is the number of physical loops in a polymer network (with no interactions, i.e. $\beta=0$) embedded in a d-dimensional lattice, and n_L is the number of vertices of functionality L. Duplantier showed that

$$\gamma(0)=1-\nu d\mathcal{L}+\sum_{L\geqslant 1}n_L\sigma_L\tag{3.3}$$

where ν is the exponent characterizing the radius of gyration, and when $d=2$, σ_L is given by

$$\sigma_L=(2-L)(9L+2)/64\tag{3.4}$$

Table 1. Theoretical values of $\gamma(0)$.

$\gamma(0)$	ISAW	ISAP	ISAS-3	ISAS-4
$d = 2$	$1\frac{11}{32} \approx 1.344$	$-\frac{1}{2}$	$1\frac{1}{16} \approx 1.063$	$\frac{1}{2}$
$d = 3$	1.18	−0.78	1.09	1.02

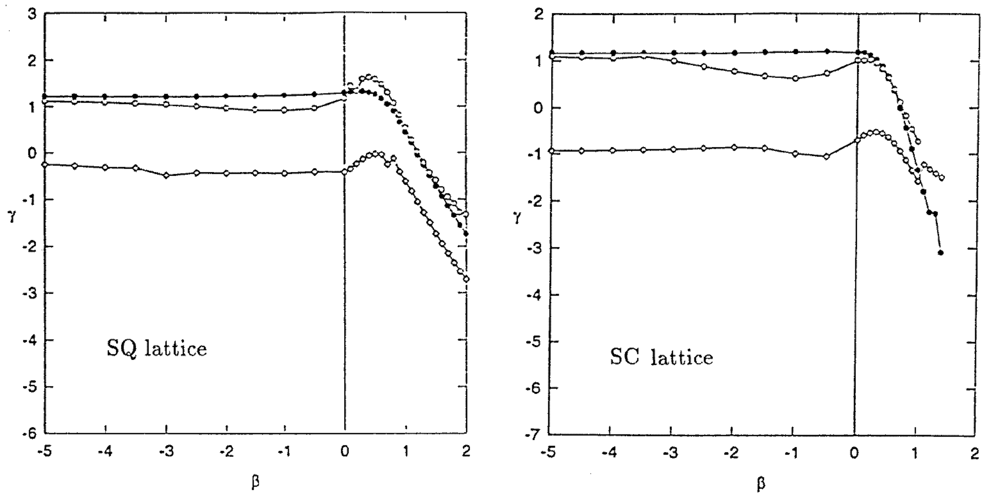

Figure 1. Estimates of $\gamma(\beta)$ for ISAW ($\bullet$), ISAP ($\Diamond$) and ISAS-3 ($\bigcirc$) on the square (SQ) and simple cubic (SC) lattices.

while when $d = 4 - \varepsilon (\varepsilon > 0)$,

$$\sigma_L = \frac{\varepsilon}{8}\frac{L}{2}(2 - L) + \left(\frac{\varepsilon}{8}\right)^2 \frac{L}{8}(L - 2)(8L - 21) + \mathrm{O}(\varepsilon^3). \tag{3.5}$$

For ISAW, ISAP, ISAS-3 and ISAS-4, one finds the theoretical values of $\gamma(0)$ given in table 1 for dimensions $d = 2$ and 3. For $\beta < \beta_c$, one expects that $\gamma(\beta) = \gamma(0)$. At $\beta = \beta_c$, a different value for the exponent is expected; for instance, for ISAW on the hexagonal lattice, Duplantier and Saleur (1987) have shown that $\gamma(\beta_c) = \frac{8}{7} < \gamma(0)$.

From the asymptotic forms in (3.1) and (3.2), it follows that the ratios $r_n \equiv Z_n(\beta)/Z_{n-1}(\beta)$ behave asymptotically as

$$r_n = \mu(\beta)\left[1 + \frac{\gamma(\beta) - 1}{n} + \mathrm{O}\left(\frac{1}{n^2}\right)\right] \tag{3.6}$$

i.e. linearly with $1/n$ as $n \to \infty$. A linear fit of the last few values gives a line with $\mu(\beta)$ as the intercept and slope $m(\beta) = \mu(\beta)[\gamma(\beta) - 1]$. In this way, the limiting reduced free energy, given by

$$\kappa(\beta) = \log \mu(\beta) \tag{3.7}$$

may be determined numerically. The above extrapolation procedures were found to work particularly well in the $\beta < 0$ region, but only up to relatively small values of $\beta > 0$. (See figures 2–4 of Yu *et al* (1997).)

We now present our results for the exponent $\gamma(\beta)$ calculated using

$$\gamma(\beta) = 1 + \frac{m(\beta)}{\mu(\beta)}. \tag{3.8}$$

Plots of $\gamma(\beta)$ for ISAW, ISAP and ISAS-3 on the square and simple cubic lattices are presented in figure 1. Plots for the triangular lattice are rather similar. Data for $f > 3$ are too short to extract reasonable estimates of $\gamma(\beta)$. It is observed that for $\beta < \beta_c$ (see, for example, the estimates in (3.14) and (3.15)), $\gamma(\beta)$ is roughly constant and consistent with Duplantier's predictions for $\gamma(0)$ given in table 1. Around $\beta = \beta_c$, a dramatic change in behaviour occurs with $\gamma(\beta)$ decreasing rapidly as β increases further. Such behaviour seems physically quite unreasonable and raises questions about the validity of the asymptotic forms in (3.1) and (3.2) for $\beta > \beta_c$. Indeed there is a conjecture (Bennett-Wood *et al* 1994) which suggests that for $\beta > \beta_c$ the asymptotic forms for Z_n in (3.1) and (3.2) should be replaced by

$$Z_n(\beta) \sim n^{\gamma(\beta)-1}\mu_0(\beta)^n\mu_1(\beta)^{n^\sigma} \tag{3.9}$$

where, most likely, $\sigma = (d-1)/d$, and $\mu_0(\beta)$ and $\mu_1(\beta)$ are unknown functions. Unfortunately, because of the number of unknowns in (3.9), Bennett-Wood *et al* (1994, 1998) were quite unable to estimate $\gamma(\beta)$ for $\beta > \beta_c$, even though they extended the series for ISAW and ISAP on the square lattice to $n = 29$ and $n = 42$, respectively.

Not surprisingly, the limiting reduced free energies determined numerically by Yu *et al* (1997) are very smooth, but approximate curves, quite unsuited to the study of the collapse transition. For estimating β_c and ϕ, the heat capacity is much more useful and, as usual, we will *assume* (Gaunt and Flesia 1990) that it may be calculated by defining the heat capacity of a polymer of size n as

$$C_n(\beta) = \frac{\partial^2\kappa_n(\beta)}{\partial\beta^2} \tag{3.10}$$

where

$$\kappa_n(\beta) = n^{-1}\log Z_n(\beta) \tag{3.11}$$

and then taking the $n \to \infty$ limit. We have therefore derived and analysed some exact enumeration and Monte Carlo simulation data for the heat capacity of f-stars. The simulations employ the Multiple Markov Chain sampling method (Tesi *et al* 1996b) and a 'pivot+local' algorithm. Thus, plots of C_n against β $(-5 < \beta < 5)$ for walks, polygons, 3-stars and 4-stars on the square, triangular and simple cubic lattices have been made. The plots are not reproduced here since they are not especially interesting and, in any case, are qualitatively very similar to the corresponding plots for collapsing lattice trees (Gaunt and Flesia 1991) and lattice animals (Flesia and Gaunt 1992). In particular, for n sufficiently large, they all exhibit a single sharp peak of height $h_n \equiv C_{n,\max}$ which is expected to increase as n increases like

$$h_n \sim n^{2\phi-1} \qquad n \to \infty. \tag{3.12}$$

The location of the peak at $\beta = \beta_{\max}(n)$ is identified with the collapse of the finite size polymer. As $n \to \infty$, $\beta_{\max}(n)$ is expected to approach β_c like

$$\beta_{\max}(n) = \beta_c + An^{-\phi} + \cdots \qquad n \to \infty \tag{3.13}$$

where A is a constant amplitude. The scaling analysis leading to (3.12) and (3.13) has been given elsewhere (Gaunt and Flesia 1991, Brak *et al* 1993) and will not be repeated here.

If the limiting free energies of interacting f-stars, self-avoiding walks and polygons are identical for all values of β (see Yu *et al* 1997, Bennett-Wood *et al* 1998 and section 2 of this paper), then β_c and ϕ should be the same for these three polymer architectures. In $d = 2$, recent results for ISAW and ISAP are consistent with a common location for the collapse transition at

$$\beta_c = 0.663 \pm 0.016 \qquad \text{(SQ)} \tag{3.14}$$

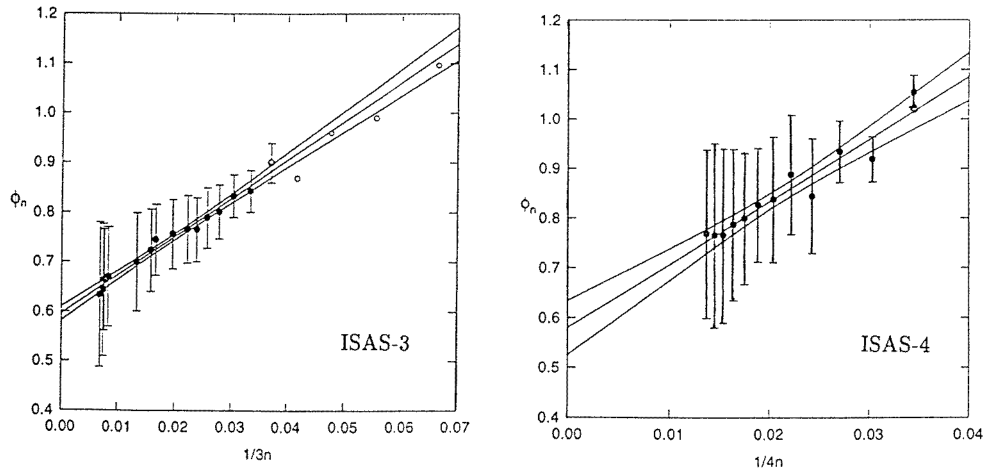

Figure 2. Estimates of ϕ for ISAS-3 and ISAS-4 on the square lattice. Monte Carlo (●) and exact enumeration (○) results.

while in $d = 3$ a common value around

$$\beta_c = 0.277 \pm 0.009 \qquad \text{(SC)} \tag{3.15}$$

is indicated (see Bennett-Wood *et al* 1998, and references therein). For ISAS-3 and ISAS-4, our series and Monte Carlo data are too limited to yield independent estimates of β_c with comparable uncertainties. However, we can confirm that the data are consistent with the above values.

For the cross-over exponent ϕ, there is the expectation that in $d = 3$, which is the upper critical dimension for tricritical walks, ϕ will have the mean-field value $\phi = \frac{1}{2}$. In common with other workers (Tesi *et al* 1996b, Grassberger and Hegger 1995a), we have simply accepted the expected theoretical value of $\phi = \frac{1}{2}$ and we know of no recent direct estimates for ISAW, ISAP or ISAS-f, although our series data are not inconsistent with $\phi = \frac{1}{2}$.

When $d = 2$, there is the conjecture of Duplantier and Saleur (1987) that $\phi = \frac{3}{7}$. However, as has been emphasized by Brak *et al* (1993), cross-over exponents are notoriously difficult to determine numerically and attempts to confirm this conjecture by direct numerical estimation have been surrounded in controversy. For ISAP, the best numerical estimate is far away from $\phi = \frac{3}{7}$ at $\phi = 0.90 \pm 0.02$ (Maes and Vanderzande 1990). For ISAW, a number of numerical estimates are somewhat closer to $\phi = \frac{3}{7}$, falling as they do in the range from $\phi = 0.48 \pm 0.07$ (Derrida and Saleur 1985) to $\phi = 0.66 \pm 0.02$ (Meirovitch and Lim 1989). Our Monte Carlo results for ISAS-3 and ISAS-4 on the square lattice are shown in figure 2. A linear least-squares fit of the larger values of n gives

$$\phi = 0.60 \pm 0.01 \quad (f = 3) \qquad \phi = 0.58 \pm 0.06 \quad (f = 4) \tag{3.16}$$

where the uncertainties represent the 95% confidence intervals shown in the figure. Our series data are consistent with these values.

The estimates in (3.16) support the conjecture that ϕ is independent of f for f-stars. They also lie within the range of ϕ-values that we quoted for ISAW, and are therefore consistent with the conjecture that walks and stars have a common value of ϕ. Unfortunately, none of the estimates for stars, walks or polygons are close to the theoretical value of $\phi = \frac{3}{7}$. However, more recent Monte Carlo work for ISAW, utilizing much larger values of n, has

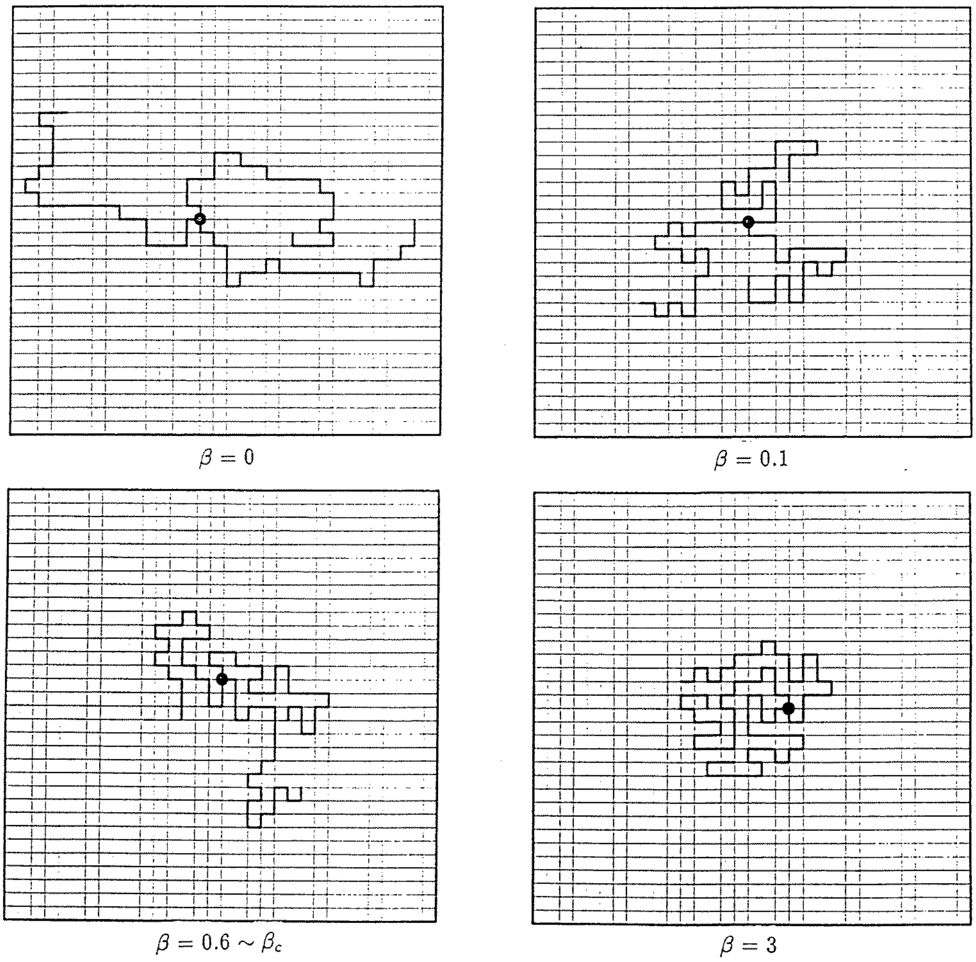

Figure 3. Typical simulation configurations at various values of β for ISAS-3 with $n = 30$ edges in each branch on the square lattice.

given $\phi = 0.430 \pm 0.006$ for the Manhattan lattice (Prellberg and Owczarek 1994) and $\phi = 0.435 \pm 0.006$ for the square lattice (Grassberger and Hegger 1995b), both of which seem to confirm $\phi = \frac{3}{7}$. Grassberger and Hegger argue that the larger values of ϕ that have been found may have resulted from the neglect of extremely large correction-to-scaling terms. So there remains the realistic hope that, when high-quality data are available for larger values of n, a correction-to-scaling analysis will yield estimates of ϕ closer to the expected theoretical value of $\phi = \frac{3}{7}$.

Finally, to understand qualitatively how an interacting uniform star polymer collapses as β increases from $\beta = 0$, interesting information can be obtained by using the Monte Carlo simulations to examine typical configurations. Figure 3 shows a 3-star on the square lattice with $n = 30$ in each branch changing its conformation from an expanded object to a compact or collapsed object as β increases. The collapse seems to occur in two stages. When $\beta = 0$, the star is expanded with relatively few intrachain interactions and even fewer interchain interactions. As β increases, each branch of the star begins to collapse individually so by

$\beta = 0.1$ there has been a large increase in the number of intrachain interactions although the number of interchain interactions is still small. This observation suggests that the conclusion implied by (2.23), namely that the limiting free energy is dominated by self-interactions within each branch at least for large d, is also true for small d. The individual chains (although quite short) seem to exhibit the blob-and-link structure observed by Grassberger and Hegger (1995b). At $\beta = 0.6$, just below β_c, not only has the average branch length of the star shrunk further, but different branches have come closer together increasing significantly the number of inter-chain contacts. At $\beta = 3.0$, well into the collapsed phase, the number of contacts is approaching its maximum value and one large blob has formed which contains most of the star. A similar process of collapse occurs when $f = 4$.

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Appendix A. Partition functions $Z_n^{(d)}(x; f)$ for ISAS-f with $f = 3, 4, 5$ and 6

A.1. $f = 3$

$$Z_1^{(d)}(x;3) = 4\binom{d}{2} + 8\binom{d}{3}$$

$$\begin{aligned}
Z_2^{(d)}(x;3) = {} & (16 + 48x + 20x^2)\binom{d}{2} + (744 + 960x + 288x^2 + 16x^3)\binom{d}{3} \\
& + (5248 + 3840x + 576x^2)\binom{d}{4} + (11\,520 + 3840x)\binom{d}{5} + 7680\binom{d}{6}
\end{aligned}$$

$$\begin{aligned}
Z_3^{(d)}(x;3) = {} & (300 + 392x + 468x^2 + 208x^3 + 12x^4)\binom{d}{2} + (54\,104 + 75\,384x + 60\,936x^2 \\
& + 25\,840x^3 + 6000x^4 + 768x^5)\binom{d}{3} + (1581\,760 + 1708\,608x + 995\,520x^2 \\
& + 310\,144x^3 + 52\,608x^4 + 5760x^5)\binom{d}{4} + (14\,527\,360 + 11\,600\,640x \\
& + 4704\,000x^2 + 956\,160x^3 + 82\,560x^4 + 3840x^5)\binom{d}{5} \\
& + (56\,732\,160 + 31\,703\,040x + 8087\,040x^2 + 806\,400x^3)\binom{d}{6} \\
& + (105\,692\,160 + 37\,094\,400x + 4515\,840x^2)\binom{d}{7} \\
& + (92\,897\,280 + 15\,482\,880x)\binom{d}{8} + 30\,965\,760\binom{d}{9}
\end{aligned}$$

$$\begin{aligned}
Z_4^{(d)}(x;3) = {} & (3604 + 5600x + 7400x^2 + 6088x^3 + 3652x^4 + 1528x^5 + 292x^6)\binom{d}{2} \\
& + (3548\,104 + 5643\,624x + 5888\,760x^2 + 4706\,320x^3 + 2650\,560x^4 \\
& + 1118\,760x^5 + 375\,384x^6 + 121\,488x^7 + 18\,384x^8 + 3744x^9)\binom{d}{3}
\end{aligned}$$

$$+(359\,019\,968 + 477\,608\,640x + 396\,898\,752x^2 + 250\,745\,408x^3$$
$$+112\,933\,056x^4 + 38\,962\,560x^5 + 10\,964\,928x^6 + 2979\,456x^7$$
$$+463\,488x^8 + 75\,648x^9 + 12\,288x^{10})\binom{d}{4}$$
$$+(9511\,981\,440 + 10\,227\,281\,280x + 6708\,929\,280x^2 + 3297\,354\,880x^3$$
$$+1128\,600\,960x^4 + 293\,410\,560x^5 + 62\,027\,520x^6 + 12\,349\,440x^7$$
$$+1148\,160x^8 + 111\,360x^9)\binom{d}{5} + (101\,525\,752\,320 + 87\,006\,965\,760x$$
$$+44\,450\,150\,400x^2 + 35\,703\,267\,840x^3 + 4044\,971\,520x^4 + 720\,437\,760x^5$$
$$+100\,277\,760x^6 + 11\,381\,760x^7)\binom{d}{6} + (540\,608\,517\,120 + 362\,266\,813\,440x$$
$$+139\,873\,950\,720x^2 + 37\,086\,013\,440x^3$$
$$+5819\,304\,960x^4 + 582\,220\,800x^5 + 39\,352\,320x^6)\binom{d}{7}$$
$$+(1600\,325\,959\,680 + 811\,442\,257\,920x + 223\,763\,742\,720x^2$$
$$+37\,896\,929\,280x^3 + 2869\,493\,760x^4 + 72\,253\,440x^5)\binom{d}{8}$$
$$+(2757\,346\,099\,200 + 998\,367\,068\,160x + 175\,854\,551\,040x^2$$
$$+14\,337\,146\,880x^3)\binom{d}{9}$$
$$+(2749\,759\,488\,000 + 635\,417\,395\,200x + 53\,880\,422\,400x^2)\binom{d}{10}$$
$$+(1471\,492\,915\,200 + 163\,499\,212\,800x)\binom{d}{11} + 326\,998\,425\,600\binom{d}{12}$$

A.2. $f = 4$

$$Z_1^{(d)}(x;4) = \binom{d}{2} + 12\binom{d}{3} + 16\binom{d}{4}$$
$$Z_2^{(d)}(x;4) = (1 + 8x + 20x^2 + 16x^3 + 2x^4)\binom{d}{2}$$
$$+(672 + 2496x + 2976x^2 + 1200x^3 + 120x^4)\binom{d}{3}$$
$$+(24\,352 + 52\,416x + 35\,136x^2 + 8064x^3 + 480x^4)\binom{d}{4}$$
$$+(210\,880 + 280\,320x + 107\,520x^2 + 11\,520x^3)\binom{d}{5}$$
$$+(681\,600 + 529\,920x + 92\,160x^2)\binom{d}{6}$$
$$+(913\,920 + 322\,560x)\binom{d}{7} + 430\,080\binom{d}{8}$$
$$Z_3^{(d)}(x;4) = (81 + 144x + 356x^2 + 368x^3 + 300x^4 + 48x^5)\binom{d}{2}$$

$$+(189\,336 + 573\,696x + 826\,704x^2 + 769\,056x^3$$
$$+446\,004x^4 + 172\,800x^5 + 33\,384x^6 + 4896x^7)\binom{d}{3}$$
$$+(32\,247\,344 + 74\,255\,424x + 80\,352\,768x^2 + 54\,632\,192x^3$$
$$+23\,236\,992x^4 + 6818\,880x^5 + 1131\,072x^6 + 142\,848x^7 + 8640x^8)\binom{d}{4}$$
$$+(1145\,229\,440 + 1231\,449\,600x + 1632\,417\,600x^2 + 823\,757\,440x^3$$
$$+255\,616\,320x^4 + 53\,779\,200x^5 + 6378\,240x^6 + 583\,680x^7 + 19\,200x^8)\binom{d}{5}$$
$$+(14\,800\,070\,400 + 24\,191\,481\,600x + 12\,198\,216\,960x^2 + 4512\,030\,720x^3$$
$$+979\,925\,760x^4 + 135\,129\,600x^5 + 9400\,320x^6 + 460\,800x^7)\binom{d}{6}$$
$$+(90\,648\,499\,200 + 75\,420\,831\,360x + 42\,022\,471\,680x^2 + 10\,870\,594\,560x^3$$
$$+1488\,614\,400x^4 + 108\,380\,160x^5 + 2580\,480x^6)\binom{d}{7}$$
$$+(299\,544\,698\,880 + 266\,080\,855\,040x + 72\,325\,693\,440x^2$$
$$+11\,766\,988\,800x^3 + 768\,552\,960x^4 + 10\,321\,920x^5)\binom{d}{8}$$
$$+(564\,908\,359\,680 + 200\,521\,117\,440x + 60\,429\,680\,640x^2$$
$$+4675\,829\,760x^3)\binom{d}{9}$$
$$+(608\,012\,697\,600 + 391\,867\,015\,680x + 19\,508\,428\,800x^2)\binom{d}{10}$$
$$+(347\,435\,827\,200 + 544\,993\,737\,600x)\binom{d}{11} + 81\,749\,606\,400\binom{d}{12}$$

A.3. $f = 5$

$$Z_1^{(d)}(x;5) = 6\binom{d}{3} + 32\binom{d}{4} + 32\binom{d}{5}$$
$$Z_2^{(d)}(x;5) = (96 + 960x + 3312x^2 + 4944x^3 + 3114x^4 + 625x^5)\binom{d}{3}$$
$$+(31\,872 + 152\,064x + 264\,864x^2 + 205\,184x^3 + 67\,632x^4 + 7104x^5)\binom{d}{4}$$
$$+(1048\,480 + 3\,166\,720x + 3412\,800x^2 + 1571\,200x^3 + 286\,880x^4$$
$$+14\,208x^5)\binom{d}{5}$$
$$+(10\,433\,664 + 21\,012\,480x + 14\,330\,880x^2 + 3793\,920x^3 + 312\,960x^4)\binom{d}{6}$$
$$+(44\,056\,320 + 58\,168\,320x + 23\,385\,600x^2 + 2795\,520x^3)\binom{d}{7}$$
$$+(89\,026\,560 + 70\,533\,120x + 12\,902\,400x^2)\binom{d}{8}$$

$$+(85\,155\,840 + 30\,965\,760x)\binom{d}{9} + 30\,965\,760\binom{d}{10}$$

A.4. $f = 6$

$$Z_1^{(d)}(x;6) = \binom{d}{3} + 24\binom{d}{4} + 80\binom{d}{5} + 64\binom{d}{6}$$

$$\begin{aligned}Z_2^{(d)}(x;6) = {} & (1 + 24x + 228x^2 + 1088x^3 + 2718x^4 + 3312x^5 + 1496x^6)\binom{d}{3}\\ & +(10\,688 + 103\,584x + 396\,096x^2 + 756\,544x^3 + 751\,008x^4\\ & +359\,616x^5 + 62\,400x^6)\binom{d}{4}\\ & +(1814\,800 + 10\,451\,040x + 23\,605\,120x^2 + 26\,364\,160x^3 + 14\,999\,040x^4\\ & +3961\,280x^5 + 353\,280x^6)\binom{d}{5}\\ & +(55\,888\,704 + 218\,165\,760x + 327\,210\,240x^2 + 235\,115\,520x^3\\ & +81\,701\,760x^4 + 11\,980\,800x^5 + 471\,040x^6)\binom{d}{6}\\ & +(616\,438\,144 + 1\,696\,611\,840x + 1731\,340\,800x^2 + 799\,339\,520x^3\\ & +160\,608\,000x^4 + 10\,483\,200x^5)\binom{d}{7}\\ & +(3172\,929\,536 + 6139\,822\,080x + 4148\,551\,680x^2 + 1135\,411\,200x^3\\ & +102\,789\,120x^4)\binom{d}{8}\\ & +(8546\,549\,760 + 11\,170\,897\,920x + 4551\,966\,720x^2 + 567\,705\,600x^3)\binom{d}{9}\\ & +(12\,412\,108\,800 + 9\,909\,043\,200x + 1857\,945\,600x^2)\binom{d}{10}\\ & +(9196\,830\,720 + 3406\,233\,600x)\binom{d}{11} + 2724\,986\,880\binom{d}{12}\end{aligned}$$

Appendix B. Partition functions $Z_n(x; f)$ for ISAS-f with $f = 3, 4, 5$ and 6 on the triangular, square and simple cubic lattices

B.1. $f = 3$

Triangular lattice

$$\begin{aligned}Z_1(x;3) &= 2 + 12x + 6x^2\\ Z_2(x;3) &= 54 + 144x + 288x^2 + 288x^3 + 324x^4 + 192x^5 + 22x^6\\ Z_3(x;3) &= 1188 + 5136x + 9468x^2 + 12\,692x^3 + 14\,598x^4 + 16\,608x^5\\ &\quad +15\,574x^6 + 10\,068x^7 + 6174x^8 + 3216x^9 + 234x^{10}\\ Z_4(x;3) &= 24\,800 + 137\,952x + 350\,556x^2 + 557\,852x^3 + 753\,330x^4 + 890\,904x^5\\ &\quad +956\,786x^6 + 895\,476x^7 + 800\,334x^8 + 641\,728x^9 + 431\,796x^{10}\end{aligned}$$

$$+244\,740x^{11} + 149\,992x^{12} + 59\,376x^{13} + 8142x^{14}$$

$$\begin{aligned}Z_5(x;3) = {} & 588\,288 + 3641\,376x + 10\,886\,382x^2 + 21\,960\,156x^3 + 34\,616\,226x^4\\ & +46\,380\,636x^5 + 55\,041\,392x^6 + 59\,417\,004x^7 + 58\,865\,532x^8\\ & +53\,771\,596x^9 + 46\,358\,190x^{10} + 37\,146\,528x^{11} + 27\,797\,382x^{12}\\ & +18\,957\,288x^{13} + 11\,613\,612x^{14} + 6472\,456x^{15} + 3326\,190x^{16}\\ & +1490\,304x^{17} + 405\,506x^{18} + 21\,708x^{19}\end{aligned}$$

Square lattice

$$\begin{aligned}Z_1(x;3) &= 4\\ Z_2(x;3) &= 16 + 48x + 20x^2\\ Z_3(x;3) &= 300 + 392x + 468x^2 + 208x^3 + 12x^4\\ Z_4(x;3) &= 3604 + 5600x + 7400x^2 + 6088x^3 + 3652x^4 + 1528x^5 + 292x^6\\ Z_5(x;3) &= 42\,532 + 96\,672x + 115\,316x^2 + 102\,224x^3 + 78\,040x^4 + 44\,760x^5\\ & \quad +17\,944x^6 + 5904x^7 + 692x^8\\ Z_6(x;3) &= 534\,496 + 1\,353\,256x + 1831\,220x^2 + 1831\,112x^3 + 1592\,956x^4\\ & \quad +1171\,072x^5 + 740\,424x^6 + 386\,920x^7 + 162\,104x^8 + 57\,216x^9\\ & \quad +14\,404x^{10} + 368x^{11}\\ Z_7(x;3) &= 6681\,352 + 18\,681\,272x + 30\,088\,516x^2 + 32\,964\,168x^3 + 29\,626\,364x^4\\ & \quad +23\,245\,648x^5 + 15\,964\,736x^6 + 9720\,160x^7 + 4987\,764x^8\\ & \quad +2195\,800x^9 + 792\,364x^{10} + 237\,272x^{11} + 49\,036x^{12} + 2056x^{13}\\ Z_8(x;3) &= 83\,718\,536 + 259\,560\,880x + 454\,134\,432x^2 + 551\,442\,112x^3 + 547\,246\,116x^4\\ & \quad +470\,484\,464x^5 + 363\,559\,608x^6 + 251\,445\,792x^7 + 157\,245\,292x^8\\ & \quad +88\,789\,472x^9 + 44\,625\,304x^{10} + 19\,683\,952x^{11} + 7535\,320x^{12}\\ & \quad +2530\,920x^{13} + 674\,604x^{14} + 74\,304x^{15} + 752x^{16}\\ Z_9(x;3) &= 1041\,176\,236 + 3588\,799\,576x + 6796\,252\,052x^2 + 9178\,842\,840x^3\\ & \quad +9870\,576\,592x^4 + 9011\,561\,928x^5 + 7317\,039\,152x^6 + 5381\,580\,712x^7\\ & \quad +3611\,035\,872x^8 + 2216\,253\,216x^9 + 1242\,947\,448x^{10} + 632\,068\,360x^{11}\\ & \quad +288\,426\,096x^{12} + 117\,920\,264x^{13} + 42\,418\,520x^{14} + 13\,008\,784x^{15}\\ & \quad +3320\,580x^{16} + 386\,928x^{17} + 4664x^{18}\end{aligned}$$

Simple cubic lattice

$$\begin{aligned}Z_1(x;3) &= 20\\ Z_2(x;3) &= 792 + 1104x + 348x^2 + 16x^3\\ Z_3(x;3) &= 55\,004 + 75\,560x + 62\,340x^2 + 26\,464x^3 + 6036x^4 + 768x^5\\ Z_4(x;3) &= 3558\,916 + 5660\,424x + 5910\,960x^2 + 4724\,584x^3 + 2661\,516x^4\\ & \quad +1123\,344x^5 + 376\,260x^6 + 121\,488x^7 + 18\,384x^8 + 3744x^9\\ Z_5(x;3) &= 240\,081\,924 + 476\,966\,568x + 533\,017\,740x^2 + 478\,165\,592x63 + 348\,581\,544x^4\\ & \quad +208\,251\,024x^5 + 104\,074\,904x^6 + 44\,993\,160x^7 + 16\,155\,852x^8\\ & \quad +5160\,712x^9 + 1161\,744x^{10} + 182\,832x^{11} + 11\,064x^{12}\end{aligned}$$

$$Z_6(x;3) = 15\,741\,417\,560 + 36\,773\,597\,544x + 47\,199\,363\,084x^2 + 47\,532\,171\,456x^3 \\ +40\,384\,978\,380x^4 + 29\,662\,886\,640x^5 + 19\,185\,018\,888x^6 \\ +11\,016\,272\,712x^7 + 5685\,178\,944x^8 + 2632\,057\,680x^9 \\ +1094\,562\,540x^{10} + 410\,593\,176x^{11} + 132\,416\,520x^{12} \\ +36\,401\,136x^{13} + 7132\,656x^{14} + 1313\,008x^{15} + 94\,104x^{16}$$

B.2. $f = 4$

Triangular lattice

$$Z_1(x;4) = 12x^2 + 3x^3$$

$$Z_2(x;4) = 120x^2 + 144x^3 + 408x^4 + 450x^5 + 606x^6 + 348x^7 + 204x^8$$

$$Z_3(x;4) = 6834x^2 + 16\,080x^3 + 26\,871x^4 + 42\,594x^5 + 66\,114x^6 + 80\,886x^7 \\ +81\,624x^8 + 79\,746x^9 + 69\,492x^{10} + 45\,180x^{11} + 26\,214x^{12} \\ +12\,492x^{13} + 1812x^{14}$$

$$Z_4(x;4) = 349\,881x^2 + 1340\,550x^3 + 3030\,567x^4 + 5202\,768x^5 + 8045\,004x^6 \\ +11\,204\,400x^7 + 14\,110\,899x^8 + 16\,113\,498x^9 + 17\,264\,310x^{10} \\ +17\,001\,672x^{11} + 15\,193\,434x^{12} + 12\,607\,500x^{13} + 9\,842\,124x^{14} \\ +6795\,702x^{15} + 4093\,800x^{16} + 2302\,518x^{17} + 1116\,612x^{18} \\ +330\,408x^{19} + 43\,656x^{20}$$

$$Z_5(x;4) = 20\,722\,203x^2 + 99\,282\,390x^3 + 278\,345\,472x^4 + 591\,516\,756x^5 + 1041\,351\,153x^6 \\ +1607\,009\,868x^7 + 2233\,356\,501x^8 + 2839\,596\,270x^9 + 3357\,300\,360x^{10} \\ +3725\,181\,450x^{11} + 3886\,242\,549x^{12} + 3830\,011\,002x^{13} \\ +3570\,218\,226x^{14} + 3141\,497\,550x^{15} + 2612\,281\,962x^{16} \\ +2049\,883\,446x^{17} + 1518\,351\,750x^{18} + 1054\,459\,248x^{19} \\ +686\,039\,850x^{20} + 410\,102\,154x^{21} + 221\,890\,572x^{22} + 109\,304\,472x^{23} \\ +47\,673\,828x^{24} + 15\,552\,288x^{25} + 2526\,804x^{26} + 65\,136x^{27}$$

Square lattice

$$Z_1(x;4) = 1$$

$$Z_2(x;4) = 1 + 8x + 20x^2 + 16x^3 + 2x^4$$

$$Z_3(x;4) = 81 + 144x + 356x^2 + 368x^3 + 300x^4 + 48x^5$$

$$Z_4(x;4) = 1831 + 3712x + 9112x^2 + 12\,080x^3 + 15\,268x^4 + 12\,944x^5 + 9460x^6 \\ +4352x^7 + 1498x^8$$

$$Z_5(x;4) = 35\,073 + 137\,280x + 286\,460x^2 + 442\,896x^3 + 545\,758x^4 + 524\,168x^5 \\ +402\,756x^6 + 253\,464x^7 + 124\,212x^8 + 44\,504x^9 + 1171x^{10} + 1232x^{11} + 6x^{12}$$

$$Z_6(x;4) = 994\,733 + 3\,935\,440x + 8972\,504x^2 + 14\,678\,840x^3 + 19\,285\,608x^4 \\ +21\,154\,064x^5 + 20\,322\,372x^6 + 17\,077\,200x^7 + 12\,674\,292x^8 \\ +8322\,272x^9 + 4785\,320x^{10} + 2407\,480x^{11} + 1008\,736x^{12} \\ +345\,856x^{13} + 91\,912x^{14} + 8440x^{15} + 168x^{16}$$

$$Z_7(x;4) = 26\,140\,609 + 110\,358\,048x + 288\,949\,584x^2 + 526\,263\,552x^3 + 750\,679\,328x^4$$

$$+876\,651\,904x^5 + 881\,820\,384x^6 + 782\,503\,976x^7 + 616\,689\,280x^8$$
$$+433\,424\,512x^9 + 269\,729\,000x^{10} + 149\,539\,040x^{11} + 73\,225\,472x^{12}$$
$$+31\,117\,600x^{13} + 11\,202\,496x^{14} + 3217\,712x^{15} + 721\,248x^{16}$$
$$+101\,992x^{17} + 3788x^{18}$$

Simple cubic lattice

$$Z_1(x;4) = 15$$
$$Z_2(x;4) = 675 + 2520x + 3036x^2 + 1248x^3 + 126x^4$$
$$Z_3(x;4) = 189\,579 + 574\,128x + 827\,772x^2 + 770\,160x^3 + 446\,904x^4 + 172\,944x^5$$
$$+33\,384x^6 + 4896x^7$$
$$Z_4(x;4) = 45\,199\,245 + 135\,993\,696x + 226\,538\,136x^2 + 287\,507\,616x^3 + 280\,970\,532x^4$$
$$+220\,013\,064x^5 + 142\,106\,076x^6 + 75\,925\,656x^7 + 34\,151\,154x^8$$
$$+12\,859\,920x^9 + 3\,885\,672x^{10} + 1\,075\,152x^{11}$$
$$+187\,860x^{12} + 22\,560x^{13} + 2016x^{14}$$

B.3. $f = 5$

Triangular lattice

$$Z_1(x;5) = 6x^4$$
$$Z_2(x;5) = 24x^4 + 24x^5 + 186x^6 + 228x^7 + 384x^8 + 312x^9 + 318x^{10} + 48x^{11}$$
$$Z_3(x;5) = 3348x^4 + 6444x^5 + 14\,502x^6 + 34\,980x^7 + 64\,098x^8 + 86\,352x^9$$
$$+123\,966x^{10} + 159\,024x^{11} + 161\,256x^{12} + 153\,624x^{13} + 136\,920x^{14}$$
$$+95\,460x^{15} + 57\,270x^{16} + 28\,008x^{17} + 7998x^{18} + 348x^{19}$$
$$Z_4(x;5) = 319\,506x^4 + 1\,386\,600x^5 + 3813\,174x^6 + 8481\,420x^7 + 16\,320\,858x^8$$
$$+27\,595\,656x^9 + 41\,873\,820x^{10} + 58\,778\,616x^{11} + 76\,658\,784x^{12}$$
$$+92\,261\,364x^{13} + 103\,081\,266x^{14} + 108\,342\,336x^{15} + 106\,631\,496x^{16}$$
$$+97\,502\,448x^{17} + 82\,466\,976x^{18} + 65\,725\,176x^{19} + 47\,990\,154x^{20}$$
$$+31\,477\,932x^{21} + 18\,842\,310x^{22} + 10\,017\,048x^{23} + 4400\,508x^{24}$$
$$+1432\,872x^{25} + 212\,994x^{26} + 4728x^{27}$$

Simple cubic lattice

$$Z_1(x;5) = 6$$
$$Z_2(x;5) = 96 + 960x + 3312x^2 + 4944x^3 + 3114x^4 + 624x^5$$
$$Z_3(x;5) = 141\,030 + 903\,624x + 2393\,844x^2 + 3\,990\,912x^3 + 4510\,350x^4 + 3641\,808x^5$$
$$+2030\,172x^6 + 762\,480x^7 + 159\,306x^8 + 21\,216x^9 + 672x^{10}$$
$$Z_4(x;5) = 133\,651\,434 + 723\,160\,992x + 1958\,676\,552x^2 + 3736\,139\,352x^3$$
$$+5512\,258\,548x^4 + 6628\,835\,832x^5 + 667\,113\,180x^6 + 5743\,689\,024x^7$$
$$+4245\,805\,926x^8 + 2729\,967\,120x^9 + 1525\,855\,860x^{10}$$
$$+732\,882\,480x^{11} + 308\,729\,046x^{12} + 109\,730\,256x^{13} + 33\,511\,488x^{14}$$
$$+8527\,440x^{15} + 1776\,924x^{16} + 252\,768x^{17} + 37\,152x^{18}$$

B.4. $f = 6$

Triangular lattice

$$Z_1(x; 6) = x^6$$
$$Z_2(x; 6) = x^6 + 12x^8 + 12x^9 + 54x^{10} + 72x^{11} + 108x^{12} + 60x^{13} + 3x^{14}$$
$$\begin{aligned}Z_3(x; 6) = {} & 322x^6 + 330x^7 + 1143x^8 + 4142x^9 + 7986x^{10} + 12\,210x^{11} + 27\,778x^{12} \\ & +43\,830x^{13} + 54\,735x^{14} + 77\,372x^{15} + 96\,096x^{16} + 89\,040x^{17} \\ & +83\,932x^{18} + 73\,404x^{19} + 42\,192x^{20} + 24\,624x^{21} + 10\,401x^{22} \\ & +1500x^{23} + 130x^{24}\end{aligned}$$
$$\begin{aligned}Z_4(x; 6) = {} & 46\,657x^6 + 199\,074x^7 + 612\,021x^8 + 1666\,800x^9 + 3935\,994x^{10} \\ & +8256\,840x^{11} + 15\,594\,412x^{12} + 27\,073\,578x^{13} + 43\,544\,964x^{14} \\ & +64\,979\,506x^{15} + 90\,682\,770x^{16} + 118\,749\,336x^{17} + 146\,078\,071x^{18} \\ & +168\,491\,262x^{19} + 183\,299\,793x^{20} + 188\,125\,048x^{21} + 180\,452\,973x^{22} \\ & +162\,116\,562x^{23} + 136\,945\,428x^{24} + 107\,421\,036x^{25} + 77\,313\,291x^{26} \\ & +51\,175\,456x^{27} + 30\,804\,522x^{28} + 16\,023\,696x^{29} + 7344\,129x^{30} \\ & +2599\,296x^{31} + 513\,204x^{32} + 26\,032x^{33}\end{aligned}$$

Simple cubic lattice

$$Z_1(x; 6) = 1$$
$$Z_2(x; 6) = 1 + 24x + 228x^2 + 1088x^3 + 2718x^4 + 3312x^5 + 1496x^6$$
$$\begin{aligned}Z_3(x; 6) = {} & 15\,625 + 180\,000x + 2713\,632x^2 + 5570\,544x^4 + 8223\,600x^5 + 9006\,456x^6 \\ & +7247\,376x^7 + 4318\,140x^8 + 1740\,464x^9 + 481\,440x^{10} + 59\,280x^{11} + 1792x^{12}\end{aligned}$$

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