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1/d-expansions for the free energy of lattice animal models of a self-interacting branched polymer

P J Peard and D S Gaunt

Department of Physics, King's College, Strand, London WC2R 2LS, UK

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Abstract. We model a self-interacting branched polymer by a nearest-neighbour contact model of lattice animals with either site or bond counting (k - and k' -models, respectively). $1/d$ -expansions for the reduced limiting free energy are derived through order $1/d^5$ in which the coefficients are temperature dependent. By evaluating the coefficients at certain special temperatures, we obtain $1/d$ -expansions for the growth constants of various types of lattice animal, again through order $1/d^5$. The $1/d$ -expansions are used to obtain numerical estimates of the growth constants and to study the temperature dependence of the reduced limiting free energies on d -dimensional simple hypercubic lattices for values of d up to the upper critical dimension. The results are compared with ones obtained by more conventional series methods. Unexpected results are obtained for a range of values of the temperature variable.

1. Introduction

Linear polymer molecules in dilute solution are expanded objects under good solvent conditions and may be modelled as a self-avoiding walk (SAW) on a lattice. If the solvent quality decreases, the linear polymer can collapse from a random coil to a globule and this phenomenon has been investigated experimentally (Slagowski *et al* 1976, Sun *et al* 1980, 1990). A convenient model for this system is a SAW with an energy term proportional to the number of nearest-neighbour *contacts*, i.e. pairs of vertices of the walk which are one lattice space apart but not connected by an edge of the walk. Many authors have used this model since its introduction by Orr (1946).

A similar collapse phenomenon is expected to occur in randomly branched polymers in dilute solution (as the solvent quality decreases) although this does not seem to have been studied experimentally. However, the collapse has been studied theoretically by various authors using lattice animals (connected subgraphs or section graphs of the lattice), lattice trees (animals with no cycles) and c -animals (animals with precisely c cycles). Different models have been suggested with the collapse being driven by a cycle fugacity (Derrida and Herrmann 1983, Dickman and Shieve 1984, 1986, Lam 1987, 1988, Chang and Shapir 1988, Gaunt and Flesia 1990, Madras *et al* 1990, Vanderzande 1993), a contact fugacity (Gaunt and Flesia 1990, 1991, Madras *et al* 1990, Gaunt 1991, Flesia and Gaunt 1992, Flesia *et al* 1992a), a solvent fugacity (Flesia *et al* 1992a, 1993, 1994, Flesia 1993) or by a combination of two such fugacities (Flesia *et al* 1992b, 1994). The techniques used to study this collapse include transfer matrix methods on two-dimensional strips (Derrida and Herrman 1983), Monte Carlo methods (Dickman and Shieve 1984, Lam 1987, 1988) and exact enumeration methods (Chang and Shapir 1988, Gaunt and Flesia 1990, 1991, Madras *et al* 1990, Gaunt 1991, Flesia and Gaunt 1992, Flesia *et al* 1992a, b, 1994).

Madras *et al* (1990) used series analysis and exact enumeration data for lattice animals on the square and simple cubic lattices to investigate the reduced limiting free energy of two different representations of the cycle model and compared these numerical results with some rigorous bounds. Similar work has been presented for contact models (Gaunt and Flesia 1990, Madras *et al* 1990, Gaunt 1991, Flesia and Gaunt 1992) and for the solvent model (Flesia 1993, Flesia *et al* 1994). New exact enumeration data, analogous to that presented in the appendices of Madras *et al* (1990), are now available for simple hypercubic lattices in dimensions $d = 4-8$, inclusive. These data allow us to derive and study the reduced limiting free energy of lattice animal models on a simple hypercubic lattice using a $1/d$ -expansion and to estimate numerically the growth constants for lattice animals in higher dimensions.

Expansions in $1/d$ were first introduced by Fisher and Gaunt (1964) and used by them to study (amongst other things) the SAW model of a dilute solution of linear polymers. They derived an expansion for μ , the SAW limit, through order $1/d^5$ and used it to obtain numerical estimates of μ in dimensions $d = 2-6$, inclusive. The validity of such an expansion was demonstrated rigorously by Kesten (1964) for sufficiently large d . The corresponding expansion for NAWs or neighbour-avoiding walks has been given by Gaunt *et al* (1984) through order $1/d^3$. An expansion through order $1/d^5$ for the amplitude A in the asymptotic form

$$c_n \sim An^{\gamma-1}\mu^n \quad n \rightarrow \infty \quad (1.1)$$

for the number, c_n , of n -step SAWs was given by Gaunt (1986).

More recently, Nemirovsky *et al* (1992a, b) and Ishinabe *et al* (1994) have studied an interacting SAW with nearest-neighbour contact energy $-\epsilon$, by deriving expansions through order $1/d^5$ for the reduced limiting free energy, $\log \mu$, and several other thermodynamic and structural quantities. The coefficients of these $1/d$ -expansions are now temperature dependent functions of $z = e^{\epsilon/kT}$. The known results for SAWs (Fisher and Gaunt 1964, Gaunt 1986) may be recovered by setting $z = 1$, while setting $z = 0$ extends the known results for NAWs (Gaunt *et al* 1984) through order $1/d^5$.

The application of $1/d$ -expansions to lattice animals was first made by Gaunt *et al* (1976). They derived an expansion for $\log \Lambda_s$ through order $1/d^2$, where Λ_s is the growth constant of strongly embeddable (i.e. section graphs of the lattice) animals with site counting. The analogous expansion through order $1/d^2$ for $\log \lambda_b$, where λ_b is the growth constant of weakly embeddable (i.e. subgraphs of the lattice) animals with bond counting, was derived by Gaunt and Ruskin (1978). An error in the coefficient of $1/d^2$ was corrected by Harris (1982), who also extended the expansion through order $1/d^5$. Recently, Gaunt *et al* (1994) extended the expansion for $\log \Lambda_s$ by one more term and derived the expansions for $\log \lambda_s$ (i.e. weakly embedded animals with site counting) and $\log \Lambda_b$ (i.e. strongly embedded animals with bond counting) through the same order (i.e. through order $1/d^3$).

Expansions for c -animals, both weakly and strongly embedded, have been given for the case $c = 0$ (i.e. lattice trees) through order $1/d^3$ (Gaunt *et al* 1982, 1994), and through lower order when $c = 1$ and 2 (Whittington *et al* 1983).

The aim of the present paper is to do, for the more difficult problem of interacting lattice animals, what Nemirovsky *et al* (1992b) did for interacting SAWs. We concentrate on the *contact model* of branched polymers and derive, for the first time, an expansion for the reduced limiting free energy through order $1/d^5$. The free energies at particular temperatures are related to the growth constants of different types of lattice animal, which we therefore obtain through the same order.

A model of branched polymers in which the collapse is driven by a nearest-neighbour contact interaction is the obvious generalization of the interacting SAW model of linear polymers. However, the techniques developed here can be applied to many other models including the cycle and solvent models.

In section 2, we outline the derivation of the 1/d-expansions and present the main results. In section 3, we compare the expansions for lattice animal growth constants with known results and for the free energy with rigorously known bounds (Madras *et al* 1990) and discuss the limitations of the 1/d-expansion for these problems. In section 4, we summarize our results and discuss further work.

2. 1/ σ -expansions

In contact models, an interaction energy is introduced between *contacts*, i.e. pairs of occupied nearest-neighbour sites of the lattice, which are not directly joined by a bond of the lattice animal. This gives each animal a weight $e^{\beta k}$, where β is proportional to the inverse temperature and k is the number of contacts in the animal. e^β is a contact fugacity. The animals are weakly embedded in the lattice, since the case of strong embeddings is trivial for a *contact model* (i.e. $k = 0$ by definition). Finally, the size of the animal can be measured either by the number (n) of sites it contains or the number (b) of bonds. This gives two different contact models; one with site counting (k -model) and one with bond counting (k' -model).

The partition function for the k -model is defined as

$$Z_n(z; k) = \sum_k a_n(k) z^k \quad (2.1)$$

where $z = e^\beta$ is the contact fugacity and $a_n(k)$ is the number (per lattice site) of weakly embedded lattice animals with n sites and k nearest-neighbour contacts on a d -dimensional simple hypercubic lattice. The coordination number $q (= \sigma + 1)$ of the lattice is given by

$$q = 2d = \sigma + 1. \quad (2.2)$$

The function Z_n is easily evaluated by direct counting for very small animals with $n = 1, 2, 3, \dots$ sites. Clearly,

$$Z_1 = 1 \quad (2.3)$$

and

$$Z_2 = \frac{q}{2} = d = \binom{d}{1} \quad (2.4)$$

since the only animal with two sites is a single bond of which there are $q/2$ per lattice site. Alternatively, the result (2.4) may be thought of as follows: a single bond may only span a single dimension and $\binom{d}{1}$ is the number of ways of choosing one dimension from d dimensions. A three-site animal has two bonds that can be either collinear or perpendicular. The linear animal occupies a single dimension and contributes $\binom{d}{1}$ to Z_3 . When the bonds

are perpendicular, there are four distinguishable (i.e. cannot be superimposed by translation) animals each spanning a two-dimensional subspace of which there are $\binom{d}{2}$. Thus,

$$Z_3 = \binom{d}{1} + 4 \binom{d}{2}. \quad (2.5)$$

A temperature dependent term first appears in Z_4 and is due to the four distinguishable animals formed by deleting one side of a square leaving one nearest-neighbour contact. These four animals span one of the $\binom{d}{2}$ two-dimensional subspaces, as do another 17 distinguishable animals with no contacts. This latter group includes 12 three-bond chains, four uniform three-stars with one bond per arm and one square. In addition, there are 32 animals, all with no contacts, which reach into a three-dimensional subspace; of these, 24 are chains and the other eight are uniform three-stars. Finally, the linear four-site animal contributes a term $\binom{d}{1}$, as before. Hence, we find

$$Z_4 = \binom{d}{1} + (17 + 4z) \binom{d}{2} + 32 \binom{d}{3}. \quad (2.6)$$

For larger values of n , Z_n have been derived using computer enumeration and are given in appendix 1 through $n = 8$. Although incomplete expressions have been derived for larger values of n , it should be emphasized that the expressions in appendix 1 hold for arbitrary d . Clearly, the first term is always $\binom{d}{1}$, since when $d = 1$ there is only one animal. At the other end, Z_n terminates with the term involving $\binom{d}{n-1}$, since those n -site clusters which occupy the greatest subspace will have no cycles and are therefore trees with each of their $(n-1)$ bonds in a different dimension. All these clusters will have zero contacts. The general form can therefore be written as

$$Z_n(z; k) = \sum_{i=1}^{n-1} \sum_{k \geq 0} f_{i,k}^{(n)} z^k \binom{d}{n-i} \quad n \geq 2 \quad (2.7)$$

where

$$f_{n-1,k}^{(n)} = \begin{cases} 1 & k = 0 \\ 0 & k > 0 \end{cases} \quad \forall n. \quad (2.8)$$

It should be noted that the terms in (2.7) appear in the reverse order to those in appendix 1.

The next step is to determine the n -dependence of the coefficients $f_{i,k}^{(n)}$. From appendix 1, we see that the sequence of coefficients $\{f_{1,0}^{(n)}\}$ is $\{1, 4, 32, 400, 6912, 153\,664, 4\,194\,309, \dots; n \geq 2\}$ and is generated by the function

$$f_{1,0}(n) = 2^{n-1} n^{n-3}. \quad (2.9)$$

This function counts trees with n sites that span $n-1$ dimensions (Gaunt *et al* 1982, equation (4.6), and Gaunt *et al* 1976, equation (2.4)) and since all these clusters have zero contacts, it is clear that

$$f_{1,k}(n) = 0 \quad \forall k > 0. \quad (2.10)$$

Similarly, we assume that the sequence $\{f_{2,0}^{(n)}\} \equiv \{1, 17, 348, 8640, 254\,800, 8\,749\,056, \dots; n \geq 3\}$ is generated by the function

$$f_{2,0}(n) = 2^{n-3}n^{n-5}(n-2)(2n^2 - 6n + 9) \tag{2.11}$$

while the sequence $\{f_{2,1}^{(n)}\} \equiv \{0, 4, 96, 2304, 62\,720, 19\,066\,080, \dots; n \geq 3\}$ is generated by

$$f_{2,1}(n) = 2^{n-3}n^{n-5}4(n-2)(n-3). \tag{2.12}$$

In addition,

$$f_{2,k}(n) = 0 \quad \forall k > 1. \tag{2.13}$$

$f_{2,0}(n)$ is, as expected, the coefficient of $\binom{d}{n-2}$ in the corresponding expansion for all strongly embeddable (i.e. zero contacts) animals with site counting (Gaunt *et al* 1976, equation (2.4)). A check on all the functions is provided by summing over k giving

$$\sum_{k \geq 0} f_{2,k}(n) = 2^{n-3}n^{n-5}(n-2)(2n^2 - 2n - 3). \tag{2.14}$$

As expected, this is the coefficient of $\binom{d}{n-2}$ in the expansion for all weakly embeddable animals with site counting and without regard to contacts (Gaunt *et al* 1994, equation (3.2)).

The $f_{i,k}(n)$ derived above can be written as

$$f_{i,k}(n) = 2^{n-2i+1}n^{n-2i-1}g_{i,k}(n) \tag{2.15}$$

where $g_{i,k}(n)$ is a polynomial in n . We assume this form to be generally valid. We have derived all $g_{i,k}(n)$ for $i = 1-6$ and the non-zero ones are presented in appendix 2. For $i = 1$ and 2, they follow from (2.9), (2.11) and (2.12). For larger values of i , they have been derived using exact enumeration data and the fact that their coefficients are constrained by the existence of a $1/\sigma$ -expansion for the reduced limiting free energy (see later).

We now rewrite the partition function (2.7) of an animal with a fixed number (n) of sites, as a function of n . Thus,

$$Z(n, z; k) = \sum_{i=1}^{n-1} \sum_{k \geq 0} 2^{n-2i+1}n^{n-2i-1}g_{i,k}(n)z^k \binom{d}{n-i} \quad n \geq 2. \tag{2.16}$$

Following Gaunt *et al* (1976), the binomial coefficients may be expanded in inverse powers of σ using

$$\begin{aligned} \binom{d}{s} &= (\sigma^s/2^s s!)[1 - s(s-2)\sigma^{-1} + \frac{1}{6}s(s-1)(3s^2 - 13s + 11)\sigma^{-2} \\ &\quad - \frac{1}{6}s(s-1)(s-2)^2(s^2 - 5s + 3)\sigma^{-3} \\ &\quad + \frac{1}{360}s(s-1)(s-2)(s-3)(15s^4 - 150s^3 + 455s^2 - 468s + 127)\sigma^{-4} \\ &\quad - \frac{1}{360}s(s-1)(s-2)^2(s-3)(s-4)(3s^4 - 34s^3 + 107s^2 - 84s + 15)\sigma^{-5} + \dots]. \end{aligned} \tag{2.17}$$

Then formally taking the logarithm of $Z(n, z; k)$, dividing by n and letting $n \rightarrow \infty$, we get

$$F(z; k) = \lim_{n \rightarrow \infty} \frac{1}{n} \log Z(n, z; k) \quad (2.18)$$

$$= \log \sigma + 1 + \lim_{n \rightarrow \infty} \sum_{i \geq 1} \sum_{j \geq 0} h_{i,j}(n) z^j \sigma^{-i}. \quad (2.19)$$

The reduced limiting free energy, F , is an intensive quantity, so the assumed existence of this expansion to all orders in $1/\sigma$ implies that the $h_{i,j}(n)$ are constants (in fact, rational numbers) in the limit $n \rightarrow \infty$. This in turn implies that the $g_{i,k}(n)$, which determine the $h_{i,j}(n)$, are constrained, as was mentioned earlier. Explicitly, we find

$$\begin{aligned} F(z; k) = & \log \sigma + 1 + (-2 + 2z)\sigma^{-1} + \left(-\frac{79}{24} - \frac{7}{2}z + \frac{9}{2}z^2\right)\sigma^{-2} \\ & + \left(-\frac{317}{24} + \frac{149}{12}z - \frac{179}{4}z^2 + \frac{130}{3}z^3\right)\sigma^{-3} \\ & + \left(-\frac{18321}{320} - \frac{1127}{12}z + \frac{1403}{4}z^2 - \frac{3667}{6}z^3 + \frac{1225}{4}z^4 + 64z^5\right)\sigma^{-4} \\ & + \left(-\frac{123307}{240} + \frac{59657}{240}z - 1418z^2 + \frac{41433}{8}z^3 - \frac{128329}{16}z^4\right. \\ & \left. + \frac{71761}{20}z^5 + 752z^6\right)\sigma^{-5} + O(\sigma^{-6}). \end{aligned} \quad (2.20)$$

On setting $z = 1$ in (2.1), we see that Z_n is the *total* number of weakly embedded lattice animals with n sites (i.e. without regard to the number of contacts). Hence, F , as defined by (2.18) will be the logarithm of the corresponding growth constant, namely $\log \lambda_s$. Thus, setting $z = 1$ in (2.20) gives

$$\log \lambda_s = \log \sigma + 1 - \frac{55}{24}\sigma^{-2} - \frac{53}{24}\sigma^{-3} - \frac{39683}{960}\sigma^{-4} - \frac{44303}{240}\sigma^{-5} + O(\sigma^{-6}). \quad (2.21)$$

Similarly, setting $z = 0$ in (2.20) gives

$$\log \Lambda_s = \log \sigma + 1 - 2\sigma^{-1} - \frac{79}{24}\sigma^{-2} - \frac{317}{24}\sigma^{-3} - \frac{18321}{320}\sigma^{-4} - \frac{123307}{240}\sigma^{-5} + O(\sigma^{-6}) \quad (2.22)$$

where Λ_s is the growth constant for strongly embedded lattice animals with site counting. These expansions agree through order σ^{-3} with the results of Gaunt *et al* (1994) but the remaining coefficients are new.

The k' -model is treated in a similar manner but with one important difference. For bond counting, the analogues of the generating functions $f_{i,k}(n)$ are more complicated. In particular, one gets *different functions* for bond animals containing *different numbers of cycles*. (This effect was first noted by Gaunt and Ruskin (1978), equation (2.4) and ensuing discussion.) It is convenient, therefore, to introduce a two-variable model with contact fugacity z and cycle fugacity y . The analogue of (2.7) is

$$Z_b(y, z; c', k') = \sum_{i=0}^{b-1} \sum_{c, k \geq 0} f_{i,k,c}^{(b)} y^c z^k \binom{d}{b-i} \quad b \geq 1 \quad (2.23)$$

where the $f_{i,k,c}^{(b)}$ are the numbers of lattice animals with b bonds, k contacts and c cycles that are weakly embeddable in a $(b-i)$ -dimensional subspace ($i = 0, 1, 2, \dots, b-1$). The numbers $f_{i,k,c}^{(b)}$ have been determined by computer enumeration and are generated by the functions

$$f_{i,k,c}(b) = 2^{b-2i+c} (b+1-c)^{b-2(i+1)+c} g_{i,k,c}(b) \quad (2.24)$$

where the non-zero $g_{i,k,c}(b)$ are polynomials in b and are given in appendix 3 for $i = 0-5$.

The partition function in (2.23) may now be written, in analogy with (2.16), as a function of b , namely $Z(b, y, z; c', k')$. As before, the binomial coefficients are expanded in inverse powers of σ . Then one takes the logarithm of $Z(b, y, z; c', k')$, divides by b and lets $b \rightarrow \infty$. Finally, setting $y = 1$ and performing the sum over all c gives the reduced limiting free energy of the k' -model as

$$\begin{aligned}
 F(z; k') = & \log \sigma + 1 + \left(\frac{-5}{2} + 2z\right)\sigma^{-1} + \left[-\left(\frac{13}{6} - \frac{1}{2e}\right) - 5z + \frac{9}{2}z^2\right]\sigma^{-2} \\
 & + \left[-\left(\frac{191}{12} + \frac{1}{4e}\right) + \left(33 + \frac{1}{2e}\right)z - \frac{135}{2}z^2 + \frac{130}{3}z^3\right]\sigma^{-3} \\
 & + \left[-\left(\frac{139}{5} - \frac{271}{48e} - \frac{1}{8e^2}\right) - \left(\frac{499}{2} + \frac{85}{4e}\right)z + (679 + \frac{37}{2e})z^2 \right. \\
 & \left. - \frac{1501}{2}z^3 + \frac{953}{4}z^4 + 64z^5\right]\sigma^{-4} \\
 & + \left[-\left(\frac{1585}{3} + \frac{1171}{32e} + \frac{3}{e^2}\right) + \left(\frac{3597}{4} + \frac{8467}{48e} + \frac{65}{12e^2}\right)z \right. \\
 & \left. - (4522 + \frac{1001}{4e})z^2 + \left(\frac{62831}{6} + \frac{443}{12e}\right)z^3 - \left(\frac{20333}{2} - \frac{68}{e}\right)z^4 \right. \\
 & \left. + \frac{56321}{20}z^5 + 752z^6\right]\sigma^{-5} + O(\sigma^{-6}). \tag{2.25}
 \end{aligned}$$

Now when we set $z = 1$, we obtain

$$\begin{aligned}
 \log \lambda_b = & \log \sigma + 1 - \frac{1}{2}\sigma^{-1} - \left(\frac{8}{3} - \frac{1}{2e}\right)\sigma^{-2} - \left(\frac{85}{12} - \frac{1}{4e}\right)\sigma^{-3} - \left(\frac{931}{20} - \frac{139}{48e} - \frac{1}{8e^2}\right)\sigma^{-4} \\
 & - \left(\frac{2777}{10} + \frac{177}{32e} - \frac{29}{12e^2}\right)\sigma^{-5} + O(\sigma^{-6}) \tag{2.26}
 \end{aligned}$$

where λ_b is the growth constant for weakly embedded lattice animals with bond counting. Setting $z = 0$ gives the corresponding result for strongly embedded animals with bond counting, namely

$$\begin{aligned}
 \log \Lambda_b = & \log \sigma + 1 - \frac{5}{2}\sigma^{-1} - \left(\frac{13}{6} - \frac{1}{2e}\right)\sigma^{-2} - \left(\frac{191}{12} + \frac{1}{4e}\right)\sigma^{-3} - \left(\frac{139}{5} - \frac{271}{48e} - \frac{1}{8e^2}\right)\sigma^{-4} \\
 & - \left(\frac{1585}{3} + \frac{1171}{32e} + \frac{3}{e^2}\right)\sigma^{-5} + O(\sigma^{-6}). \tag{2.27}
 \end{aligned}$$

The expansion for $\log \lambda_b$ agrees through order σ^{-5} with that given by Harris (1982), while that for $\log \Lambda_b$ agrees through order σ^{-3} with the result of Gaunt *et al* (1994), the last two coefficients being new.

Equations (2.20) and (2.25) are the central results of this paper. They are the analogues, for the k - and k' -models of a self-interacting *branched* polymer, of Nemirovsky *et al* (1992b), equation (19), for the contact model of a self-interacting *linear* polymer.

3. Growth constants and the free energy

The $1/\sigma$ -expansions for the growth constants and for the reduced limiting free energies are expected to be asymptotic rather than convergent (Kesten 1964, Gerber and Fisher 1974, Fisher and Singh 1990, Hara and Slade 1995). In a given dimension, numerical estimates of the four growth constants may be obtained by truncation after the term of least modulus. Table 1 compares estimates of the logarithm of the growth constants obtained from $1/\sigma$ -expansions (indicated by the superscript σ), with series estimates (indicated by the superscript s) (Gaunt 1980, Flesia and Gaunt 1992, P J Peard, unpublished), for $d = 2$ through $d = 8$ (the upper critical dimension). The errors quoted on the estimates from

the $1/\sigma$ -expansions are the magnitudes of the term of least modulus (Gaunt and Ruskin 1978). When the uncertainties are taken into account, the agreement between the series and $1/\sigma$ -estimates improves monotonically as d increases. In all cases, the pairs of estimates overlap and the $1/\sigma$ -estimates appear to be the more accurate when $d \geq 6$. Surprisingly, the two estimates of $\log \lambda_b$ overlap for all $d = 2-8$. It is interesting that, on taking the uncertainties into account, the $1/\sigma$ -expansion overestimates $\log \lambda_s$ for all d , but tends to underestimate in all the other cases.

As pointed out by Gaunt *et al* (1994), the coefficients in the $1/\sigma$ -expansions (2.21), (2.22), (2.26) and (2.27) for the logarithm of the growth constants, suggest the ordering

$$\lambda_s > \lambda_b > \Lambda_s > \Lambda_b \quad (3.1)$$

for any dimension d . Both sets of numerical estimates in table 1 conform to (3.1) for all $d = 2-8$. In fact, all except the last of the inequalities in (3.1) have been proven rigorously (Whittington and Soteros 1990, Gaunt *et al* 1994).

Finally, we may use the $1/\sigma$ -expansions (2.20) and (2.25), to study the temperature dependence of the reduced limiting free energies of the k - and k' -models in a given dimension. This is done by evaluating the temperature-dependent coefficients at a given temperature (or z), substituting the appropriate value of $\sigma (= 2d - 1)$ and truncating the expansion after the term of least modulus. As before, the uncertainties are taken to be of the order of the term of least modulus. The process is then repeated for different values of z and/or σ .

The $1/\sigma$ -estimates obtained as above may be compared with more conventional series estimates and with some rigorous upper and lower bounds that have been derived (Madras *et al* 1990). Series estimates of $F(\beta; k)$ and $F(\beta; k')$ for the square ($d = 2$) and simple cubic ($d = 3$) lattices have been tabulated for a range of values of $\beta (= \log z)$ by Flesia and Gaunt (1992), table 1. They are plotted for the k' -model by Flesia and Gaunt (1992), figures 1 and 2, and for the k -model by Madras *et al* (1990), figure 3, for $d = 2$ and by Gaunt (1991), figure 1, for $d = 3$.

In figure 1, we give as an example $1/\sigma$ -estimates and series estimates of $F(\beta; k)$ plotted against β on the simple cubic lattice, together with the rigorous bounds. The curve derived by more conventional series methods is expected to be essentially exact over most of the range plotted. For values of $\beta > 1$, series methods fail to provide reliable estimates of F but, in any case, the collapse transition is believed to occur around $\beta = \beta_c \simeq 0.3$ (Flesia and Gaunt 1992). The abrupt changes in the $1/\sigma$ -plot occur at temperatures where there is a change in the order of the term at which truncation of the $1/\sigma$ -expansion occurs. The $1/\sigma$ -plot is not too bad, especially when one remembers that it is derived from an asymptotic $1/d$ -expansion by setting $d = 3$. It is never that far from the plot derived by conventional series methods—sometimes below it, other times above it. In some regions, it lies within the rigorous bounds, while in other regions, it lies just outside. Essentially comparable figures are obtained for the k' -model in $d = 3$, and for the k - and k' -models on the square lattice.

One might expect that asymptotic $1/d$ -expansions would give even better results for larger values of d . This does indeed appear to be the case *but, for reasons that we do not understand, only for $\beta \leq 0$ (or $0 \leq z \leq 1$)*. Unfortunately, conventional series estimates of $F(\beta)$ are not available for comparison when $d > 3$, except at the temperatures $\beta = -\infty$ ($z = 0$) and $\beta = 0$ ($z = 1$)—see table 1. We have seen earlier that for $d \geq 6$, $1/\sigma$ -estimates of the free energy at these two special temperatures are extremely accurate (more so than the conventional series estimates) and this seems likely to be true at all temperatures in

Table 1. Comparison of series and 1/σ - expansion estimates of the logarithm of various growth constants for d = 2-8.

d	2	3	4	5	6	7	8
$\log \lambda_s^{(s)}$	1.704 ± 0.002	2.434 ± 0.004	2.862 ± 0.006	3.153 ± 0.010	3.371 ± 0.013	3.55 ± 0.01	3.70 ± 0.05
$\log \lambda_s^{(\sigma)}$	1.762 ± 0.082	2.500 ± 0.018	2.893 ± 0.006	3.166 ± 0.003	3.373 ± 0.001	3.5484 ± 0.0005	3.6962 ± 0.0002
$\log \lambda_b^{(s)}$	1.651 ± 0.002	2.364 ± 0.005	2.791 ± 0.025	3.096 ± 0.035	3.323 ± 0.035	3.50 ± 0.045	3.65 ± 0.05
$\log \lambda_b^{(\sigma)}$	1.397 ± 0.259	2.354 ± 0.056	2.768 ± 0.017	3.090 ± 0.005	3.322 ± 0.002	3.5063 ± 0.0008	3.6603 ± 0.0004
$\log \Lambda_s^{(s)}$	1.4019 ± 0.0005	2.121 ± 0.003	2.592 ± 0.015	2.93 ± 0.02	3.19 ± 0.04	3.38 ± 0.02	3.56 ± 0.04
$\log \Lambda_s^{(\sigma)}$	1.066 ± 0.366	1.880 ± 0.092	2.531 ± 0.024	2.899 ± 0.009	3.172 ± 0.003	3.382 ± 0.001	3.5544 ± 0.0007
$\log \Lambda_b^{(s)}$	1.355 ± 0.002	2.0677 ± 0.0005	2.540 ± 0.002	2.881 ± 0.004	3.142 ± 0.007	3.35 ± 0.01	3.53 ± 0.06
$\log \Lambda_b^{(\sigma)}$	1.045 ± 0.220	1.861 ± 0.041	2.491 ± 0.011	2.869 ± 0.004	3.140 ± 0.002	3.3527 ± 0.0009	3.5273 ± 0.0005

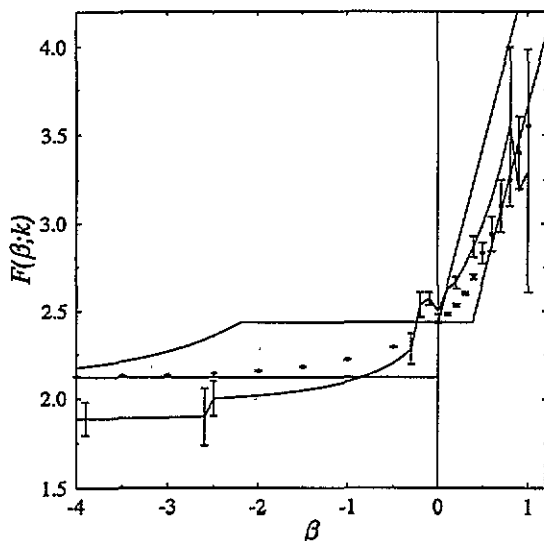


Figure 1. Series (•) and $1/\sigma$ -estimates of the reduced limiting free energy $F(\beta)$ of the k -model on the simple cubic lattice, together with their uncertainties. Rigorous upper and lower bounds are also shown.

between (i.e. for all $\beta < 0$). This conclusion is supported by the following observations: the $1/\sigma$ -estimates have very small uncertainties, they lie entirely within the rigorous upper and lower bounds (which are quite tight for large d) and they approach the rigorous lower bound asymptotically as $\beta \rightarrow -\infty$, as they must (Madras *et al* 1990).

For $\beta > 0$ ($z > 1$) and d large, the $1/\sigma$ -estimates are apparently very precise (providing β is not too large) and the corresponding $1/\sigma$ -plot is a smooth continuation of the curve for $\beta \leq 0$. However, except for β very small, the plot lies well outside the region delineated by the rigorous bounds, which are parallel straight lines with slopes $(d-1)$. Even worse, the discrepancy between the $1/\sigma$ -plot and the rigorous bounds increases as d increases. Hence, even when d is large, asymptotic $1/d$ -expansions appear not to be valid for $\beta > 0$, except possibly for very small β .

4. Discussion

In this paper, we have studied a self-interacting branched polymer with the aid of a nearest-neighbour contact model of lattice animals with either site or bond counting (k - and k' -models, respectively). Asymptotic expansions in inverse powers of σ have been derived through order $1/\sigma^5$ for the reduced limiting free energy. These expansions have been derived using the 'elementary' methods that we have used in the past. None of the interesting theoretical developments discussed by Harris (1982), Nemirovsky *et al* (1992b) and Hara and Slade (1995) are actually needed for the practical problem of series derivation through order $1/d^5$. Evaluating the temperature-dependent coefficients at the special temperatures $\beta = -\infty$ ($z = 0$) and $\beta = 0$ ($z = 1$) gives $1/\sigma$ -expansions, through the same order, for the logarithm of the growth constants Λ_s and Λ_b , and λ_s and λ_b , respectively. For λ_b , the expansion (2.26) agrees with that derived by Harris (1982) while for λ_s , Λ_s and Λ_b , our results (2.21), (2.22) and (2.27) extend the previously known results (Gaunt *et al* 1994) by two terms. The $1/\sigma$ -expansions (2.20) and (2.25) for the reduced limiting free energy are

entirely new, and are the analogues of Nemirovsky *et al* (1992b), equation (19), for the contact model of a self-interacting linear polymer. (There is no need to distinguish between site and bond counting for linear polymers.)

We have used the 1/σ-expansions to estimate the growth constants and the reduced limiting free energies for all *d* upto *d* = 8, the upper critical dimension. The 1/σ-estimates have been compared with estimates obtained by more conventional series methods and, in the case of the free energies, with rigorously derived bounds. For β ≤ 0, the 1/σ-estimates get more accurate as *d* increases. In particular, by *d* = 6, the 1/σ-estimates of the growth constants (or, equivalently, the reduced limiting free energies at β = -∞ and β = 0) overlap with the series estimates in all cases and, furthermore, the 1/σ-estimates are the more accurate.

For β > 0, 1/σ-estimates consistent with the rigorously known bounds on the reduced limiting free energy are only obtained for β small. The range of β over which the 1/σ-plot and the rigorous bounds are consistent *shrinks* as *d* increases, and outside this range the separation between the 1/σ-plot and the bounds *increases* as *d* increases. Both of these findings were contrary to our expectations. One might speculate that the range of validity of 1/σ-expansions is determined by the collapse transition at β_c(*d*). On the other hand, it may be that the 1/σ-expansions are not valid for any β > 0. Further work is needed to understand the intriguing nature of the 1/σ-expansions for β > 0.

In a future publication, our methods will be extended to yield 1/σ-expansions for the growth constants of lattice trees (animals with no cycles), and the reduced limiting free energy of other lattice animal models of interacting branched polymers (Gaunt and Flesia 1990, Flesia 1993), including two-variable models (Flesia *et al* 1992b, 1994).

Finally, we have not thus far addressed, in higher dimensions, the existence of the collapse transition, nor the possibility of a collapse-collapse transition (Flesia *et al* 1992b, 1994) in a two-variable model. These important questions will also be the subject of a future publication.

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Appendix 1.

Partition function, Z_n, of the *k*-model for all *n* ≤ 8 on a *d*-dimensional simple hypercubic lattice.

$$Z_1(z; k) = 1$$

$$Z_2(z; k) = \binom{d}{1}$$

$$Z_3(z; k) = \binom{d}{1} + 4 \binom{d}{2}$$

$$Z_4(z; k) = \binom{d}{1} + (17 + 4z) \binom{d}{2} + 32 \binom{d}{3}$$

$$Z_5(z; k) = \binom{d}{1} + (61 + 32z) \binom{d}{2} + (348 + 96z) \binom{d}{3} + 400 \binom{d}{4}$$

$$Z_6(z; k) = \binom{d}{1} + (214 + 174z + 30z^2) \binom{d}{2} + (2836 + 1596z + 180z^2) \binom{d}{3} \\ + (8640 + 2304z) \binom{d}{4} + 6912 \binom{d}{5}$$

$$Z_7(z; k) = \binom{d}{1} + (758 + 828z + 332z^2) \binom{d}{2} + (21\,225 + 17\,880z + 4968z^2 + 400z^3) \binom{d}{3} \\ + (129\,288 + 68\,160z + 9408z^2) \binom{d}{4} + (254\,800 + 62\,720z) \binom{d}{5} \\ + 153\,664 \binom{d}{6}$$

$$Z_8(z; k) = \binom{d}{1} + (2723 + 3730z + 2258z^2 + 336z^3) \binom{d}{2} \\ + (154\,741 + 172\,368z + 77\,958z^2 + 15\,308z^3 + 408z^4 + 384z^5) \binom{d}{3} \\ + (1\,688\,424 + 1\,313\,408z + 377\,280z^2 + 40\,256z^3) \binom{d}{4} \\ + (6\,160\,640 + 2\,961\,920z + 407\,040z^2) \binom{d}{5} + (8\,749\,056 + 19\,066\,080z) \binom{d}{6} \\ + 4\,194\,309 \binom{d}{7}.$$

Appendix 2.

Polynomials $g_{i,k}(n)$ for all $i \leq 6$. (See equation (2.16).)

$$g_{1,0}(n) = 1$$

$$g_{2,0}(n) = (n-2)(9-6n+2n^2)$$

$$g_{2,1}(n) = 4(n-2)(n-3)$$

$$g_{3,0}(n) = \frac{1}{6}(n-3)(-1560 + 1122n - 679n^2 + 360n^3 - 104n^4 + 12n^5)$$

$$g_{3,1}(n) = 2(n-3)(n-4)(45 + 11n - 16n^2 + 4n^3)$$

$$g_{3,2}(n) = 2(n-3)(n-4)(n-5)(21 + 4n)$$

$$g_{4,0}(n) = \frac{1}{6}(n-4)(204\,960 - 114\,302n + 41\,527n^2 - 17\,523n^3 + 7404n^4 - 2930n^5 + 828n^6 \\ - 128n^7 + 8n^8)$$

$$g_{4,1}(n) = \frac{2}{3}(n-4)(n-5)(336 - 986n - 541n^2 - 91n^3 + 342n^4 - 116n^5 + 12n^6)$$

$$g_{4,2}(n) = 4(n-4)(n-5)(-5376 + 1034n + 526n^2 - 114n^3 - 19n^4 + 4n^5)$$

$$g_{4,3}(n) = \frac{8}{3}(n-4)(n-5)(n-6)(-2268 + 30n + 39n^2 + 4n^3)$$

$$g_{5,0}(n) = \frac{1}{360}(n-5)(-3\,731\,495\,040 + 1\,923\,269\,040n - 535\,510\,740n^2 + 150\,403\,080n^3 \\ - 42\,322\,743n^4 + 12\,397\,445n^5 - 4\,062\,240n^6 + 1\,335\,320n^7 \\ - 356\,232n^8 + 62\,240n^9 - 6000n^{10} + 240n^{11})$$

$$g_{5,1}(n) = \frac{1}{3}(n-5)(n-6)(1\,300\,320 - 480\,180n - 28\,423n^2 + 46\,140n^3 - 6037n^4 + 2124n^5 \\ - 3908n^6 + 1652n^7 - 272n^8 + 16n^9)$$

$$g_{5,2}(n) = \frac{1}{3}(n-5)(n-6)(-4\,712\,400 + 2\,381\,074n + 350\,045n^2 - 267\,582n^3 - 14\,129n^4 \\ + 15\,580n^5 + 120n^6 - 548n^7 + 48n^8)$$

$$g_{5,3}(n) = \frac{4}{3}(n-5)(n-6)(n-7)(-901\,800 + 188\,085n + 48\,724n^2 - 10\,737n^3 - 720n^4 \\ + 76n^5 + 16n^6)$$

$$g_{5,4}(n) = \frac{2}{3}(n-5)(n-6)(n-7)(2\,398\,680 - 374\,331n - 28\,056n^2 + 1611n^3 + 280n^4 + 16n^5)$$

$$g_{5,5}(n) = 1024(n-5)(n-6)(n-7)n^2$$

$$g_{6,0}(n) = \frac{1}{360}(n-6)(1\,785\,362\,705\,280 - 939\,451\,308\,048n + 248\,868\,418\,932n^2 \\ - 56\,265\,094\,748n^3 + 11\,984\,445\,891n^4 - 2\,448\,081\,038n^5 \\ + 535\,284\,255n^6 - 127\,651\,774n^7 + 33\,940\,138n^8 - 9\,580\,440n^9 + 2\,398\,912n^{10} \\ - 440\,688n^{11} + 51\,856n^{12} - 3424n^{13} + 96n^{14})$$

$$g_{6,1}(n) = \frac{1}{90}(n-6)(n-7)(-23\,113\,537\,920 + 7909\,985\,232n - 651\,579\,924n^2 + 79\,125\,128n^3 \\ + 2\,066\,043n^4 - 16\,478\,588n^5 + 4\,688\,465n^6 - 1\,000\,940n^7 \\ + 673\,856n^8 - 299\,032n^9 + 62\,720n^{10} - 6240n^{11} + 240n^{12})$$

$$g_{6,2}(n) = \frac{2}{3}(n-6)(n-7)(-61\,205\,760 + 90\,113\,856n + 7\,880\,092n^2 - 19\,205\,706n^3 \\ + 2\,322\,958n^4 + 963\,640n^5 - 128\,379n^6 - 42\,081n^7 + 4880n^8 \\ + 1564n^9 - 316n^{10} + 16n^{11})$$

$$g_{6,3}(n) = \frac{4}{9}(n-6)(n-7)(3\,254\,929\,920 - 1\,752\,427\,152n + 56\,884\,146n^2 + 113\,254\,335n^3 \\ - 14\,059\,494n^4 - 2\,923\,902n^5 + 554\,129n^6 + 10\,682n^7 - 3140n^8 \\ - 476n^9 + 48n^{10})$$

$$g_{6,4}(n) = \frac{2}{3}(n-6)(n-7)(n-8)(866\,871\,720 - 279\,374\,382n - 10\,748\,979n^2 + 10\,615\,978n^3 \\ - 462\,859n^4 - 82\,444n^5 - 378n^6 + 368n^7 + 32n^8)$$

$$g_{6,5}(n) = \frac{8}{15}(n-6)(n-7)(n-8)(-1\,188\,380\,160 + 308\,727\,756n - 8\,194\,524n^2 - 1\,901\,385n^3 \\ - 55\,350n^4 + 9815n^5 + 456n^6 + 16n^7)$$

$$g_{6,6}(n) = 512(n-6)(n-7)(n-8)(n-9)n^2(135 + 8n).$$

Appendix 3.

Polynomials $g_{i,k,c}(b)$ for all $i \leq 5$. (See equation (2.24).)

$$g_{0,0,0}(b) = 1$$

$$g_{1,0,0}(b) = (b-1)(7-3b+2b^2)$$

$$g_{1,1,0}(b) = 4(b-1)(b-2)$$

$$g_{2,0,0}(b) = \frac{1}{6}(b-2)(-237+185b-115b^2+115b^3-56b^4+12b^5)$$

$$g_{2,0,1}(b) = (b-2)(b-3)$$

$$g_{2,1,0}(b) = 4(b-2)(b-3)(44-6b-3b^2+2b^3)$$

$$g_{2,2,0}(b) = 2(b-2)(b-3)(b-4)(25+4b)$$

$$g_{3,0,0}(b) = \frac{1}{6}(b-3)(126212-76155b+16024b^2-2240b^3+446b^4-345b^5 \\ + 254b^6-76b^7+8b^8)$$

$$g_{3,0,1}(b) = (b-3)(b-4)(50+5b-9b^2+2b^3)$$

$$g_{3,1,0}(b) = \frac{2}{3}(b-3)(b-4)(15930-7243b-245b^2+771b^3-49b^4-56b^5+12b^6)$$

$$g_{3,1,1}(b) = 2(b-3)(b-4)(b-5)(9+2b)$$

$$g_{3,2,0}(b) = 2(b-3)(b-4)(-16990+5541b+376b^2-325b^3-2b^4+8b^5)$$

$$g_{3,3,0}(b) = \frac{8}{3}(b-3)(b-4)(b-5)(-2195+120b+51b^2+4b^3)$$

$$g_{4,0,0}(b) = \frac{1}{360}(b-4)(-1739544030+863175477b-185751094b^2+55226901b^3 \\ - 16404778b^4+2667383b^5-235546b^6+41399b^7-50472b^8 \\ + 22040b^9-3840b^{10}+240b^{11})$$

$$g_{4,0,1}(b) = \frac{1}{6}(b-4)(b-5)(19152-3408b-2550b^2+293b^3+399b^4-128b^5+12b^6)$$

$$g_{4,0,2}(b) = \frac{1}{2}(b-4)(b-5)(b-6)(5+b)$$

$$g_{4,1,0}(b) = \frac{2}{3}(b-4)(b-5)(2076048-1271592b+129810b^2+74215b^3-19649b^4-2245b^5 \\ + 1215b^6+82b^7-76b^8+8b^9)$$

$$g_{4,1,1}(b) = 2(b-4)(b-5)(-10416+1754b+573b^2-89b^3-24b^4+4b^5)$$

$$g_{4,2,0}(b) = \frac{1}{3}(b-4)(b-5)(-18852936+9863406b-839975b^2-433169b^3+75835b^4 \\ + 11071b^5-2516b^6-212b^7+48b^8)$$

$$g_{4,2,1}(b) = 2(b-4)(b-5)(b-6)(-1848-9b+33b^2+4b^3)$$

$$g_{4,3,0}(b) = \frac{8}{3}(b-4)(b-5)(b-6)(-739567+205831b+12154b^2-6809b^3 \\ - 131b^4+82b^5+8b^6)$$

$$\begin{aligned}
g_{4,4,0}(b) &= \frac{2}{3}(b-4)(b-5)(b-6)(b-7)(-285\,224 + 20\,350b + 6195b^2 + 472b^3 + 16b^4) \\
g_{4,5,0}(b) &= 1024(b-4)(b-5)(b-6)(b+1)^2 \\
g_{5,0,0}(b) &= \frac{1}{360}(b-5)(859\,767\,624\,432 - 478\,442\,764\,026b + 117\,239\,639\,733b^2 \\
&\quad - 22\,126\,013\,137b^3 + 3\,761\,312\,903b^4 - 610\,561\,813b^5 \\
&\quad + 144\,141\,417b^6 - 30\,677\,939b^7 + 3\,646\,965b^8 - 144\,101b^9 \\
&\quad + 116\,374b^{10} - 84\,344b^{11} + 21\,120b^{12} - 2320b^{13} + 96b^{14}) \\
g_{5,0,1}(b) &= \frac{1}{6}(b-5)(b-6)(4\,402\,944 - 1\,535\,520b - 113\,032b^2 + 92\,370b^3 + 6755b^4 - 4004b^5 \\
&\quad - 1947b^6 + 966b^7 - 148b^8 + 8b^9) \\
g_{5,0,2}(b) &= \frac{1}{2}(b-5)(b-6)(-7536 + 339b + 515b^2 - 21b^3 - 19b^4 + 2b^5) \\
g_{5,1,0}(b) &= \frac{1}{90}(b-5)(b-6)(6\,124\,470\,480 - 7\,849\,886\,514b + 2\,259\,675\,805b^2 + 397\,569\,014b^3 \\
&\quad - 239\,603\,363b^4 + 6\,791\,226b^5 + 10\,861\,455b^6 - 1\,223\,814b^7 \\
&\quad - 353\,857b^8 + 53\,128b^9 + 14\,840b^{10} - 3840b^{11} + 240b^{12}) \\
g_{5,1,1}(b) &= \frac{1}{3}(b-5)(b-6)(-13\,214\,880 + 4\,439\,508b + 421\,968b^2 - 275\,323b^3 - 3930b^4 \\
&\quad + 8123b^5 + 450b^6 - 316b^7 + 24b^8) \\
g_{5,1,2}(b) &= \frac{2}{3}(b-5)(b-6)(b-7)(-1558 - 31b + 18b^2 + 3b^3) \\
g_{5,2,0}(b) &= \frac{1}{3}(b-5)(b-6)(-3\,921\,287\,832 + 2\,648\,871\,214b - 471\,107\,213b^2 - 69\,916\,963b^3 \\
&\quad + 31\,801\,960b^4 - 673\,016b^5 - 913\,689b^6 + 53\,705b^7 + 19\,934b^8 \\
&\quad - 1340b^9 - 328b^{10} + 32b^{11}) \\
g_{5,2,1}(b) &= 2(b-5)(b-6)(b-7)(-825\,120 + 135\,060b + 27\,458b^2 - 4259b^3 \\
&\quad - 437b^4 + 22b^5 + 8b^6) \\
g_{5,3,0}(b) &= \frac{4}{9}(b-5)(b-6)(9\,792\,754\,944 - 5\,701\,715\,159b + 895\,497\,136b^2 + 93\,886\,183b^3 \\
&\quad - 37\,524\,016b^4 + 530\,123b^5 + 639\,104b^6 - 22\,511b^7 - 5744b^8 \\
&\quad - 44b^9 + 48b^{10}) \\
g_{5,3,1}(b) &= \frac{4}{3}(b-5)(b-6)(b-7)(b-8)(-118\,935 + 2118b + 2001b^2 + 186b^3 + 8b^4) \\
g_{5,4,0}(b) &= \frac{2}{3}(b-5)(b-6)(b-7)(1\,288\,218\,912 - 490\,453\,936b + 25\,861\,226b^2 + 9\,692\,991b^3 \\
&\quad - 846\,932b^4 - 85\,811b^5 + 2574b^6 + 608b^7 + 32b^8) \\
g_{5,4,1}(b) &= 1088(b-5)(b-6)(b-7)b^2 \\
g_{5,5,0}(b) &= \frac{8}{15}(b-5)(b-6)(b-7)(-888\,455\,136 + 289\,054\,916b - 12\,970\,573b^2 - 2\,121\,755b^3 \\
&\quad - 8955b^4 + 12\,887b^5 + 568b^6 + 16b^7) \\
g_{5,6,0}(b) &= 512(b-5)(b-6)(b-7)(b-8)(8b+143)(b+1)^2.
\end{aligned}$$

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