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Area-weighted moments of convex polygons on the square lattice

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Abstract. When constructing series expansions for the zero-field partition function of the q-state Potts model on the square lattice using the finite-lattice method, the series can be extended by one term by adding a correction of $(q-1)$ times the number of convex polygons of an appropriate order. By virtue of duality, such corrections apply for both high- and low-temperature series. For low-temperature series, corrections to the field-dependent partition function are of the same order in the temperature variable as the zero-field correction. The general corrections are given by area-weighted moments of the number of convex polygons. We obtain conjectured closed-form expressions for the two generating functions that give corrections to the first two field derivatives of the low-temperature partition function. These solutions are also of interest as exact solutions in the study of restricted self-avoiding-walk problems, in this instance restricted by convexity. They also solve what has been described by Delest and Viennot as a major problem. We note that our generating functions satisfy the analogue of the scaling relation $\alpha+2\beta+\gamma=2$.

We are currently engaged in a program of using the finite-lattice method (de Neef and Enting 1977) to extend series expansions for various lattice statistics models. We have made a number of improvements to various finite-lattice algorithms but the main reason that we have been able to extend various series is the increasing availability of powerful computers with large amounts of memory.

In the early applications of the finite-lattice method, nearly a decade ago, increases of 50 to 100% in the number of series terms were obtained. Repeating these early calculations using modern computers gives further increases of typically 50 to 100% in the number of series terms. Our studies have concentrated on self-avoiding polygons on two-dimensional lattices (using refinements of the algorithm described by Enting (1980a)) and the Potts model on two-dimensional lattices (see Enting 1978, 1980b) and in three dimensions (currently in progress).

In the course of our polygon enumeration on the square lattice we noted (Guttmann and Enting 1988a) that if the finite-lattice method gave the polygon generating function correct to order x^m then the next term was also complete apart from a relatively small correction given by $c_{m+2}x^{m+2}$ where c_n is the number of convex polygons of n steps. These convex polygons are such that any straight line on the bonds of the dual lattice cuts the bonds of the convex polygon at most twice. In our studies of the q-state Potts model on the square lattice we have noted that the first correction to the finite-lattice calculations of the partition function is of the form $(q-1)c_nv^n$ for high-temperature series and by duality $(q-1)c_n z^n$ for low-temperature series. The low-temperature series for the Potts model partition function, Z, is of the form (Wu 1982)

$$\lim_{n\to\infty} Z_N^{1/N} = Z(z,\mu) = 1+(q-1)z^{\nu}\mu+\ldots = 1+\sum_n z^n\phi_n(\mu) \tag{1}$$

where ν is the lattice coordination number and $z=\exp(-\Delta E/kT)$, $\mu=\exp(-H/kT)$, ΔE is the energy per pair of non-identical neighbours and H is the energy per non-zero spin. The $\phi_n(\mu)$ are polynominals in μ.

For the low-temperature series, the convex polygons are the graphs describing the corrections to the finite-lattice method in a general field. However the correction term involves area-weighted moments of the convex polygons rather than simply their number. The finite-lattice expression for low-temperature expansions of the partition function approximates the full expansion (1) by the finite product:

$$Z(z,\mu) \approx \prod_{\substack{j,k \\ j+k\leqslant 2w+1}} Z_{j,k}(z,\mu). \tag{2}$$

In order to reduce the complexity of the calculations we have generally made the substitution $\mu=1-y$ and truncated the expansion in y at order y^2. This is sufficient to give us the low-temperature partition function, order parameter and susceptibility. If $c_{n,m}$ is the number of convex polygons with $n=4w+4$ steps and area m, then the correction to (2) of lowest order in z is given by $(q-1)\Sigma_m c_{n,m} z^n(1-y)^m$. Our interest in corrections to expansions truncated at order y^2 leads us to consider the three generating functions

$$P_0(z)=\sum_n\sum_m c_{n,m}z^n \tag{3a}$$

$$P_1(z)=\sum_n\sum_m c_{n,m}mz^n \tag{3b}$$

$$P_2(z)=\sum_n\sum_m c_{n,m}\tfrac{1}{2}m(m-1)z^n. \tag{3c}$$

We obtain the $P_j(z)$ by calculating the low-order coefficients using a transfer matrix technique and then fitting a recurrence relation which enables us to determine the function, assuming that we have calculated sufficient terms. We used this approach (Guttmann and Enting 1988b) to determine

$$P_0(z)=x^2[(1-6x+11x^2-4x^3)/(1-4x)^2-4x^2/(1-4x)^{3/2}] \tag{4}$$

with $x=z^2$. This result had the status of a conjectured exact result.

Unknown to us, this result had previously been obtained by Delest and Viennot (1984) using the theory of algebraic languages. The result was subsequently confirmed by Lin and Chang (1988). Although our method is not rigorous, it is particularly convenient and we have used it to obtain

$$P_1(x)=x^2[(1-12x+50x^2-76x^3+42x^4-48x^5+32x^6)/(1-4x)^4+4x^2/(1-4x)^{5/2}] \tag{5}$$

and

$$P_2(x)=x^3[R(x)/(1-4x)^6+S(x)/(1-4x)^{9/2}] \tag{6a}$$

where

$$R(x)=2+5x-224x^2+1306x^3-3352x^4+4536x^5-3424x^6+1664x^7-512x^8 \tag{6b}$$

and

$$S(x) = -29x + 172x^2 - 356x^3 + 312x^4 - 120x^5. \tag{6c}$$

While the derivation of $P_1(x)$ followed that of $P_0(x)$, described in Guttmann and Enting (1988b), the derivation of $P_2(x)$ was rather more complicated. Our computer program obtained a recurrence relation with non-integer coefficients in this case (unlike the case of $P_0(x)$ and $P_1(x)$), and some ingenuity was required to establish equation (6*c*). In particular, it was clear from the differential approximants that $P_2(x)$ was of the form (6*a*). We therefore considered the series expansion of

$$Q(x) = (1-4x)^{9/2} P_2(x)/x^4 = R(x)/(1-4x)^{3/2} + S(x). \tag{6d}$$

As $S(x)$ is a polynomial of degree n_s, it contributes only to the first n_s terms of the power series expansion of (6*d*). We therefore multiply the last known coefficients of $Q(x)$ by $(1-4x)^{3/2}$, and if our initial assumption of a functional form given by (6*a*) is correct, a polynomial will result. This was indeed the case, giving the results (6*b*) and (6*c*) above. Again, these results have the status of conjectured exact results. However, to determine (5) required 19 terms out of the known 24 non-zero terms, while the more ingenious method used to determine (6*a*) required 16 terms out of the known 23 non-zero terms. The additional terms were then predicted. As these are integers with up to 18 digits, the likelihood that the conjectured exact results are wrong is extraordinarily small. The solution so obtained solves what Delest and Viennot (1984) have termed a 'major problem'.

The series used to derive these generating functions were obtained by a simple modification of the expressions given by Guttmann and Enting (1988b). We considered four sets of partial enumerations which we denoted R_{ij}^k, S_{ij}^k, T_{ij}^k, U_{ij}^k and defined relations of the form

$$X_{mn}^{k+1} = \sum_1 R_{ij}^k + \sum_2 S_{ij}^k + \sum_3 T_{ij}^k + \sum_4 U_{ij}^k \tag{7}$$

where X represents one of R, S, T or U and the precise range of each summation over i and j depends on which variable X represents, as well as on m and n. We generalise these relations to include the y dependence in R, S, T and U. The equations (7)–(10) of Guttmann and Enting (1988b) which we represent by the generic relation (7) are generalised to the form

$$X_{mn}^{k+1}(y) = (1-y)^{i-j}\left(\sum_1 R_{ij}^k(y) + \sum_2 S_{ij}^k(y) + \sum_3 T_{ij}^k(y) + \sum_4 U_{ij}^k(y)\right) \tag{8}$$

with the ranges of each sum remaining unchanged. Our calculations only retain the y dependence to order y^2.

While we have mainly considered the generating functions $P_1(z)$ and $P_2(z)$ in their role of correction terms to Potts model expansions, they are interesting quantities in their own right. They represent new, presumably exact, solutions of additional geometrical properties of convex self-avoiding rings.

It is of some interest to relate these quantities to a 'Potts-like' model in which the convex polygons are the only terms contributing, i.e.

$$Z^*(z, \mu = 1-y) = 1 + P_0(z) - yP_1(z) + y^2 P_2(z). \tag{9}$$

In this representation, the exponent α is the dominant exponent of

$$\frac{\partial^2}{\partial z^2} \ln Z^* = \frac{\partial}{\partial z}[P_0'(z)/(1+P_0(z))] \qquad \text{i.e. } \alpha = 2. \tag{10}$$

The exponent β is given by the dominant exponent of $P_1(z)/(1+P_0(z))$, i.e. $\beta=-2$. The exponent γ is given by the dominant exponent of $P_2(z)/(1+P_0(z))$. Thus $\gamma=4$. These exponents satisfy the scaling relation $\alpha+2\beta+\gamma=2$. However, since P_1/P_0 diverges ($\beta=-2$), this quantity does not seem to have any obvious interpretation as an order parameter. It should be noted that these definitions of analogues of thermodynamic quantities are related to the low-temperature Potts/Ising expansions. Alternative relations could give other sets of exponents. In particular Lin and Chang (1988) were able to determine the asymptotic form of the mean-square radius of gyration of convex polygons and, with what was essentially an analogue of high-temperature series, found the exponents $\alpha=4$, $\nu=1$. Thus the extension of convex polygon statistics to produce analogues of all the conventional exponents α, β, γ, δ, ν... can be performed in more than one way. Presumably the same is true for unrestricted self-avoiding polygons.

In conclusion, we comment on the correction terms for finite-lattice expansions for the Potts model on the simple cubic lattice. In the absence of duality, different graphs are involved for high and low temperatures. For neither case do we have a closed-form solution but for $q\neq 2$ we can exploit our knowledge of the q dependence of the corrections, and multiply the corrections for the Ising ($q=2$) case by $(q-1)$. The calculation of Ising model series is easier than for larger q values and so the Ising series can usually be obtained to higher order. The low-temperature corrections are given by a particular class of tree graphs and they give corrections for the next *two* terms in each low-temperature expansion. The graphs that give corrections to the high-temperature series are what we call 'maximally extended polygons'. These are the three-dimensional generalisation of convex polygons. Any plane face of the dual lattice cuts the bonds of a maximally extended polygon at most twice. We have enumerated suitably restricted self-avoiding walks to determine that on the simple cubic lattice there are 3, 22, 201, 2160, 24 680, 285 384, 3278 484, 37 154 172 such polygons with 4, 6, ..., 18 steps respectively. This does not give enough steps for us to determine a recurrence relation. The generalisation of our transfer matrix approach seems to be too complicated to be practical because the additional dimension removes a number of constraints that simplified the square lattice formalism. It remains to be seen whether the algebraic language approach of Delest and Viennot or the generating function approach of Lin and Chang encounters similar difficulties in going from two to three dimensions.

References

Delest M P and Viennot G 1984 *Theor. Comput. Sci.* **34** 169-206
de Neef T and Enting I G 1977 *J. Phys. A: Math. Gen.* **10** 801-5
Enting I G 1978 *Aust. J. Phys.* **31** 515-22
—— 1980a *J. Phys. A: Math. Gen.* **13** 3713-22
—— 1980b *J. Phys. A: Math. Gen.* **13** L133-6
Guttmann A J and Enting I G 1988a *J. Phys. A: Math. Gen.* **21** L165-72
—— 1988b *J. Phys. A: Math. Gen.* **21** L467-74
Lin K Y and Chang S J 1988 *J. Phys. A: Math. Gen.* **21** 2635-42
Wu F Y 1982 *Rev. Mod. Phys.* **54** 235-68