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Lattice Animals: Supplementation of Perimeter Polynomial Data by Graph-Theoretic Methods

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Application of graph-theoretic methods to new perimeter polynomials for connected clusters on a lattice yields extra data on the total number of clusters and for the coefficients in the series expansion for the mean size of clusters at low densities. The lattices studied are the square, the square with next nearest neighbors, the triangular, and the simple cubic.

KEY WORDS: Cluster enumeration; perimeter polynomials.

Recently, Mertens[(1)] has described an enumeration algorithm for deriving perimeter polynomials and has given new data for four lattices: the square, the square with next nearest neighbors, the triangular, and the simple cubic. He points out that his data could usefully be supplemented by graph-theoretic methods. We have performed the necessary calculations. Since the theoretical background has been adequately described before,[(2–4)] we simply report the results.

We follow the notation of Mertens and denote for any lattice the total number of strong embeddings of connected clusters of n sites by g_n and the probability that a site is occupied by p. We write the expansion for the mean size of clusters at low densities in the form

$$S(p) = \sum b_n p^n \tag{1}$$

with $b_0 = 1$. We also define $q = 1 - p$.

We have used the techniques described in detail by Sykes and Wilkinson.[(5)] If perimeter polynomials $D_n(q)$ are available for a lattice for

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all clusters through n sites, then the number of clusters with $n+1$ sites (g_{n+1}) is determined, together with the coefficients in the expansion of $S(p)$ through b_n. For lattices for which the *total* number of clusters with two further sites (g_{n+2}) is available an extra coefficient (b_{n+1}) can be added for $S(p)$ [ref. 5, Eq. (2.9)]. For the square lattice, Mertens used his perimeter polynomials through D_{22} and the value of g_{24} given by Redelmeier[5] to obtain b_{23}. For lattices of high coordination number the rapid growth in the total number of clusters makes computer enumeration extremely costly in terms of cpu time. However, alternative combinatorial methods described by Sykes[7-10] and developed and implemented by Martin[11] can be used to avoid direct enumeration. For the simple cubic lattice detailed results are reported by Madras *et al.*,[12] Appendix B, from which the values $g_{16} = 1\,435\,074\,454\,755$ and $g_{17} = 10\,977\,812\,452\,428$ can be added to Mertens' Table I. Using Mertens' polynomials through D_{14} for this lattice, we calculate $b_{15} = 327\,024\,444$ to extend his Table II.

An alternative technique can be used for lattices for which the expansion for the mean number of clusters at low densities

$$K(p) = \sum k_n p^n \tag{2}$$

is available through k_{n+2}. Combined with perimeter polynomials through D_n, k_{n+2} determines both b_{n+1} and g_{n+2} [ref. 5, Eq. (2.8)]. For two-dimensional lattices the mean number expansion can often be derived by special methods.[2,3] Thus, for the triangular lattice we can exploit the fact that the lattice is self-matching and obtain the low-density expansion $K(p)$ from the corresponding high-density expansion in powers of q. The calculation requires the information contained in the perimeter polynomials to be regrouped in powers of q. The values through D_{18} for the triangular lattice are not sufficient to derive the value of k_{20} in this way, but the necessary additional data are given by Sykes *et al.*[13] [Eqs. (2.11) and (2.12)]. Using their data, we find $k_{20} = 14\,289$ and thence can supplement Mertens' Tables I and II with the values $g_{20} = 2\,599\,804\,551\,168$ and $b_{19} = 20\,763\,036$.

A similar procedure applies to the square lattice with next nearest neighbors. The coefficient k_{n+2} can be derived from the mean number expansion at high densities on the matching lattice, which in this case is the square lattice.[2] The data required are implicit in ref. 13 or could alternatively be got by regrouping Mertens' perimeter polynomials for the square lattice. From the result $k_{15} = -4\,400$ for the second-neighbor lattice we can supplement Mertens' Tables I and II with the values $g_{15} = 74\,570\,549\,714$ and $b_{14} = 11\,450\,284$.

If the two techniques outlined above are combined, then a knowledge of the perimeter polynomials through D_n, together with the values of g_{n+3} and k_{n+3}, determines the extra coefficient b_{n+2}. This procedure was used in ref. 5 to obtain b_{12} for the simple cubic lattice. The combinatorial data used to derive the more recent results for this lattice reported in ref. 12 are in principle sufficient (using the results of ref. 4) to determine k_{17}; combined with Mertens' perimeter polynomials through D_{14}, this should eventually enable us to determine b_{16}.

The generating function methods of refs. 7–10 can be further developed to derive the expansion of $S(p)$ without recourse to perimeter polynomials and it seems likely that for lattices of high coordination number such techniques will prove the better; for lattices of low coordination number, direct enumeration has much to commend it.

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