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SERIES EXPANSION FOR RECTILINEAR POLIMERS ON THE SQUARE LATTICE

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Разложение в ряд для прямолинейных полимеров на квадратной решетке

Число способов, при использовании которых можно полностью покрыть квадратную решетку данным числом прямолинейных r -меров, (r≥2) оценивается с помощью комбинаторного метода, включающего разложение в ряд.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Priezzhev V.B.

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Series Expansion for Rectilinear Polimers on the Square Lattice

A number of ways in which a quadratic lattice can be fully covered with given numbers of rectilinear r -mers (r≥2) is estimated by a combinatorial method involving series expansion.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1978

1. INTRODUCTION

One of the simplest, yet unsolved, problems in lattice statistics is the pure r -mer problem in which each site of lattice is singly occupied by one element of a rectilinear r-mer molecule. The pure r -mer problem is characterized by the residual entropy or "molecular freedom" per r-mer ϕ_r, defined so that the number of arrangements of n r-mers on a lattice of $n\times r$ sites is asymptotically $(\phi_r)^n$. The exact solution for the case of dimers was obtained by Fisher [1] and Kasteleyn [4] for the square lattice and subsequently for other two-dimensional lattices (Kasteleyn [5]). No rigorous treatments of the general r-mer problem have yet been given.

The Bethe approximation on a lattice of coordination number c leads to

$$\phi_r = \left(\frac{cr}{2}\right)\left[1-\frac{2}{cr}(r-1)\right]^{cr/2-r+1} \qquad (1.1)$$

and becomes invalid as r increases (ϕ_r is less than unity already for $r>3$ in the case of a square lattice). There are enough data, provided by the matrix method of Kramers-Wannier (Van Craen [10]), the Kikuchi method (Kaye and Burley [6]), series expansions (Van Craen and Bellemans [11]) to obtain fair estimates of the exact solution of trimer problem.

Recently Kowalsky and Priezzhev [7] and Gagunashvili and Priezzhev [2] have investigated rigorously lower and upper bounds of ϕ_r for arbitrary $r \geq 2$. Their results are summarized in the following three inequalities:

$$\phi_r \leq \left(\frac{r}{2}\right)^{1/r} \exp\left\{\frac{4G}{\pi r}\right\} \quad \text{for } r \text{ even}, \tag{1.2}$$

$$\phi_r \leq \left(\frac{r-1}{2}\right)^{1/r} \exp\left\{\frac{1}{\pi r}\int_0^{\pi} \operatorname{arch}\left(\frac{2r}{r-1} - \cos\phi\right) d\phi\right\} \text{ for } r \text{ odd} \tag{1.3}$$

$$\phi_r \geq \exp\left\{\frac{4G}{\pi r}\right\}, \tag{1.4}$$

where $G = 0.915965\ldots$ (Catalan's constant).

In the present paper we develop a method of approaching the problem which is an extension of these works. This method based on the combinatorial principle of inclusion and exclusion provides a series technique for estimating the molecular freedom per r-mer for arbitrary $r \geq 2$.

2. RECTILINEAR POLIMERS ON THE SUPERLATTICE

Consider a planar quadratic $mr \times nr$ lattice to which one can attach rectilinear r-mers in such a way that every r-mer occupies r lattice points and the lattice is fully occupied by r-mers. We denote the lattice points by (x, y) and define points of quadratic $m \times n$ suparlattice as points with coordinates (X, Y) which obey

$$X (\mathrm{mod}\, r) = 0,$$
$$Y (\mathrm{mod}\, r) = 0.$$

To estimate ϕ_r, we use the following proposition (Kowalsky and Priezzhev [7]):

Proposition 1. Let $r(mn)$ points of the lattice be occupied by mn r-mers, arranged on the superlattice, then the rest of points may be covered with r-mers not more than in one manner.

So, any arbitrary configuration of r-mers is defined by arrangement of mn r-mers on the superlattice. There are $2r$ different ways in which a superlattice site may be occupied and consequently there are altogether $(2r)^{mn}$ possibilities. Many of them, however, are unacceptable because of incompatibilities between arrangements of different r-mers on the superlattice.

Let us consider the reasons for which the r-mer configuration C on the superlattice may be unacceptable. The simplest of them is the intersection of r-mers covering neighbouring superlattice points. To clarify other cases we introduce some auxiliary notions.

By reduced coordinates of the point (x, y) we understand the pair of integers $[i, j]$ defined by

$$i = x (\mathrm{mod}\, r) \qquad i \in (0, 1, \ldots, r-1)$$

$$j = y (\mathrm{mod}\, r) \qquad j \in (0, 1, \ldots, r-1).$$

Let C be a configuration of r-mers on the superlattice and $B(C)$ be a set of a superlattice bounds partially covered by r-mers from C. Each bound appears in $B(C)$ 0,1,2 times if there are 0,1 or 2 r-mers covering this bound. A digraph is defined as a collection of superlattice sites and collection of bounds B(C). A cycle of a digraph is a collection of bounds of the form $p_1p_2, p_2p_3, \ldots, p_{k-1}p_1$, where p_ip_j denote the bounds joining superlattice points p_i and p_j, and all points in the collection save p_1 are distinct. A cycle is closed relative to reduced coordinates $[i,j]$ $i \neq 0$, $j \neq 0$ if all points of the basic $mr \times nr$ lattice belonging to its bounds and having reduced coordinates $[i,0]$, $[0,j]$ are covered by r-mers from C.

The cycle p_1p_2, p_2p_1 resulting from intersection of two neighbouring r-mers from C in the basic lattice points is closed, too, with respect to reduced coordinates of these points. We call any closed cycle the contour and we use $g(i_1j_1; i_2j_2; \ldots; i_sj_s)$ to denote the contour closed with respect to coordinates $[i_1,j_1], [i_2,j_2], \ldots, [i_s,j_s]$ or g if the values of these coordinates are not essential. We will say that the configuration C generates the contour g. Note that different configurations can generate the same contour and a few contours can correspond to one cycle.

Proposition 2. (Gagunashvili, Priezzhev[2]). If the r-mers configuration C on the superlattice generates at least one contour g, then the dense packed configuration on the basic lattice involving C does not exist.

Thus, in order to get an explicit expression for ϕ_r, we need to exclude from the total number $(2r)^{nm}$ of r-mers configurations on the superlattice those generating contours. Consider the set of all distinct contours $\{g_s\}$, $s=1$ to k, where k is the maximum number of contours for given lattice. Let

P be the total number of r-mers configurations on the superlattice. Let P_i be the number of configurations generating the contour g_i and $P_{i_1,i_2,\ldots,i_s}$ be the number generating the contours $g_{i_1}, g_{i_2}, \ldots, g_{i_s}$. Then by the principle of inclusion and exclusion the number of configurations P_0 generating none of the contours is given by

$$P_0 = P - \sum_i P_i + \sum_{i_1<i_2} P_{i_1,i_2} + \ldots + (-1)^s \times \\ \times \sum_{i_1<i_2<\ldots<i_s} P_{i_1,\ldots,i_s} + \ldots + (-1)^k P_{1,2,\ldots,k} \quad . \tag{2.1}$$

One may take on trust that excluding of the configurations generating the contours exhausts the set of all unacceptable configurations. At least we have the following statement (Priezzhev[9]):

Proposition 3. In the case $r=2$ P_0 is the number of all possible dense and nonoverlapping arrangements of dimers on the square lattice .

Conjecture. The proposition 3 is valid for all $r \geq 2$.

If the conjecture holds, we obtain the expression for the molecular freedom of r-mers on the basic $mr \times nr$ lattice:

$$\phi_r = (P_0)^{1/rmn} \quad . \tag{2.2}$$

In the opposite case the right-hand side of equation (2.2) is the upper bound of ϕ_r.

3. DERIVATION OF THE SERIES EXPANSION

Let G_s be the set of contours $g_1, g_2, \ldots, g_\nu$ generated by r-mer configuration on the superlattice. The index s denotes the number of superlattice points belonging to contours from G_s; $\nu(G_s)$ denotes the number of contours in the set G_s. Note, that one may arrange an r-mer on each of mn-s superlattice points which do not belong to G_s in $2r$ independent ways. We define $W(G_s)$ by

$$\sum_C{}'(-1)^{\nu(G_s)} = (2r)^{mn-s}\, W(G_s), \qquad (3.1)$$

where the prime denotes the summation over configurations C generating the set G_s. By definition $|W(G_s)|$ is the number of arrangements of s r-mers on the s superlattice sites which lead to the set of contours G_s. According to (2.1), in notations introduced we have

$$P_0 = P + \sum_{G_2}\sum_C{}'(-1)^{\nu(G_2)} + \sum_{G_3}\sum_C{}'(-1)^{\nu(G_3)} + \ldots + \sum_{G_{mn}}\sum_C{}'(-1)^{\nu(G_{mn})} =$$

$$= (2r)^{mn} + (2r)^{mn-2}\sum_{G_2} W(G_2) + \qquad (3.2)$$

$$+ (2r)^{mn-3}\sum_{G_3} W(G_3) + \ldots + \sum_{G_{mn}} W(G_{mn}).$$

We define the generating function

$$\Lambda_N(x) = (2r)^N\{1 + \sum_{s=2}^{N}\omega_N(s)x^s\}, \qquad (3.3)$$

where $N = mn$ and

$$\omega_N(s) = \sum_{G_s} W(G_s).$$

In the thermodynamic limit

$$\Lambda(x) = \lim_{N\to\infty}[\Lambda_N]^{1/N} = 2r\{1 + \sum_{s=2}^{\infty}\omega(s)x^s\}, \qquad (3.4)$$

where it can be shown that

$$\omega(s) = \omega_N(s)|_{N=1}.$$

From (2.2), (3.2), (3.3) and (3.4) it follows that

$$\phi_r = [\Lambda(\tfrac{1}{2r})]^{1/r} = (2r)^{1/r}\{1 + \sum_{s=2}^{\infty}\omega(s)(\tfrac{1}{2r})^s\}^{1/r}. \qquad (3.5)$$

From the boundedness of ϕ_r for each fixed r the convergence of the series in equation (3.5) follows: so $\omega(s)/r^s \to 0$ for $s\to\infty$. We shall see below that the convergence is rapid enough to estimate ϕ_r using the first few terms of the series.

4. GRAPH DATA

To begin the calculation of the coefficients $\omega(s)$, let us consider a few simple cases.

1. Case $s=2$, $r=3$. In this case G_2 contains only contour ($\nu(G_2)=1$) from the collection $g(1,0)$, $g(2,0)$, $g(1,0;2,0)$, $g(0,1)$, $g(0,2)$, $g(0,1;0,2)$. The r-mer configurations corresponding to the first three contours are shown in fig.1(b),(c),(d). The remaining three contours correspond to vertical r-mers. Thus, for $r=3$ $\omega_N(2) = -6N$ and $\omega(2) = -6$. A simple calculation shows that for arbitrary r

$$\omega_N(2) = -2\frac{r(r-1)}{2}N, \quad \omega(2) = r(r-1).$$

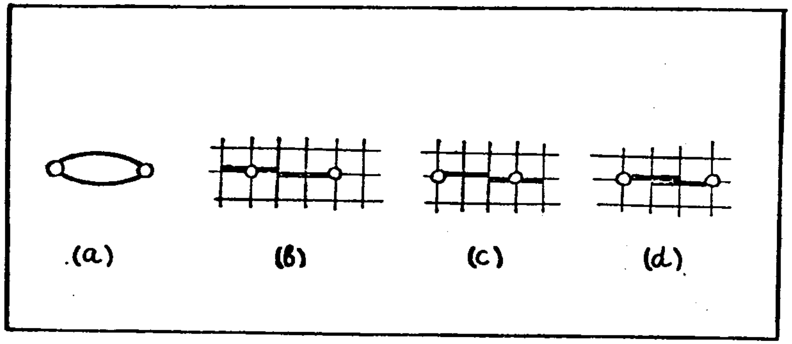


Fig. 1. Case $s=2$, $r=3$. Open circles denote superlattice points. (a) A cycle, (b), (c), (d) r-mer configurations generating contours $g(1,0)$, $g(2,0)$, $g(1,0;2,0)$.

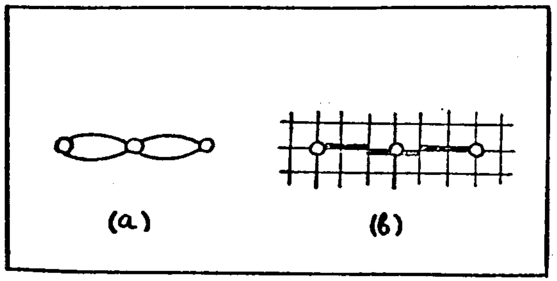


Fig. 2. (a) Two connected cycles in case $s=3$. (b) The r-mer configuration ($r=3$) generating contours $g(1,0)$ and $g(2,0)$.

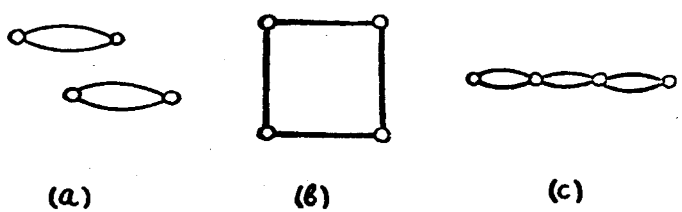


Fig. 3. Cycles contributing in the coefficient $\omega(4)$.

2. Case $s=3$, $r=3$. One of the two configurations appearing in this case is shown in fig. 2. We see that $\omega_N(3)=2N$, $\omega(3)=2$. For arbitrary $r>2$ we have

$$\omega_N(3) = 2\sum_{i=2}^{r-1}\frac{i(i-1)}{2}N, \quad \omega(3) = \sum_{i=2}^{r-1} i(i-1).$$

3. Case $s=4$. This case is illustrated in fig. 3. The enumeration of the contours corresponding to cycles of the type (a) leads to

$$N(2N-7)\left[\frac{r(r-1)}{2}\right]^2.$$

Similarly, for the cycles of the type (b) we have

$$2N\left[\frac{r(r-1)}{2}\right]^2$$

and for those of type (c):

$$\begin{cases} 2N\sum_{i=3}^{r-1}\sum_{j=2}^{i-1}\frac{i(i-1)}{2} & (r>3) \\ 0 & (r=2 \text{ or } r=3) \end{cases}$$

Using these expressions, we obtain

$$\omega(4) = -7\left[\frac{r(r-1)}{2}\right]^2 - 2\sum_{i=3}^{r-1}\sum_{j=2}^{i-1}\frac{i(i-1)}{2},$$

where we use conventions that a sum is equal to zero, if in the summation the lower index exceeds the upper one.

To consider more general cases, let us make first some preliminary remarks. Among the set of contours arising on a digraph there can appear such pairs of contours g and g′ that for any configuration of r-mers the presence of g′ necessitates the presence of g, but the inverse does not hold. In that case following the principle of inclusion and exclusion when calculating the coefficient $\omega(s)$ we should take into account only the contribution from contour g.

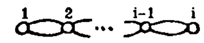
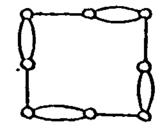
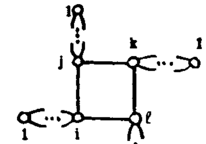
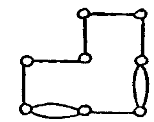
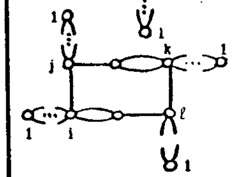
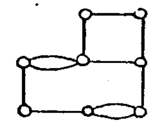
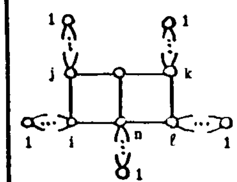
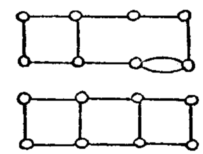
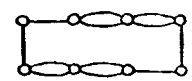
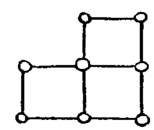
Now let us derive general expressions for $\omega(s)$ up to eighth order. To this end consider all possible types of connected cycles entering into the 8-th order expansion (Table 1) and calculate the numbers of r-mers configurations generating different contours which correspond to each of these cycles. These numbers will be denoted by $K^{(r)}$ for each value of the r-mer length, their dependence on other indices is shown in Table 1. Indices i, j, k, ℓ, n take such values that the total number of cycle vertices does not exceed eight. Formulae for calculating the number of r-mer configurations $K^{(r)}$ can be found in Appendix A. Appendix B contains formulae for calculating the coefficients $\omega(s)$ expressed through $K^{(r)}$.

5. RESULTS

The expansion coefficients $\omega(s)$, $s = 2,3,\ldots,8$ obtained by evaluating expressions A1-A11 and B1-B7 for first twenty values of r are listed in Table 2. The series in eq. (3.5) has been truncated after the eight term and resulting values of the molecular freedom

$$\phi_r = (2r)^{1/r}\{1 + \sum_{s=2}^{8}\omega(s)(\frac{1}{2r})^s\}^{1/r}$$

Table 1

n	Type of cycle	$K^{(r)}$	n	Type of cycle	$K^{(r)}$
1		$K_1^{(r)}(i)$	6		$K_6^{(r)}$
2		$K_2^{(r)}(i,j,k,\ell)$	7		$K_7^{(r)}$
3		$K_3^{(r)}(i,j,k,\ell)$	8		$K_8^{(r)}$
4		$K_4^{(r)}(i,j,k,\ell,n)$	10		$K_{10}^{(r)}$
5		$K_5^{(r)}$	11		$K_{11}^{(r)}$

are listed in the last column of Table 2. These expansions are not long enough to lead to an accurate estimate of ϕ_r by using the Pade technique. Nevertheless, to make a comparison with results of the previous papers we have estimated ϕ_2 and ϕ_3 by evaluating the Pade approximants P(2,2) and

Table 2

Expansion coefficients $\omega(s)$ and molecular freedom ϕ_r

r	ω(2)	ω(3)	ω(4)	ω(5)	ω(6)	ω(7)	ω(8)	φ_r
2	-2	0	-7	0	-50	0	-472	1.82
3	-6	2	-63	72	-1302	2552	-35912	1.66
4	-12	8	-254	576	-10596	40464	-596041	1.55
5	-20	20	-710	2402	-49900	280600	-4757065	1.48
6	-30	40	-1605	7212	-170702	1263200	-24714755	1.42
7	-42	70	-3157	17682	-473354	4336502	-96842767	1.38
8	-56	112	-5628	37744	-1131368	12346448	-310832678	1.34
9	-72	168	-9324	72828	-2420664	30641256	-859905270	1.32
10	-90	240	-14595	130104	-4753770	68450640	-2120515650	1.29
11	-110	330	-21835	218724	-8718974	140699460	-4771407850	1.27
12	-132	440	-31482	350064	-15124428	270315584	-9963307607	1.26
13	-156	572	-44018	537966	-25047204	491091744	-19551975079	1.24
14	-182	728	-59969	798980	-39887302	851161168	-36408772309	1.23
15	-210	910	-79905	1152606	-61426610	1417146770	-64824333305	1.22
16	-240	1120	-104440	1621536	-91892816	2279043680	-111022357660	1.21
17	-272	1360	-134232	2231896	-134028272	3555894896	-183801981692	1.20
18	-306	1632	-169983	3013488	-191163810	5402319840	-295328614140	1.19
19	-342	1938	-212439	4000032	-267297510	8015955600	-462094556508	1.18
20	-380	2280	-262390	5229408	-367178420	11645870640	-706072161205	1.17

P(4,4) to the series

$$-2x^2 - 7x^4 - 50x^6 - 472x^8$$

at $x = 1/4$ and

$$-6x^2 + 2x^3 - 63x^4 + 72x^5 - 1302x^6 + 2552x^7 - 35912x^8$$

at $x = 1/6$.

These results of calculation are listed in Table 3, together with the results of Nagle/8/, Gaunt/3/, Van Craen and Bellemans /11/. Table 3 clearly demonstrates the accuracy

Table 3

Values of the molecular freedom ϕ_2 per dimer and ϕ_3 per trimer for square lattice

	Truncated series	Pade approximant
ϕ_2* Nagle,1966	1.7694	1.7905
ϕ_2 Gaunt, 1969	1.7728	1.78-1.80
ϕ_2 this paper	1.8202	1.8067
ϕ_3** Van Craen and Bellemans, 1972	-	1.57
ϕ_3 this paper	1.66	1.64

*Exact value of $\phi_2 = 1.7916$ (Kasteleyn/4/, Fisher /1/).

** Estimate of $\phi_3 = 1.6 \pm 0.001$ obtained by matrix method (Van Craen, 1975).

of calculation of ϕ_r at $r = 2$ and $r = 3$. Information about the calculational accuracy at larger r can be obtained by comparing the calculated ϕ_r with its upper and lower bounds reported in the Introduction. For instance, at $r=20$ from equations (1.2), (1.4), we have $1.19 \geq \phi_{20} \geq 1.06$, $\phi_{20}=1.17$ so that the accuracy is not worse than (-10%, +2%).

APPENDIX A

$$K_1^{(r)}(i) = \sum_{m_i=i-1}^{r-1} \sum_{m_{i-1}=i-2}^{m_i-1} \cdots \sum_{m_1=0}^{m_2-1} 1 , \tag{A1}$$

$$K_2^{(r)}(i,j,k,\ell) = K_1^{(r)}(i+k)\, K_1^{(r)}(j+\ell) , \tag{A2}$$

$$K_3^{(r)}(i,j,k,\ell) = K_1^{(r)}(j+\ell) \times$$
$$\times \left\{ \sum_{m_i=i}^{r-1} \sum_{m_{i-1}=i-1}^{m_i-1} \cdots \sum_{m_1=1}^{m_2-1} \sum_{m=m_1}^{r-1} \sum_{n=1}^{m_1} \sum_{n_k=\max(n,k)-1}^{m_1-1} \sum_{n_{k-1}=k-2}^{n_k-1} \sum_{n_1=0}^{n_2-1} 1 \right\}, \tag{A3}$$

$$K_4^{(r)}(i,j,k,\ell,n) = K_1^{(r)}(i+\ell+1) \times$$
$$\times \left\{ \sum_{m_j=j}^{r-1} \sum_{m_{j-1}=j-1}^{m_j-1} \cdots \sum_{m_1=1}^{m_2-1} \sum_{p_k=k}^{r-1} \sum_{p_{k-1}=k-1}^{p_k-1} \cdots \sum_{p_1=1}^{p_2-1} \sum_{q_n=n-1}^{\min(m_1,p_1)-1} \sum_{q_{n-1}=n-2}^{q_n-1} \cdots \sum_{q_1=0}^{q_2-1} 1 \right\}, \tag{A4}$$

$$K_5^{(r)} = K_1^{(r)}(2) \left\{ \sum_{m_3=1}^{r-1} \sum_{m_2=1}^{m_3} \sum_{m_1=1}^{m_2} \sum_{m=1}^{m_1} (m_1-m+1)(m_1-m+2)/2 \right\}, \tag{A5}$$

$$K_6^{(r)} = \left\{ \sum_{m_1=1}^{r-1} \sum_{m=1}^{m_1} m(m+1)/2 \right\}^2 \tag{A6}$$

$$K_7^{(r)} = \left\{ \sum_{m_1=1}^{r-1} \sum_{m=1}^{r-1} \min(m,m_1)\left[\min(m,m_1)+1\right]/2 \right\}^2 \tag{A7}$$

$$K_8^{(r)} = K_1^{(r)}(3) \left\{ \sum_{m_2=1}^{r-1} \sum_{m_1=1}^{m_2} \sum_{m=1}^{m_1} m(2r-m-1)/2 \right\}, \tag{A8}$$

$$K_9^{(r)} = \left(\sum_{n=1}^{r-1} n^2 \right) \left\{ \sum_{m_1=2}^{r-1} \sum_{m=1}^{m_1-1} m(r-m)(m+1)/2 \right\}, \tag{A9}$$

$$K_{10}^{(r)} = K_1^{(r)}(4) \sum_{m_1=1}^{r-1} \sum_{m=1}^{r-1} \min(m,m_1)\, m , \tag{A10}$$

$$K_{11}^{(r)} = \left(\sum_{m_1=2}^{r-1} \sum_{m=1}^{m_1-1} m^2 \right) \left\{ \sum_{n_1=2}^{r-1} \sum_{n=1}^{n_1-1} n(2r-n-1)/2 \right\} \tag{A11}$$

APPENDIX B

$$\omega(2) = -2K_1^{(r)}(2) , \tag{B1}$$

$$\omega(3) = 2K_1^{(r)}(3) , \tag{B2}$$

$$\omega(4) = -7\left[K_1^{(r)}(2)\right]^2 - 2K_1^{(r)}(4) , \tag{B3}$$

$$\omega(5) = 24K_1^{(r)}(2)K_1^{(r)}(3) + 2K_1^{(r)}(5) , \tag{B4}$$

$$\omega(6) = -2K_1^{(r)}(6) - 46\left[K_1^{(r)}(2)\right]^3 - 20\left[K_1^{(r)}(3)\right]^2 \tag{B5}$$
$$-34K_1^{(r)}(2)K_1^{(r)}(4) - 4K_3^{(r)}(1,1,1,1) + 4K_4^{(r)}(1,1,1,1,1),$$

$$
\begin{aligned}
\omega(7) = {} & 2K_1^{(r)}(7) + 44\,K_1^{(r)}(2)K_1^{(r)}(5) + 56\,K_1^{(r)}(3)K_1^{(r)}(4) \\
& + 276\left[K_1^{(r)}(2)\right]^2 K_1^{(r)}(3) + 8K_3^{(r)}(2,1,1,1) + 8K_3^{(r)}(1,2,1,1) \\
& - 8K_4^{(r)}(2,1,1,1,1) - 8K_4^{(r)}(1,2,1,1,1) - 4K_4^{(r)}(1,1,2,1,1),
\end{aligned}
\tag{B6}
$$

$$
\begin{aligned}
\omega(8) = {} & -2K_1^{(r)}(8) - 382\left[K_1^{(r)}(2)\right]^4 - 520K_1^{(r)}(2)\left[K_1^{(r)}(3)\right]^2 \\
& - 420\left[K_1^{(r)}(2)\right]^2 K_1^{(r)}(4) - 39\left[K_1^{(r)}(4)\right]^2 - 54K_1^{(r)}(2)K_1^{(r)}(6) \\
& - 72\,K_1^{(r)}(3)K_1^{(r)}(5) - 60K_1^{(r)}(2)K_3^{(r)}(1,1,1,1) \\
& + 60K_1^{(r)}(2)K_4^{(r)}(1,1,1,1,1) - 8K_3^{(r)}(3,1,1,1) - 8K_3^{(r)}(1,3,1,1) \\
& + 8K_4^{(r)}(3,1,1,1,1) + 8K_4^{(r)}(1,3,1,1,1) - 4K_3^{(r)}(2,1,2,1) \\
& - 4K_3^{(r)}(1,2,1,2) - 8K_3^{(r)}(2,1,1,2) - 8K_3^{(r)}(2,2,1,1) \\
& + 4K_4^{(r)}(2,1,1,1,2) + 4K_4^{(r)}(1,2,1,2,1) + 16K_4^{(r)}(2,2,1,1,1) \\
& + 4K_4^{(r)}(1,1,3,1,1) + 8K_4^{(r)}(2,1,2,1,1) + 8K_4^{(r)}(1,2,2,1,1) \\
& - 4K_5^{(r)} - 2K_6^{(r)} - 8K_7^{(r)} + 8K_8^{(r)} + 8K_9^{(r)} - 4K_{10}^{(r)} - 8K_{11}^{(r)}.
\end{aligned}
\tag{B7}
$$

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