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Size dependence of virial coefficients for classical gases†

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Abstract. It is known that size dependence of virial coefficients $B_k(N)$ for a system of N molecules can be expressed in terms of virial coefficients for the infinite system. We prove this property by using a graphic approach. A simple method to derive $B_k(N)$ from this approach is described and illustrated.

1. Introduction

In computer simulations of thermodynamic systems, finite numbers of particles are considered. To relate properties of finite systems to those of similar infinite systems, shape and size effects should be considered. These effects may enter into virial coefficients at quite low densities. There have been many studies on the finiteness corrections of the equation of state for classical gases (Oppenheim and Mazur 1957, Lebowitz and Percus 1961, Hubbard 1971a, b, Percus 1982, Kratky 1980, 1985). The size correction of virial coefficients in particular has been calculated extensively by Kratky (1985).

The virial expansion of the pressure P for a classical gas is expressed as

$$P/k_{\mathrm{B}}T = \rho + \sum_{k=2}^{\infty} B_k\rho^k \tag{1}$$

where $\rho = N/V$ is the density of the system. The virial coefficients B_k, in the thermodynamical limit $N \to \infty$, are

$$B_k = -(k-1)\sum_{\alpha} \frac{I(s_\alpha^{(k)})}{S(s_\alpha^{(k)})} \tag{2}$$

where the summation goes over all k-point stars, $S(s_\alpha^{(k)})$ and $I(s_\alpha^{(k)})$ are, respectively, the symmetry number and the graph integral of the αth star of k points $s_\alpha^{(k)}$ (Mayer and Mayer 1940, Uhlenbeck and Ford 1962, Domb 1974, Chen 1984).

In the thermodynamic limit, the graph integrals $I(g)$ depend on the temperature T and the intermolecular potential. For finite systems $I(g)$ will also depend on the shape and the size of the volume. It is very difficult to study the shape correction (or implicit correction) for general systems. With periodic boundary conditions and for $k \leq L/R$ (R is the range of intermolecular interactions and L is the length of the system), graph integrals $I(s_\alpha^{(k)})$ are independent of the size and the shape of the system, and are equal to those for the infinite system. In this case the shape effect does not exist, only the size effect (or explicit finiteness effect) needs to be considered.

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One important result found for the size-dependence virial coefficients $B_k(N)$ is that they can be expressed in terms of virial coefficients for the infinite system, that is

$$B_k(N) = \sum_{(p_1, p_2, \ldots, p_n)} F(N, p_1, p_2, \ldots, p_n) \prod_{i=1}^{n} B_{p_i} \tag{3}$$

where the summation goes over all sets of integers $\{p_i\} = (p_1, p_2, \ldots, p_n)$, with $p_i \geq 2$ such that

$$\sum_{i=1}^{n} (p_i - 1) = k - 1 \tag{4}$$

where $F(N, \{p_i\})$ are polynomials of N^{-1}, and are independent of the intermolecular potential and dimensionality of the system.

The fact that $B_k(N)$ can be expressed in terms of B_i $(2 \leq i \leq k)$ for any k and for any system has been shown by different approaches and several methods of deriving $B_k(N)$ have been studied (Hubbard 1971a, Percus 1982, Kratky 1985). One purpose of this paper is to present a new proof of this property by using a graphic approach, as done in § 2. We follow closely the graph terminology of Domb (1974) and a previous paper (Chen 1984). From this approach a simple method of calculating $F(N, \{p_i\})$ is described in § 3. The coefficients we obtain are compared to those of Kratky (1985). A summary and discussion are given in § 4.

2. Expressing $B_k(N)$ in terms of B_i

The kth virial coefficient $B_k(N)$ for a system of N molecules with periodic boundary conditions and for $k \leq L/R$ can be written formally as (Chen 1984):

$$B_k(N) = \frac{-(k-1)}{N^k} \sum_{(p_1, p_2, \ldots, p_n)} \sum_{m=1}^{n} \frac{(-1)^{m-1}}{m} \sum_{\{g\}}^{(m)} W\{g\} I\{g\} \tag{5}$$

where the first summation is the same as that of (3). The last summation $\Sigma_{\{g\}}^{(m)}$ is taken over all sets of m graphs (m_i of them are graphs g_i) such that when all graphs are decomposed into stars (by cutting at all cutpoints (or cutvertices)), there are a star of p_1 points (denoted $s_{\alpha_1}^{(p_1)}$), a star of p_2 points ($s_{\alpha_2}^{(p_2)}$), etc, and a star of p_n points ($s_{\alpha_n}^{(p_n)}$). Some of the stars may be the same. For the set of m graphs

$$I\{g\} = \prod_{i=1}^{n} I(s_{\alpha_i}^{(p_i)}) \tag{6}$$

and

$$W\{g\} = \frac{m!}{m_1! m_2! \ldots} [w(g_1)]^{m_1} [w(g_2)]^{m_2} \ldots \tag{7}$$

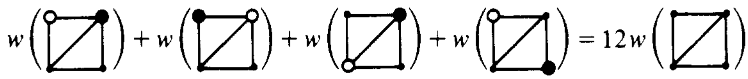
where $w(g_i)$ are weak lattice constants of graph g_i on the complete graph of N points.

It is impractical to calculate $B_k(N)$ from (5) for $k > 6$, because the number of terms involved increases rapidly with k. In what follows we first show that $\Sigma\ W\{g\} I\{g\}$ in (5) can be written as products of virial coefficients for the infinite system. This property simplifies our calculation of $B_k(N)$ significantly.

We first consider some properties of vertex colouring of graphs. For an uncoloured graph of p points, denoted $g_\alpha^{(p)}$ (the αth p-point graph), if q points of the graph are coloured differently then we obtain several different coloured graphs $g_{\alpha,\beta}^{(p,q)}$. Here $g_{\alpha,\beta}^{(p,q)}$ denotes the βth coloured graph obtained from colouring q points of the graph $g_\alpha^{(p)}$. The sum of weak lattice constants of these coloured graphs is nothing but the weak lattice constant of $g_\alpha^{(p)}$ multiplied by the number of permutations of p distinct points taken q at a time, that is

$$\sum_\beta w(g_{\alpha,\beta}^{(p,q)}) = w(g_\alpha^{(p)})p!/(p-q)!. \tag{8}$$

For example, when two points of the four-vertex graph on the right-hand side of (9) are coloured (by ● and ○), we have



(9)

When some points of a graph are coloured, the symmetry number $S(g)$ of the coloured graph is smaller than (or equal to) that of the uncoloured graph, while the weak lattice constant $w(g)$ of the coloured graph is larger than (or equal to) that of the uncoloured graph. They are related by

$$w(g_{\alpha,\beta}^{(p,q)}) = w(g_\alpha^{(p)})S(g_\alpha^{(p)})/S(g_{\alpha,\beta}^{(p,q)}). \tag{10}$$

Combining (8) and (10) we obtain

$$\sum_\beta S^{-1}(g_{\alpha,\beta}^{(p,q)}) = S^{-1}(g_\alpha^{(p)})p!/(p-q)! \tag{11}$$

where $S^{-1}(g) = [S(g)]^{-1}$.

All graphs can be considered as consisting of stars. The constituent stars, considered as blocks, are connected together at cutvertices. The connectivity among blocks can be represented by a block-cutvertex (BC) diagram (Bollobás 1979). Figure 1 shows the BC diagram for a graph of eight blocks. Each block is represented schematically by a loop. For a given BC diagram, we obtain graphs by allocating stars to the blocks. For instance, we allocate a star $s_{\alpha_1}^{(p_1)}$ to block b_1, a star $s_{\alpha_2}^{(p_2)}$ to block b_2, etc. There are many different ways to allocate a star of p points to a block having q cutvertices. Each method of allocation can be described by a coloured graph which is obtained by colouring q points of the p-point star.

Consider a term in $\Sigma_{\{g\}}^{(m)}$, which is described by a set of m graphs $\{g\}$. There are n blocks in the set of m BC diagrams of the graphs. A star of p_1 points $s_{\alpha_1}^{(p_1)}$ is allocated to block b_1 (having q_1 cutvertices) in a way described by the coloured graph $s_{\alpha_1,\beta_1}^{(p_1,q_1)}$, a star of p_2 points $s_{\alpha_2}^{(p_2)}$ is allocated to block b_2 (having q_2 cutvertices) in a way described by $s_{\alpha_2,\beta_2}^{(p_2,q_2)}$, etc. If we reallocate any star $s_{\alpha_i}^{(p_i)}$ in the block b_i in a different way which is described by $s_{\alpha_i,\beta_i'}^{(p_i,q_i)}$, we obtain a new term in the summation $\Sigma_{\{g\}}^{(m)}$. We

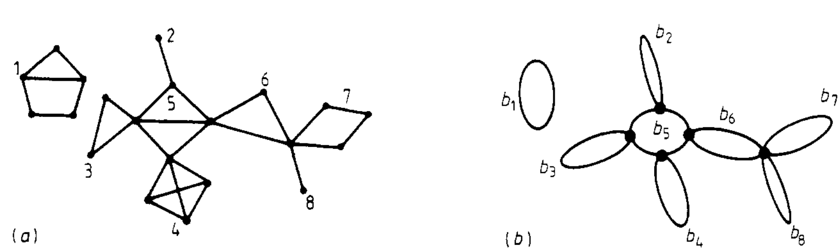


Figure 1. A graph (a) consisting of eight stars and its block-cutvertex diagram (b).

also get a new term if a star $s_{\alpha_i}^{(p_i)}$ is replaced by $s_{\alpha_i'}^{(p_i)}$, a different star having the same number of points. Similarly, if the stars in the blocks are rearranged (permuted), or if the stars are allocated to different sets of m BC diagrams, we obtain new terms in $\Sigma_{\{g\}}^{(m)}$.

Therefore, $\Sigma\ W\{g\}I\{g\}$ can be decomposed into a sequence of summations

$$\sum_{\{g\}}^{(m)} W\{g\}I\{g\} = \sum_{bcd} \sum_{\text{permu}} \sum_{\{\alpha\}} \sum_{\{\beta\}} W\{g\}I\{g\}. \tag{12}$$

Here Σ_{bcd} sums over all sets of m BC diagrams such that the total number of block is n. Σ_{permu} is carried out over all different arrangements of stars $s_{\alpha_i}^{(p_i)}$ in the blocks. Permutations of stars in equivalent blocks do not give new terms (in figure 1 blocks b_2, b_3, b_4 are equivalent, b_7 amd b_8 are equivalent). The third summation is taken over all different stars of p_i points, and the last summation is over all different methods that each star $s_{\alpha_i}^{(p_i)}$ is allocated to the block. Note that, if some of the stars are the same, different $\{\beta\}$ may describe the same term.

For a p-point graph g (coloured or uncoloured), the weak lattice constant of g on the complete graph of N points (denoted K_N) is

$$w(g) = N![(N-p)!S(g)]^{-1} = N_p/S(g). \tag{13}$$

We will use the shorthand notation N_p for $N!/(N-p)!$ hereafter. If all stars that make up the graph are different, the symmetry number of the graph is equal to the product of the symmetry numbers of the constituent coloured stars (the cutvertices are coloured). Hence

$$W\{g\} = m! \prod_{j=1}^{m} N_{v_j} \left(\prod_{i=1}^{n} S(s_{\alpha_i,\beta_i}^{(p_i,q_i)}) \right)^{-1} \tag{14}$$

where v_j is the number of vertices of the jth graph. The denominator $m_1!m_2!\ldots$ in (7) is equal to one as the n stars are assumed to be different. The graph integrals $I\{g\}$ are independent of the structure of the BC diagrams and how the stars are allocated to the block. They are given by (6).

Summing over all $\{\beta\}$ and using (11), we obtain

$$\sum_{\{\beta\}} W\{g\}I\{g\} = m! \prod_{j=1}^{m} N_{v_j} \prod_{i=1}^{n} \frac{p_i!\,I(s_{\alpha_i}^{(p_i)})}{(p_i-q_i)!\,S(s_{\alpha_i}^{(p_i)})}. \tag{15}$$

We then sum over $\{\alpha\}$ to obtain

$$\sum_{\{\alpha\}} \sum_{\{\beta\}} W\{g\}I\{g\} = m! \prod_{j=1}^{m} N_{v_j} \prod_{j=1}^{n} \frac{p_i!\,B_{p_i}}{(1-p_i)(p_i-q_i)!} \tag{16}$$

where we have used (2). For different permutations of the stars in the blocks, the only change in the above equation is that $(p_i-q_i)!$ should be replaced by $(p_i-q_{i'})!$. (The star $s_{\alpha_i}^{(p_i)}$ which was allocated to block b_i is now allocated to block $b_{i'}$.) If we further sum over all different permutations, we obtain

$$\sum_{\text{permu}} \sum_{\{\alpha\}} \sum_{\{\beta\}} W\{g\}I\{g\} = f_{bcd}(N, p_1, p_2, \ldots, p_n) \prod_{i=1}^{n} B_{p_i} \tag{17}$$

where $f_{bcd}(N, \{p_i\})$ depends on the set of m BC diagrams and the set $(p_1, p_2, \ldots, p_n)$. The coefficient $f_{bcd}(N, \{p_i\})$ is a polynomial in N. It can be calculated from (16).

To reach (17) we have assumed that all stars are different, and hence all p_i are different. If some of the stars are the same, the following symmetries should be considered. (i) Some of the m graphs may have higher symmetry and additional symmetry factors should be included in the denominator of (14). (ii) Some of the m graphs may be the same. The factors $m_1!m_2!\ldots$ in (7) should be considered. (iii) Different $\{\beta\}$ or different permutations of stars may describe the same term in $\Sigma_{\{g\}} W\{g\}I\{g\}$.

Consider a set of n stars, n_1' of them are the star s_{α_1}, n_2' of them are the star s_{α_2}, etc. To take all the symmetries into account, it is most convenient to calculate $\Sigma_{\text{permu}} \Sigma_{\{\beta\}} W\{g\}I\{g\}$ by assuming that all stars have different colours (then all stars are different), and dividing the result by $(n_1'!n_2'!\ldots)$, that is

$$\sum_{\text{permu}} \sum_{\{\beta\}} W\{g\}I\{g\} = [n_1'!n_2'!\ldots]^{-1} \sum_{\text{permu}} \sum_{\{\beta\}} \tilde{W}\{g\}I\{g\} \tag{18}$$

where $\tilde{W}\{g\}$ is the constant corresponding to $W\{g\}$ when all stars are considered to have different colours.

If $p_1, p_2, \cdots, p_n$ are not all different, say n_1 of them are p_{i_1}, n_2 of them are p_{i_2}, etc, equation (17) should be modified as

$$\sum_{\text{permu}} \sum_{\{\alpha\}} \sum_{\{\beta\}} = (n_1!n_2!\ldots)^{-1} f_{bcd}(N, p_1, p_2, \ldots, p_n) \prod_{i=1}^{n} B_{p_i}. \tag{19}$$

We obtain (19) from (18) by summing over various stars of p_i points ($\Sigma_{\{\alpha\}}$), having used the multinomial expansion

$$\frac{(x_1 + x_2 + \cdots)^{n_i}}{n_i!} = \sum \left(\frac{x_1^{n_1'}}{n_1'!}\right)\left(\frac{x_2^{n_2'}}{n_2'!}\right) \cdots \tag{20}$$

where the summation extends over all positive integers n_α' such that $n_1' + n_2' + \ldots = n_i$. Equation (19) shows that the total contribution of terms described by the same set of BC diagrams can be expressed in terms of $\Pi_i B_{p_i}$. This property holds true for all sets of BC diagrams and is independent of the model of the system. It follows that $B_k(N)$ can be expressed in terms of virial coefficients for the infinite system.

3. Derivation of $B_k(N)$

The fact that $B_k(N)$ can be expressed in terms of $\Pi_i B_{p_i}$ simplifies our calculations of $B_k(N)$ significantly. We only have to consider one star for each p_i (i.e. one term in $\Sigma_{\{\alpha\}}$). The simplest stars to be considered are the complete graphs K_{p_i} (graphs with p_i points and $p_i(p_i-1)/2$ lines). There is only one term in $\Sigma_{\{\beta\}}$ because only one coloured graph is obtained when a fixed number of points are coloured from a complete graph. Contributions of other stars to $B_k(N)$ are known from the property that contributions of different stars having the same number of points must be proportional to $I(s_{\alpha_i}^{(p_i)})/S(s_{\alpha_i}^{(p_i)})$.

Therefore, (5) is reduced to the form of (3):

$$B_k(N) = \sum_{(p_1, p_2, \ldots, p_n)} \left(N^{-k} D(p_1, p_2, \ldots, p_n) \sum_{m=1}^{n} (-1)^{m-1}(m-1)!\, W_n^{(m)}\right) \prod_{i=1}^{n} B_{p_i} \tag{21}$$

where $(p_1, p_2, \ldots, p_n)$ satisfies (4) and

$$D(p_1, p_2, \ldots, p_n) = (1-k) \prod_{i=1}^{n} \left(\frac{(p_i)!}{1-p_i}\right) \frac{1}{n_1!n_2!\ldots}. \tag{22}$$

The last factor in (22) indicates that if some of the p_i are equal (n_1 of them are p_{i_1}, n_2 of them are p_{i_2}, etc) then the symmetry factor should be included. The only quantities to be determined in (21) are $W_n^{(m)}$. They are given by

$$W_n^{(m)} = \sum_{bcd} \sum_{\text{permu}} \tilde{W}\{K_{p_i}\} \tag{23}$$

where $\tilde{W}\{K_{p_i}\}$ are products of weak lattice constants (on K_N) of the m graphs obtained by allocating a set of n graphs $K_{p_1}, K_{p_2}, \cdots, K_{p_n}$ (all have different colours) to a set of m BC diagrams. The summations are over all different sets of BC diagrams and over all different permutations of K_{p_i} in the blocks.

To illustrate our method consider $n = 3$ for example. All possible sets of BC diagrams having three blocks are shown in figure 2. The first set (a) contains three BC diagrams ($m = 3$), the next two sets (b, c) contain two BC diagrams ($m = 2$) and the last four sets (d)-(g) have only one BC diagram ($m = 1$). There is only one way to allocate three complete graphs $K_{p_1}, K_{p_2}, K_{p_3}$ to the three blocks for sets (a), (d) and (g) (all blocks are equivalent for these sets of BC diagrams). There are three different methods to allocate K_{p_i} to the three blocks for sets (b), (c), (e) and (f) (there are two equivalent blocks for these BC diagrams).

It is straightforward to calculate the $W_3^{(m)}$. They are

$$W_3^{(3)} = N_{p_1} N_{p_2} N_{p_3} / p_1 ! p_2 ! p_3 ! \tag{24}$$

$$W_3^{(2)} = (p_1 p_2 N_{(p_1+p_2-1)} N_{p_3} + p_2 p_3 N_{(p_2+p_3-1)} N_{p_1} + p_1 p_3 N_{(p_1+p_3-1)} N_{p_2}$$
$$+ N_{(p_1+p_2)} N_{p_3} + N_{(p_2+p_3)} N_{p_1} + N_{(p_1+p_3)} N_{p_2}) / p_1 ! p_2 ! p_3 ! \tag{25}$$

$$W_3^{(1)} = [p_1 p_2 p_3 (p_1 + p_2 + p_3 - 2) N_{(p_1+p_2+p_3-2)} + (p_1 p_2 + p_2 p_3 + p_1 p_3) N_{(p_1+p_2+p_3-1)}$$
$$+ N_{(p_1+p_2+p_3)}] / p_1 ! p_2 ! p_3 ! \tag{26}$$

where we have used (13) and (14) (excluding the factor $m!$ which was considered in (21)). The coefficient $F(N, p_1, p_2, p_3)$ in (3) can then be obtained.

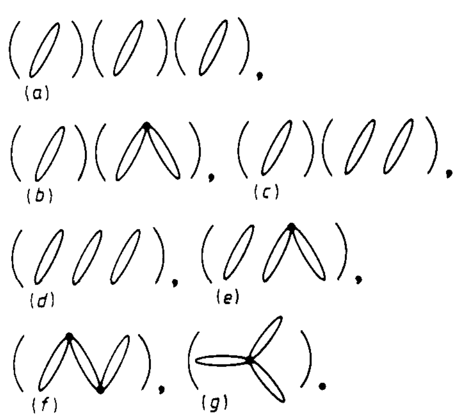


Figure 2. All sets of block-cutvertex (BC) diagrams having three blocks ($n = 3$). Set (a) has three BC diagrams; sets (b) and (c) have two BC diagrams; sets (d)-(g) contain one BC diagram.

We have calculated $F(N, p_1, p_2, \ldots, p_n)$ for general values of $\{p_i\}$ for $n \leq 5$. For $n = 1, 2$ and 3, they are

$$F(N, p_1) = N^{-k} N_{p_1} \tag{27}$$

$$F(N, p_1, p_2) = \frac{(1-k)N^{-k}}{(1-p_1)(1-p_2)} (p_1 p_2 N_{(p_1+p_2-1)} + N_{(p_1+p_2)} - N_{p_1} N_{p_2}) \tag{28}$$

$$F(N, p_1, p_2, p_3) = \frac{(1-k)p_1!p_2!p_3!N^{-k}}{(1-p_1)(1-p_2)(1-p_3)} (2W_3^{(3)} - W_3^{(2)} + W_3^{(1)}) \tag{29}$$

where k and p_i are related by (4) and $W_3^{(m)}$ are given by (24)-(26). The right-hand side of (28) and (29) should be divided by 2 if two of the p_i are equal, and divided by 3! if three p_i are equal. For $n = 4$ and 5, $F(N, \{p_i\})$ are too lengthy to be presented here.

We can use our expressions of $F(N, \{p_i\})$ to check the coefficients $B_k(N)$ previously obtained by Kratky (1985). We find that our results agree with those of Kratky completely for $k \leq 7$. However, there are discrepancies in $B_8(N)$. Our results which are not in agreement with those of Kratky are the following:

$$\begin{aligned}
F(N, 2, 4, 4) &= -112N^{-1} + 3024N^{-2} - 28\,784N^{-3} + 130\,704\,N^{-4} - 303\,072N^{-5} \\
&\quad + 339\,360N^{-6} - 141\,120N^{-7} \\
F(N, 3, 3, 4) &= -126N^{-1} + 3339N^{-2} - 30\,996N^{-3} + 137\,361N^{-4} - 311\,850N^{-5} \\
&\quad + 343\,392N^{-6} - 141\,120N^{-7} \\
F(N, 2, 2, 3, 4) &= 504N^{-1} - 17\,472N^{-2} + 196\,056N^{-3} - 996\,576N^{-4} + 2498\,832N^{-5} \\
&\quad - 2951\,424N^{-6} + 1270\,080N^{-7} \\
F(N, 2, 3, 3, 3) &= 189N^{-1} - 6426N^{-2} + 70\,308N^{-3} - 348\,705N^{-4} + 856\,170N^{-5} \\
&\quad - 994\,896N^{-6} + 423\,360N^{-7} \\
F(N, 2, 2, 2, 2, 4) &= -224N^{-1} + 9520N^{-2} - 123\,872N^{-3} + 701\,792N^{-4} - 1903\,328N^{-5} \\
&\quad + 237\,4512N^{-6} - 1058\,400N^{-7} \\
F(N, 2, 2, 2, 3, 3) &= -504N^{-1} + 21\,000N^{-2} - 266\,364N^{-3} + 1472\,100N^{-4} \\
&\quad - 3909\,528N^{-5} + 4800\,096N^{-6} - 2116\,800N^{-7}.
\end{aligned} \tag{30}$$

Kratky (private communication) has recalculated $B_8(N)$ using his correct formalism. An error in his old calculation which leads to the above discrepancies has been found. Our results, as expected, satisfy the sum rules conjectured and proved by Kratky (1985).

4. Summary and discussion

From properties of weak lattice constants of graphs we have shown that virial coefficients $B_k(N)$ for a finite system with periodic boundary conditions can be expressed in terms of virial coefficients for the infinite system. Contributions of various graphs to $B_k(N)$ are classified according to the block-cutvertex diagrams of the graphs. A simple method for calculating the coefficients $F(N, p_1, p_2, \ldots, p_n)$ for $B_k(N)$ (see equation (3)) has been described and illustrated for general values of $\{p_i\}$.

As $B_k(N)$ reduce to B_k in the thermodynamic limit (3) can be rewritten as

$$B_k(N) = B_k + \sum_{(p_1, p_2, \cdots, p_n)} \sum_{j=1}^{k-1} a^{(j)}_{(p_1, \cdots, p_n)} N^{-j} \sum_{i=1}^{n} B_{p_i}. \tag{31}$$

A general expression $F(N, p_1, p_2, \cdots, p_n)$ can be used to determine some constant $a^{(j)}_{\{p_i\}}$ in $B_k(N)$ for all values of k. For example, (28) can be used to determine $a^{(j)}_{(2,7)}$, $a^{(j)}_{(3,6)}$ and $a^{(j)}_{(4,5)}$ for $B_8(N)$; it can also be used to determine $a^{(j)}_{(2,8)}$, $a^{(j)}_{(3,7)}$, $a^{(j)}_{(4,6)}$ and $a^{(j)}_{(5,5)}$ for $B_9(N)$, etc.

The expressions $F(N, p_1, p_2, \cdots, p_n)$ for general values of $\{p_i\}$ are very complicated and difficult to derive for $n > 5$; but they are not too difficult to calculate for small values of $\{p_i\}$, because many BC diagrams do not contribute to $W^{(m)}_n$ (see equation (23)). To determine $B_7(N)$ and $B_8(N)$, we had to calculate $F(N, \{p_i\})$ for $\{p_i\} = (2, 2, 2, 2, 2, 2)$, $(2, 2, 2, 2, 2, 3)$ and $(2, 2, 2, 2, 2, 2, 2)$, respectively. They are in agreement with those of Kratky (1985).

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