

ON THE CAYLEY GRAPHS OF BOOLEAN FUNCTIONS

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Abstract. A Boolean function is a function $f : \mathbb{Z}_2^n \rightarrow \{0, 1\}$ and we denote the set of all n -variable Boolean functions by BF_n . For $f \in BF_n$ the vector $[W_f(a_0), \dots, W_f(a_{2^n-1})]$ is called the Walsh spectrum of f , where $W_f(a) = \sum_{x \in V} (-1)^{f(x) \oplus ax}$, where V_n is the vector space of dimension n over the two-element field F_2 . In this paper, we shall consider the Cayley graph Γ_f associated with a Boolean function f . We shall also find a complete characterization of the bent Boolean functions of order 16 and determine the spectrum of related Cayley graphs. In addition, we shall enumerate all orbits of the action of automorphism group on the set BF_n .

Keywords: Boolean function; Walsh spectrum; Cayley graph; automorphism group.

1. Introduction

Suppose V_n is the vector space of dimension n over the two-element field F_2 , namely the set of all n -tuples of elements in the field F_2 and \oplus denotes the addition operator over both F_2 and the vector space V_n , where V_n is the vector space of dimension n over the two-element field F_2 . A Sylvester-Hadamard matrix of order 2^n denoted by H_n is defined recursively as

$$(1.1) \quad H_0 = 1, \quad H_1 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \dots, H_n = H_1 \otimes H_{n-1}, \quad n = 1, 2, \dots$$

where \otimes denotes to Kronecker product or Tensor product.

For two vectors $a, b \in \mathbb{Z}_2^n$, where $a = (a_1, \dots, a_n)$ and $b = (b_1, \dots, b_n)$, we define their scalar product as $a \cdot b = a_1 b_1 \oplus \dots \oplus a_n b_n$. A Boolean function f on n -variables is a map from V_n to V_1 . Suppose the vectors $v_0 = (0, 0, \dots, 0)$, $v_1 = (0, 0, \dots, 1), \dots, v_{2^n-1} = (1, 1, \dots, 1)$ are ordered by lexicographical order. The $(0, 1)$ sequence $(f(v_0), f(v_1), \dots, f(v_{2^n-1}))$ is called the truth table of f and BF_n denotes the set of all n -variable Boolean functions.

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2. Walsh spectrum of Boolean functions

For the Boolean function f , the support of f denoted by Ω_f is $\Omega_f = \{x \in \mathbb{Z}_2^n, f(x) = 1\}$. The Walsh transform of an n -variable Boolean function f is an integer valued function $W_f : V_n \rightarrow [-2^n, 2^n]$ defined by

$$W_f(u) = \sum_{x \in F_2^n} f(x)(-1)^{u \cdot x}.$$

For the Boolean function f , the vector $[W_f(0), \dots, W_f(2^n - 1)]$ is called the Walsh spectrum of f , see [4,7,15,16]

Consider the Cayley graph $\Gamma_f = Cay(\mathbb{Z}_2^n, \Omega_f)$, the vertex set of the Cayley graph Γ_f is V_n and two vertices $u, v \in V_n$ are adjacent if and only if $f(u \oplus v) = 1$. This means that $E_f = \{(u, v) | u, v \in V_n, f(u \oplus v) = 1\}$. Since for every $a \in V_n, a \oplus a = 0$, one can verify that for $\Omega_f \subseteq V_n$, we have $x = -x \in \Omega_f$. We denote this class of Cayley graphs constructed by a Boolean function as B-Cayley graphs. In Appendix I, all Boolean functions of order 16 (where $|\Omega_f| = 2$) and the spectra of B- Cayley graphs are given. In Appendix II, the characterization of Boolean functions in terms of spectrum of B-Cayley graph Γ_f associated with f is given. In [5], it is proved that for given Boolean function f , the Walsh spectrum of B-Cayley graph $Cay(\mathbb{Z}_2^n, \Omega_f)$ is equal with $H_n \cdot f$. For example, let $f = [1,0,0,1]$ be a Boolean function. Then the Walsh spectrum of B-Cayley graph $Cay(\mathbb{Z}_2^n, \Omega_f)$ is

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = [0^2, 2^2].$$

For $g = [1,1,1,1]$ we have $H_n \cdot g = [0^3, 4]$ and for $h = [0,0,1,1]$ we have $H_n \cdot h = [-2, 0^2, 2]$.

Theorem 2.1. *Let f be a Boolean function whose related B-Cayley graph Γ_f is a bipartite regular graph with exactly three distinct eigenvalues and -2 is the smallest eigenvalue. Then $f \in F_2$ and $f = (0, 1, 1, 0)$.*

Proof. Suppose f satisfies in above conditions. We can suppose the spectrum of Γ_f is $Spec(\Gamma_f) = \{[-2]^{m_1}, [\lambda_1]^{m_2}, [\lambda_2]^{m_3}\}$. Since, Γ_f is bipartite, $\lambda_1 = 0$ and $\lambda_2 = 2$, see [6]. On the other hand, Γ_f is regular and so $m_3 = m_1 = 1$. If $\lambda_1, \dots, \lambda_n$ are eigenvalues of a graph, it is a well-known fact that $\sum_{i=1}^n \lambda_i^2 = 2m$. This implies that $2m = 8$ and so $m=4$. Since Γ_f is 2-regular, it is isomorphic with the cycle graph C_4 . In addition, suppose $V_n = \{00, 01, 10, 11\}$ is the set of vertices of a square as depicted in Figure 2.1. Then we have $00 + 01 = 01 \in \Omega_f$ and $11 + 01 = 10 \in \Omega_f$. Hence, $f(00) = f(11) = 0$ and $f(01) = f(10) = 1$ which yields that $f=(0,1,1,0)$. \square

Example 1. Suppose $V_3 = \{000, 001, 010, 100, 011, 101, 110, 111\}$. If $a = 110$ and $f = (0,0,0,0,1,1,1,10)$, then the related Walsh spectrum is reported in Table 1.

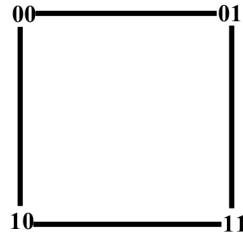


FIG. 2.1: The labeling of vertices of a square.

Table 2.1: The Walsh spectrum of $f = (0,0,0,0,1,1,1,1,1,0)$.

x	$a.x$	f	$f(x) \oplus a.x$	$(-1)^{f(x) \oplus a.x}$	$W(f)(a)$
000	0	0	0	1	0
001	0	0	0	1	
010	1	0	1	-1	
100	1	0	1	-1	
011	1	1	0	1	
101	1	1	0	1	
110	0	1	1	-1	
111	0	1	1	-1	

3. Coloring the B-Cayley graphs

Let G be a group and X a nonempty set. An action of G on X is denoted by $(G|X)$ and X is called a G -set. It induces a group homomorphism φ from G into the symmetric group S_X on X , where $\varphi(g)x = gx$ for all $x \in X$. The orbit of x will be indicated as x^G and defines as the set of all $\varphi(g)x, g \in G$. Suppose g is a permutation of n symbols with exactly λ_1 orbits of size 1, λ_2 orbits of size 2, \dots , and λ_n orbits of size n . Then the cycle type of g is defined as $1^{\lambda_1} 2^{\lambda_2} \dots n^{\lambda_n}$. Let $G = \mathbb{Z}_2^n$ and $f \in BF_n$ is a Boolean function. In [17] it is showed that the automorphism group $\text{Aut}(G)$ acts on the set BF_n as follows:

$$\forall x_i \in \mathbb{Z}_2^n, \alpha \in \text{Aut}(G) : f^\alpha(x_i) = f(\alpha(x_i)).$$

Hence, the conjugacy class of f under this action can be computed directly from the definition and it is $[f] = f^{\text{Aut}(G)} = \{f^\alpha : \alpha \in \text{Aut}(G)\}$.

Let x_1, x_2, \dots, x_n be distinct colors. Denote by $C_{m,n}$ the set of all functions $f: \{1, 2, \dots, m\} \rightarrow \{x_1, x_2, \dots, x_n\}$. The action of $p \in S_m$ induced on $C_{m,n}$ is defined by $\hat{p}(f) = f \circ p^{-1}, f \in C_{m,n}$. Treating the colors x_1, x_2, \dots, x_n that comprise the range of $f \in C_{m,n}$ as independent variables the weight of f is $W(f) = \prod_i f(i)$. Evidently, $W(f)$ is a monomial of (total) degree m . Suppose G is a permutation group of degree $m, \hat{G} = \{\hat{p} : p \in G\}, \hat{p}$ is as defined above. Let p_1, p_2, \dots, p_t be the distinct orbits of \hat{G} . The weight of p_i is the common value of $W(f), f \in p_i$. The sum of the weights of the orbits is the pattern inventory

$$W_G(x_1, x_2, \dots, x_n) = \sum_{i=1}^t w(p_i).$$

Theorem 2 [14]. (Pólya’s Theorem) If G is a subgroup of S_m , then the pattern inventory for the orbits of $C_{m,n}$ modula \hat{G} is

$$W_G(x_1, x_2, \dots, x_n) = \frac{1}{|G|} \sum_{p \in G} M_1^{C_1(p)} M_2^{C_2(p)} \dots M_m^{C_m(p)},$$

where $M_k = x_1^k + x_2^k + \dots + x_n^k$, the k^{th} power sum of the x ’s, and $(C_1(p), \dots, C_m(p))$ is the cycle type of the permutation p . We now introduce the notion of cycle index. Let G be a permutation group. The cycle index of G acting on X is the polynomial $Z(G, X)$ over Q in terms of in determinates $x_1, x_2, \dots, x_t, t = |X|$, defined by

$$(3.1) \quad Z(G, X) = \frac{1}{|G|} \sum_{C \in \text{Conj}(G)} |C| \prod_{i=1}^t x_i^{C_i(g_c)},$$

where $\text{Conj}(G)$ is the set of all conjugacy classes of G with representatives $g_C \in C$.

Let us consider the number of ways of assigning one of the colors green or blue to each corner of a square. Since there are two colors and four corners there are basically $2^4 = 16$ possibilities. However, when we take account of the symmetry of the square we see that some of the possibilities are essentially the same. For example, the first coloring, as in Figure 2 is the same as the second one after rotation through 180° .

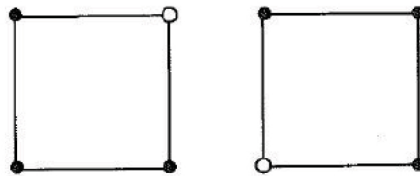


FIG. 3.1: Two indistinguishable colorings.

From above, we regard two colorings as being indistinguishable if one is transformed into the other by symmetry of the square. It is easy to find the distinguishable colorings (in this example) by trial and error: there are just six of them, as shown in the Figure 3.

Now consider a n bead necklace. Let us each corner of it to be colored green or blue. How many different colorings are there? One could argue for 2^n . For example,

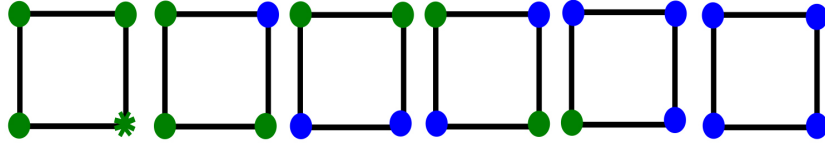


FIG. 3.2: The six distinguishable colorings.

if $n = 4$ and the corners are numbered 0,1,2,3 in clockwise order around the necklace, then there are only 6 ways of coloring the necklace $RRRR$, $BBBB$, $RRRB$, $RBBB$, $RRBB$ and $RBRB$, see Figure 4. On the other hand, all colorings $RBBB$, $BRBB$, $BBRB$, $BBBR$ are in the same class. We say that they are equivalent. In other words, the number of all non-equivalent colorings is six. This relation introduces an equivalence relation. All equivalences are

$$(3.2) \quad \begin{aligned} & \{BBBB\}, \\ & \{BBBR\}, \{BBRB\}, \{BRBB\}, \{RBBB\}, \\ & \{BBRR\}, \{BRRB\}, \{RBBR\}, \{RRBB\}, \\ & \{BRBR\}, \{RBRB\}, \\ & \{BRRR\}, \{RBRR\}, \{RRBR\}, \{RRRB\}, \\ & \{RRRR\}. \end{aligned}$$

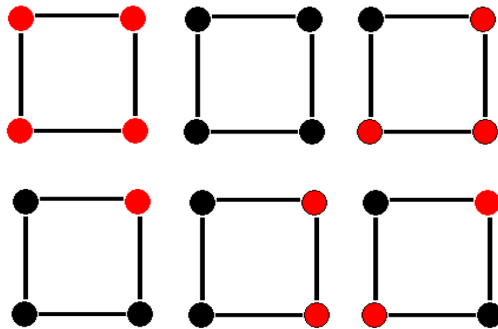


FIG. 3.3: Distinguish colorings of 4 bead necklace.

Hence, any Boolean function can be considered as a coloring of a hyper cube by two colors 0 and 1. The different colorings yields that there are 2^{2^n} Boolean functions on n variables.

Definition 3.1. Consider the Boolean function f and B-Cayley $\Gamma_f = Cay(\mathbb{Z}_2^n, \Omega_f)$. Then f is permutational symmetric (PS) if and only if for any $(x_1, \dots, x_n) \in V_n$, we have $f(\alpha(x_1, \dots, x_n)) = f(x_1, \dots, x_n)$, for any $\alpha \in \text{Aut}(\Gamma_f)$.

Note that there are $2n$ different input values corresponding to a function. From the above definition, it is clear that for PS functions, the function f possesses the

same value corresponding to each of the subsets generated from the automorphism group. As example, for $n = 4$, one gets the following partitions:

$$(3.3) \quad \begin{aligned} &\{(0, 0, 0, 0)\}, \\ &\{(0, 0, 0, 1)\}, \{(0, 0, 1, 0)\}, \{(0, 1, 0, 0)\}, \{(1, 0, 0, 0)\}, \\ &\{(0, 0, 1, 1)\}, \{(0, 1, 1, 0)\}, \{(1, 0, 0, 1)\}, \{(1, 1, 0, 0)\}, \\ &\{(0, 1, 0, 1)\}, \{(1, 0, 1, 0)\}, \\ &\{(0, 1, 1, 1)\}, \{(1, 0, 1, 1)\}, \{(1, 1, 0, 1)\}, \{(1, 1, 1, 0)\}, \\ &\{(1, 1, 1, 1)\}, \end{aligned}$$

Therefore, there are six different subsets which partition the 16 input patterns and any 4-variable PS Boolean function can have a specific value corresponding to each subset. If we replace in Eq.(3.3) 0 by R and 1 by B , then all above partitions are corresponded to the different colorings of the 2-cube or cycle C_4 as given in Eq.(3.2). Hence, there is a 1-1 correspondence between non-equivalent colorings of a n -cube and 4-variable PS Boolean functions. Let us denote

$$\Lambda_n(x_1, \dots, x_n) = \{f(\alpha(x_1, \dots, x_n)) = f(x_1, \dots, x_n) : \alpha \in \text{Aut}(\Gamma_f)\}$$

that is, the orbit of (x_1, \dots, x_n) under the action of $\text{Aut}(\Gamma_f)$ on V_n . It is clear that $\Lambda_n(x_1, \dots, x_n)$ generates a partition in the set V_n . Let $\lambda_n = |\Lambda_n(x_1, \dots, x_n)|$. It is clear that there are 2^{λ_n} number of n -variable PS Boolean functions. Let Γ_f is B-Cayley graph constructed by given Boolean function f . From Polyá's Theorem, we get that

$$\lambda_n = \frac{1}{|\text{Aut}(\Gamma_f)|} \sum_{C \in \text{Conj}(G)} |C| \prod_{i=1}^t 2^{C_i(g_c)}$$

in which every variable in Eq. (3.1) is replaced by 2. Hence, we proved the following theorem.

Theorem 3.1. *For given Boolean function f , the number of PS Boolean functions is*

$$\lambda_n = \frac{1}{|\text{Aut}(\Gamma_f)|} \sum_{C \in \text{Conj}(G)} |C| \prod_{i=1}^t 2^{C_i(g_c)}.$$

4. Application in chemistry: Enumeration of hetero-fullerenes

Enumeration of chemical compounds has been accomplished by various methods. The Polyá-Redfield theorem [14] has been a standard method for combinatorial enumerations of graphs, polyhedra, chemical compounds, and so forth. Combinatorial enumerations have found a wide-ranging application in chemistry, since chemical structural formulas can be regarded as graphs or three-dimensional objects, see [9]. Ghorbani et al. in a series of papers in [1-3,10-12] enumerated the number of hetero-fullerenes with different orders.

The fullerene era was started in 1985 with the discovery of a stable C_{60} cluster and its interpretation as a cage structure with the familiar shape of a soccer ball, by Kroto and his co-authors, see [8,13]. The well-known fullerene, the C_{60} molecule, is a closed-cage carbon molecule with three-coordinate carbon atoms tiling the spherical or nearly spherical surface with a truncated icosahedral structure formed by 20 hexagonal and 12 pentagonal rings. Such molecules made up entirely of n carbon atoms and having 12 pentagonal and $(n/2 - 10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20, see [22-30]. As an application of Pólya-Theorem in fullerenes, in Appendix III, the number of hetero-fullerenes of molecule C_{60} is given.

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Appendix I

Boolean functions of order 16 where $\Omega_f = 2$ and spectra of their B -Cayley graphs.

$f := [1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 2, 0, 2, 0, 2, 0, 2, 0, 2, 0, 2, 0, 2, 0]
 $f := [1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 2, 0, 0, 2, 2, 0, 0, 2, 2, 0, 0, 2, 2, 0, 0]
 $f := [1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 0, 2, 2, 0, 0, 2, 2, 0, 0, 2, 2, 0, 0, 2]
 $f := [1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 2, 2, 2, 0, 0, 0, 0, 2, 2, 2, 2, 0, 0, 0, 0]
 $f := [1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 2, 0, 0, 2, 0, 2, 0, 2, 0, 2, 0, 2, 0, 2]
 $f := [1, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 2, 0, 0, 0, 0, 2, 2, 2, 2, 0, 0, 0, 0, 2, 2]
 $f := [1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 0, 2, 0, 2, 2, 0, 2, 0, 0, 2, 0, 2, 2, 0]
 $f := [1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 2, 2, 2, 2, 2, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0]
 $f := [1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 2, 0, 2, 0, 2, 0, 2, 0, 2, 0, 2, 0, 2, 0]
 $f := [1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0]$ Spec(G) := [2, 2, 0, 0, 2, 2, 0, 0, 0, 0, 2, 2, 0, 0, 2, 2]
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 $f := [1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0]$ Spec(G) := [2, 0, 2, 0, 0, 2, 0, 2, 0, 2, 0, 2, 0, 2, 0, 2]
 $f := [1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0]$ Spec(G) := [2, 2, 0, 0, 0, 0, 2, 2, 0, 0, 2, 2, 2, 2, 0, 0]
 $f := [1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1]$ Spec(G) := [2, 0, 0, 2, 0, 2, 2, 0, 0, 2, 2, 0, 2, 0, 0, 2]
 $f := [0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 0, -2, 2, 0, 0, -2, 2, 0, 0, -2, 2, 0, 0, -2]
 $f := [0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, -2, 0, 0, 2, -2, 0, 0, 2, -2, 0, 0, 2, -2, 0, 0]
 $f := [0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 2, 0, 0, -2, 0, -2, 2, 0, 2, 0, 0, -2, 0, -2]
 $f := [0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, -2, 2, -2, 0, 0, 0, 0, 2, -2, 2, -2, 0, 0, 0, 0]
 $f := [0, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 0, -2, 0, -2, 2, 0, 2, 0, 0, -2, 0, -2, 2, 0]
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 $f := [0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, -2, 0, 0, 2, -2, 0, 0, 0, 0, 2, -2, 0, 0, 2, -2]
 $f := [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 2, 0, 0, -2, 0, -2, 0, -2, 0, -2, 2, 0, 2, 0]
 $f := [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0]$ Spec(G) := [2, -2, 2, -2, 0, 0, 0, 0, 0, 0, 0, 0, 2, -2, 2, -2]
 $f := [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0]$ Spec(G) := [2, 0, 0, -2, 0, -2, 2, 0, 0, -2, 2, 0, 2, 0, 0, -2]
 $f := [0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0]$ Spec(G) := [2, -2, 0, 0, 0, 2, -2, 0, 0, 2, -2, 2, -2, 0, 0, 0]
 $f := [0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, -2, 0, 2, 0, -2, 0, 2, 0, -2, 0, 2, 0, -2, 0]
 $f := [0, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 2, 0, 0, 0, 0, -2, -2, 2, 2, 0, 0, 0, 0, -2, -2]
 $f := [0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 0, -2, 0, 2, -2, 0, 2, 0, 0, -2, 0, 2, -2, 0]
 $f := [0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 2, -2, -2, 0, 0, 0, 0, 2, 2, -2, -2, 0, 0, 0, 0]
 $f := [0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, -2, 0, 0, 2, 0, -2, 2, 0, -2, 0, 0, 2, 0, -2]
 $f := [0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 2, 0, 0, 2, 2, 0, 0, 0, 0, -2, -2, 0, 0, -2, -2]
 $f := [0, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 0, -2, 2, 0, 0, -2, 0, 2, -2, 0, 0, 2, -2, 0]
 $f := [0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0]$ Spec(G) := [2, 2, -2, -2, 2, 2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0]
 $f := [0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0]$ Spec(G) := [2, 0, -2, 0, 2, 0, -2, 0, 0, 2, 0, -2, 0, 2, 0, -2]
 $f := [0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0]$ Spec(G) := [2, 2, 0, 0, 0, 0, -2, -2, 0, 0, 0, -2, -2, 2, 2, 0, 0]
 $f := [0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0]$ Spec(G) := [2, 0, 0, -2, 0, 2, -2, 0, 0, 2, -2, 0, 2, 0, 0, -2]
 $f := [0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0]$ Spec(G) := [2, 2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 2, -2]

$f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, -2, 0, 0, 0, 0, 2, -2, 0, 0, -2, 2, -2, 2, 0, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, -2, 0, 0, 2, 0, -2, 0, -2, 0, 2, -2, 0, 2, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0]$ Spec(G) := [2, -2, -2, 2, 0, 0, 0, 0, 0, 0, 0, -2, 2, 2, -2]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0]$ Spec(G) := [2, 0, 0, 2, -2, 0, 0, -2, 0, -2, -2, 0, 0, 2, 2, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0]$ Spec(G) := [2, -2, 0, 0, -2, 2, 0, 0, 0, 0, -2, 2, 0, 0, 2, -2]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0]$ Spec(G) := [2, 0, -2, 0, -2, 0, 2, 0, 0, -2, 0, 2, 0, 2, 0, -2]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1]$ Spec(G) := [2, -2, -2, 2, -2, 2, 2, -2, 0, 0, 0, 0, 0, 0, 0, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 2, 0, 2, 0, 2, 0, -2, 0, -2, 0, -2, 0, -2, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 2, 0, 0, 2, 2, 0, 0, -2, -2, 0, 0, -2, -2, 0, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 0, 2, 2, 0, 0, 2, -2, 0, 0, -2, -2, 0, 0, -2]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0]$ Spec(G) := [2, 2, 2, 2, 0, 0, 0, 0, -2, -2, -2, -2, 0, 0, 0, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0]$ Spec(G) := [2, 0, 2, 0, 2, 0, 2, 0, -2, 0, -2, 0, 0, -2, 0, -2]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0]$ Spec(G) := [2, 2, 0, 0, 0, 0, 2, 2, -2, -2, 0, 0, 0, -2, -2]
 $f := [0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1]$ Spec(G) := [2, 0, 0, 2, 0, 2, 2, 0, -2, 0, 0, -2, 0, -2, -2, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, 0, -2, 2, 0, 0, -2, -2, 0, 0, 2, -2, 0, 0, 2]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0]$ Spec(G) := [2, -2, 0, 0, 2, -2, 0, 0, -2, 2, 0, 0, -2, 2, 0, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0]$ Spec(G) := [2, 0, 2, 0, 0, -2, 0, -2, -2, 0, -2, 0, 0, 2, 0, 2]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0]$ Spec(G) := [2, -2, 2, -2, 0, 0, 0, 0, -2, 2, -2, 2, 0, 0, 0, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0]$ Spec(G) := [2, 0, 0, -2, 0, -2, 2, 0, -2, 0, 0, 2, 0, 2, -2, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0]$ Spec(G) := [2, -2, 0, 0, 0, 0, 2, -2, -2, 2, 0, 0, 0, -2, 2]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0]$ Spec(G) := [2, 0, -2, 0, 2, 0, -2, 0, -2, 0, 2, 0, -2, 0, 2, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0]$ Spec(G) := [2, 2, 0, 0, 0, 0, -2, -2, -2, 0, 0, 0, 0, 2, 2, 2]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0]$ Spec(G) := [2, 0, 0, -2, 0, 2, -2, 0, -2, 0, 0, 2, 0, -2, 2, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0]$ Spec(G) := [2, 2, -2, -2, 0, 0, 0, 0, -2, -2, 2, 2, 0, 0, 0, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0]$ Spec(G) := [2, 0, -2, 0, 0, 2, 0, -2, -2, 0, 2, 0, 0, -2, 0, 2]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1]$ Spec(G) := [2, 0, -2, 0, 0, 2, 0, -2, -2, 0, 2, 0, 0, -2, 0, 2]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0]$ Spec(G) := [2, 0, 0, 2, 0, -2, -2, 0, -2, 0, 0, -2, 0, 2, 2, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1]$ Spec(G) := [2, -2, 0, 0, 0, 0, -2, 2, -2, 2, 0, 0, 0, 0, 2, -2]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0]$ Spec(G) := [2, 0, -2, 0, 0, -2, 0, 2, -2, 0, 2, 0, 0, 2, 0, -2]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0]$ Spec(G) := [2, 0, 2, 0, -2, 0, -2, 0, -2, 0, -2, 0, 2, 0, 2, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0]$ Spec(G) := [2, 2, 0, 0, -2, -2, 0, 0, -2, -2, 0, 0, 2, 2, 0, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0]$ Spec(G) := [2, 0, 0, 2, -2, 0, 0, -2, -2, 0, 0, -2, 2, 0, 0, 2]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0]$ Spec(G) := [2, 0, 0, -2, -2, 0, 0, 2, -2, 0, 0, 2, 2, 0, 0, -2]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1]$ Spec(G) := [2, -2, 0, 0, -2, 2, 0, 0, -2, 2, 0, 0, 2, -2, 0, 0]
 $f := [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1]$ Spec(G) := [2, 0, -2, 0, -2, 0, 2, 0, -2, 0, 2, 0, 2, 0, 2, 0, -2, 0]

Appendix II: All Boolean functions of order 16.

Boolean function f	Eigenvalues
(0,1,0,0,0,0,0,0,0,1,0,0,0,0,0)	$-2^4, 0^8, 2^4$
(0,1,1,1,0,0,0,0,0,0,0,0,0,0,0)	$-1^{12}, 3^4$
(0,1,1,0,1,0,0,0,0,0,0,0,0,0,0)	$-3^2, -1^6, 1^6, 3^2$
(0,1,0,0,1,1,0,0,0,0,0,0,0,0,0)	$-1^{12}, 3^4$
(0,1,1,1,1,0,0,0,0,0,0,0,0,0,0)	$-2^6, 0^6, 2^2, 4^2$
(0,1,1,0,0,1,1,0,0,0,0,0,0,0,0)	$-4^2, 0^{12}, 4^2$
(0,1,1,0,0,0,1,0,0,0,0,0,0,1,0)	$-4, -2^4, 0^6, 2^4, 4$
(0,1,1,1,1,1,0,0,0,0,0,0,0,0,0)	$-3^2, -1^8, 1^4, 5^2$
(0,1,1,1,1,0,0,0,1,0,0,0,0,0,0)	$-3^2, -1^8, 1^4, 5^2$
(0,1,1,1,1,0,0,0,1,0,0,0,0,0,0)	$-3^3, -1^6, 1^4, 3^2, 5$
(0,1,1,0,1,0,0,1,0,1,0,0,0,0,0)	$-5, -3, -1^6, 1^6, 3, 5$
(0,1,0,1,1,0,0,0,1,0,0,0,0,0,1)	$-3^5, 1^{10}, 5$
(0,1,1,1,1,1,0,0,1,0,0,0,0,0,0)	$-4, -2^5, 0^6, 2^2, 4, 6$
(0,1,1,1,1,0,0,0,1,0,0,0,1,0,0)	$-2^9, 2^6, 6$
(0,1,1,1,1,0,0,0,1,0,0,0,0,1,0)	$-4^2, -2^3, 2^4, 0^6, 6$
(0,1,0,0,1,0,1,0,1,0,1,0,0,1,0)	$-6, -2^3, 0^8, 2^3, 6$
(0,1,0,0,0,0,1,1,0,0,1,1,1,0,0)	$-2^6, 0^8, 6^2$
(0,1,1,1,1,1,1,0,0,0,0,0,0,0,0)	$-1^{14}, 7^2$
(0,1,1,1,1,1,1,0,1,0,0,0,0,0,0)	$-3^2, -1^7, 1^4, 5, 7$
(0,1,1,1,1,1,0,0,1,1,0,0,0,0,0)	$-5, -1^{11}, 3^3, 7$
(0,1,1,1,1,1,0,0,1,0,1,0,0,0,0)	$-3^4, -1^5, 1^4, 3^2, 7$
(0,1,1,1,1,1,0,0,1,0,0,0,0,0,1)	$-5, -3^2, -1^5, 1^6, 3, 7$
(0,0,0,0,0,0,0,0,1,0,1,1,1,1,1)	$-7, -1^7, 1^7, 7$
(0,1,1,1,1,1,1,1,0,1,0,0,0,0,0)	$-2^7, 0^7, 6, 8$
(0,1,1,1,1,1,1,0,1,1,0,0,0,0,0)	$-4, -2^6, 0^5, 2^2, 4, 8$
(0,1,1,1,1,1,1,0,1,0,0,0,0,0, 1)	$-4^3, 0^{11}, 4, 8$
(0,1,1,1,1,1,0,0,1,1,0,0,0,0,1)	$-6, -2^4, 0^7, 2^3, 8$
(0,1,0,1,1,0,1,0,1,0,1,0,0,1,0,1)	$-8, 0^{14}, 8$
(0,1,1,1,1,1,1,1,1,0,0,0,0,0,0)	$-3^3, -1^8, 1^3, 5, 9$
(0,1,1,1,1,1,1,0,1,0,1,1,0,0,0)	$-3^4, -1^6, 1^3, 3^2, 9$
(0,1,1,1,1,1,1,0,1,1,0,0,0,0,1)	$-5, -3^2, -1^6, 1^5, 3, 9$
(0,1,1,0,1,0,1,1,1,0,1,1,0,0,0,1)	$-3^6, 1^9, 9$
(0,1,1,0,0,1,1,1,1,0,0,1,1,0,0,1)	$-7, -1^8, 1^6, 9$
(0,1,0,1,1,1,1,0,1,1,0,1,0,0,0,1)	$-3^6, 1^9, 9$
(0,1,1,1,1,1,1,1,1,0,1,0,0,0,0)	$-4, -2^6, 0^6, 2, 4, 10$
(0,1,1,1,1,1,1,0,1,1,0,1,0,1,0)	$-2^{10}, 2^5, 10$
(0,1,1,1,1,1,1,0,1,1,0,0,0,0,1)	$-6, -2^4, 0^8, 2^2, 10$
(0,1,1,1,1,1,1,0,1,0,1,0,1,0, 1)	$-4^2, -2^4, 0^6, 2^3, 10$
(0,1,1,1,1,1,1,1,1,1,1,1,0,0,0)	$-5, -1^{12}, 3^2, 11$
(0,1,1,1,1,1,1,1,1,1,1,0,1,0,0)	$-3^4, -1^6, 1^4, 3, 11$
(0,1,1,1,1,1,1,0,1,1,1,0,0,0,1)	$-5, -3^2, -1^6, 1^6, 11$
(0,1,1,1,1,1,1,1,1,1,1,1,1,0,0)	$-4, -2^6, 0^6, 2, 12$
(0,1,1,1,1,1,1,0,1,1,1,0,0,1,1)	$-4^3, 0^{12}, 12$
(0,1,1,1,1,1,1,1,1,1,1,1,1,0,0)	$-3^3, -1^8, 1^4, 13$
(0,1,1,1,1,1,1,1,0,1,1,1,1,1,1)	$-2^7, 0^8, 14$
(0,1,1,1,1,1,1,1,1,1,1,1,1,1,1)	$-1^{15}, 15$

Appendix III: The number of $C_{60-k}B_k$ molecules.

$k, 60 - k$	Number of hetero-fullerenes $C_{60-k}B_k$
0,60	1
1,59	1
2,58	37
3,57	577
4,56	8236
5,55	91030
6,54	835476
7,53	6436782
8,52	42650532
9,51	246386091
10,50	1256602779
11,49	5711668755
12,48	23322797475
13,47	86114390460
14,46	289098819780
15,45	886568158468
16,44	2493474394140
17,43	6453694644705
18,42	15417163018725
19,41	34080036632565
20,40	69864082608210
21,39	133074428781570
22,38	235904682814710
23,37	389755540347810
24,36	600873146368170
25,35	865257299572455
26,34	1164769471671687
27,33	1466746704458899
28,32	1728665795116244
29,31	1907493251046152
30,30	1971076398255692