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Extremal Λ-Inequalities for Ising Models with Pair Interactions

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Abstract. The inequalities for spin correlation functions of ferromagnetic Ising models with pair interactions derived in a previous paper are studied in more detail. It is shown that each of these inequalities is a positive linear combination of a finite number of "extremal" inequalities, which can in principle be determined and of which a number of examples is given.

1. Introduction

In a recent paper [1], to be referred to as I, two classes of relations between spin correlation functions of Ising models with pair interactions were studied. One of these classes consists of correlation-function inequalities, for ferromagnetic Ising models, of the type $\sum_{B\subset A} \lambda_B\langle\sigma_B\rangle\langle\sigma_B\sigma_D\rangle \geqq 0$, where A is an arbitrary set of spins of the system, D a subset of A, and $\{\lambda_B\}_{B\subset A}$ a set of real numbers which are independent of the coupling parameters of the system. In this paper this class of correlation-function inequalities (called Λ-inequalities) will be studied in more detail. In particular, we shall show that for every set of spins A with $|A|$ even there is a unique finite set of Λ-inequalities with $D=A$ from which all other Λ-inequalities with $D=A$ which are generally valid (i.e. valid for all Ising models containing the set A) can be derived by taking positive linear combinations. The method by which these extremal Λ-inequalities can, at least in principle, be found will be sketched. Examples of extremal Λ-inequalities valid for arbitrary sets A will be derived, and for the cases $|A|=4$ and $|A|=6$ all extremal Λ-inequalities will be given. The generalization to the more general case $D\subset A$ will form the subject of a subsequent paper.

2. Definitions and Notation

As in I, a *graph* G is defined as a pair $(V(G), E(G))$, where $V(G)$ is a set of elements called vertices and $E(G)$ a set of unordered pairs $\{v, v'\}$ of distinct vertices, called edges. G is *finite* if $V(G)$ and $E(G)$ are finite.

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An *Ising model* on a finite graph G is defined as a triple $(G, \mathscr{S}, K)$, where $\mathscr{S}$ is the set of all functions $\sigma: V(G) \to \{-1, 1\}$ and K a complex function on $E(G)$. The spin variable σ_v is the value of σ at the vertex v, the coupling parameter K_e is the value of K at the edge e. An Ising model is called *ferromagnetic* if $K_e \geqq 0$ for all $e \in E(G)$.

For any set $A \subset V(G)$ we define

$$\sigma_A = \prod_{v \in A} \sigma_v; \tag{1}$$

for $A = \emptyset$ we have $\sigma_\emptyset = 1$.

The Hamiltonian of the Ising model $(G, \mathscr{S}, K)$ is defined by

$$H(\sigma) = -\sum_{e \in E(G)} K_e \sigma_e, \qquad \sigma \in \mathscr{S}, \tag{2}$$

the unnormalized and normalized *spin correlation functions* (σ_A) and $\langle \sigma_A \rangle$, respectively, for any set $A \subset V(G)$ by

$$\begin{aligned} (\sigma_A) &= \sum_{\sigma \in \mathscr{S}} \sigma_A e^{-H(\sigma)}, \\ \langle \sigma_A \rangle &= (\sigma_A) Z^{-1} \quad \text{if} \quad Z \neq 0, \end{aligned} \tag{3}$$

where Z, the canonical partition function, is defined by $Z = (1)$; we have taken $kT = 1$. Since the Hamiltonian is quadratic in the σ_v, the correlation function (σ_A) vanishes if $|A|$ is odd. Therefore, we shall henceforth consider only correlation functions (σ_A) for *even* sets A, i.e. for sets with $|A|$ even. The family of all even subsets of A will be denoted by $\mathscr{P}_e(A)$.

Consider a graph G and a set $A \subset V(G)$. By $\pi(A, G)$ we denote the partition of A *induced* by G, i.e. the partition in which two vertices of A are in the same block if and only if they are in the same connected component of G. If H is a *spanning subgraph* of G, i.e. if $V(H) = V(G)$, $E(H) \subset E(G)$, the partition $\pi(A, H)$ is a *refinement* of $\pi(A, G)$, i.e., the blocks of $\pi(A, H)$ are subsets of those of $\pi(A, G)$. The set of all *even* partitions of A (i.e. partitions of A into even subsets) is denoted by Π_A^e, and the set of all even partitions of A induced by spanning subgraphs of G by $\Pi_A^e(G)$. We furthermore define for any set $B \subset A$ and any partition $\pi \in \Pi_A^e$

$$\eta_\pi(B) = \begin{cases} 1 & \text{if the number of elements of } B \text{ in every block of } \pi \text{ is even} \\ 0 & \text{otherwise.} \end{cases}$$

Observe that $\eta_\pi(A \backslash B) = \eta_\pi(B)$. In I we have derived the following theorem.

Theorem 1 (= Theorem 2 of I). *If A is an even set of vertices of a finite graph G and $\{\lambda_B\}_{B \in \mathscr{P}_e(A)}$ a family of real numbers such that $\lambda_B = \lambda_{A \backslash B}$ for all $B \in \mathscr{P}_e(A)$, then*

$$\sum_{B \in \mathscr{P}_e(A)} \lambda_B (\sigma_B)(\sigma_{A \backslash B}) \geqq 0 \tag{4}$$

for every ferromagnetic Ising model on G if and only if

$$\sum_{B \in \mathscr{P}_e(A)} \eta_\pi(B) \lambda_B \geqq 0 \tag{5}$$

for every partition $\pi \in \Pi_A^e(G)$. The equality sign in Eq. (4) *holds for every Ising model on G if and only if the equality sign in Eq.* (5) *holds for every partition $\pi \in \Pi_A^e(G)$.*

Every inequality of the form Eq. (4) will be called a Λ-inequality (with respect to Λ). The set of Eq. (5) is a finite set of linear inequalities. In the following section we shall present some general properties of such sets of linear inequalities.

3. Polyhedral Convex Cones

Consider for any vector $x \in \mathbb{R}^n$ the following set of linear combinations of the components x_k of x, where I is a finite index set,

$$\sum_{k=1}^{n} \alpha_{ik} x_k ; \qquad i \in I , \tag{6}$$

with $\alpha_{ik} \in \mathbb{R}$ for all i and k. We define the set

$$C_\alpha = \left\{ x \in \mathbb{R}^n \,\middle|\, \sum_{k=1}^{n} \alpha_{ik} x_k \geqq 0 , \quad \text{for all} \quad i \in I \right\} . \tag{7}$$

The set C_α is a *convex cone*, i.e., if $x^{(1)}$, $x^{(2)} \in C_\alpha$ then every *positive linear combination* of $x^{(1)}$ and $x^{(2)}$ (i.e. every vector $c_1 x^{(1)} + c_2 x^{(2)}$ with c_1, $c_2 \geqq 0$) also belongs to C_α. In view of its definition and the fact that I is finite C_α is called a *polyhedral convex cone*.

For any $J \subset I$ we define

$$F_J = \left\{ x \in \mathbb{R}^n \,\middle|\, \sum_{k=1}^{n} \alpha_{ik} x_k > 0 \quad \text{for all} \quad i \in J ; \quad \sum_{k=1}^{n} \alpha_{ik} x_k = 0 \quad \text{for all} \quad i \in I \backslash J \right\} . \tag{8}$$

If F_J is nonempty it is called a *face* of C_α; $F_\emptyset$ is called the *null-face*. If d_J is the number of independent vectors satisfying $\sum_{k=1}^{n} \alpha_{ik} x_k = 0$, for all $i \in I \backslash J$, we call F_J a face of dimension d_J. It is clear that there are no faces of dimension smaller then $d \equiv d_\emptyset$, that there is exactly one face of dimension d, and that there are at most $2^{|I|}$ faces.

A face F_J of C_α is called an *extremal face* of C_α if no vector in F_J can be expressed as a positive linear combination of two vectors in $C_\alpha \backslash F_J$.

We now state without proof the following facts about C_α [2]:

1) The extremal faces of C_α are the d-dimensional null-face $F_\emptyset$ and the $(d+1)$-dimensional faces (if any). Vectors in $(d+1)$-dimensional faces we call *extremal vectors*.

2) If in each extremal face F_J with $d_J = d+1$ we select an arbitrary vector x^J, and if the vectors $x^{(1)}, \ldots, x^{(d)}$ form a basis of $F_\emptyset$, every vector x in C_α can be written in the form

$$x = \sum_{J \subset I : d_J = d+1} c_J x^J + \sum_{r=1}^{d} c_r x^{(r)} , \tag{9}$$

with $c_J \geqq 0$ for all J. For a given choice of $x^{(1)}, \ldots, x^{(d)}$ and extremal vectors x^J, the decomposition is in general not unique. For $d > 0$ the choice of the x^J is not unique either. For $d = 0$, however, it is unique, apart from a positive normalization factor in each of the x^J[1]; in this case, to which we shall restrict ourselves in this paper, the x^J can be found by the following procedure. Select in all possible ways a set of $n-1$ linearly independent equations $\sum_{k=1}^{n} \alpha_{ik} x_k = 0$; if a vector x satisfying these equations lies in C_α, it is an extremal vector. For a general reference to linear inequalities see [2].

4. Extremal Λ-Inequalities

In this paper we shall consider graphs G and sets A for which $\Pi_A^e(G) = \Pi_A^e$ (cf. the remark at the end of Sect. 5), and in this section we shall investigate the set of linear inequalities

$$\sum_{B \in \mathscr{P}_e(A)} \eta_\pi(B) \lambda_B \geqq 0, \qquad \pi \in \Pi_A^e. \tag{10}$$

Because $\eta_\pi(B) = \eta_\pi(A \backslash B)$ and $\lambda_B = \lambda_{A \backslash B}$ for all $B \in \mathscr{P}_e(A)$, we select from the even subsets of A a maximal family of subsets $\mathscr{P}'_e(A)$, such that if $B \in \mathscr{P}'_e(A)$ then $A \backslash B \notin \mathscr{P}'_e(A)$; we assume that $\emptyset \in \mathscr{P}'_e(A)$.

Let us denote the two-block partitions of A by $\{B, A \backslash B\}$, $B \in \mathscr{P}'_e(A)$. If for convenience we write the one-block partition $\{A\}$ as $\{\emptyset, A\}$ we can introduce a square matrix η with elements

$$\eta_{B,B'} = \eta_{\{B, A \backslash B\}}(B'); \qquad B, B' \in \mathscr{P}'_e(A). \tag{11}$$

From the definition of $\eta_\pi(B')$ it follows that

$$\eta_{B,B'} = \tfrac{1}{2}(1 + (-1)^{|B \cap B'|}); \qquad B, B' \in \mathscr{P}'_e(A). \tag{12}$$

It is not difficult to see that η has an inverse η^{-1} with elements

$$(\eta^{-1})_{B,B'} = -\delta_{B,\emptyset}\delta_{B',\emptyset} + 2^{-|A|+3}(-1)^{|B \cap B'|}; \qquad B, B' \in \mathscr{P}'_e(A). \tag{13}$$

Let us introduce the family $\lambda = \{\lambda_B\}_{B \in \mathscr{P}'_e(A)}$, considered as a vector in $\mathbb{R}^n (n = |\mathscr{P}'_e(A)| = 2^{|A|-2})$. The set of vectors λ which satisfy Eq. (10) for all $\pi \in \Pi_A^e$ will form a convex cone C_η. It is convenient to carry over the concepts "extremal" and "positive linear combination" from the vectors λ to the corresponding Λ-inequalities.

We can now combine the results of the preceding section with Theorem 1. Since η has an inverse, we are in the case $d = 0$, and the following theorem holds.

Theorem 2. *Let G be a finite graph and $A \subset V(G)$. If $\Pi_A^e(G) = \Pi_A^e$, there exists a unique finite set of extremal Λ-inequalities with respect to A, i.e. a set from which every Λ-inequality with respect to A can be derived by taking positive linear combinations.*

To illustrate Theorem 2, we consider a set A consisting of four vertices, say $A = \{1, 2, 3, 4\}$. Π_A^e consists of the following partitions (in an obvious notation)

$$(\emptyset|1234), (12|34), (13|24), (14|23). \tag{14}$$

1 This proviso will not be repeated explicitly in the sequel

Let $\mathscr{P}'_e(A)=\{\emptyset,\{1,2\},\{1,3\},\{1,4\}\}$. The matrix η has the following form

$$\eta=\begin{pmatrix}1&1&1&1\\1&1&0&0\\1&0&1&0\\1&0&0&1\end{pmatrix}, \tag{15}$$

where the order of rows and columns is that of the partitions in (14) and the sets in $\mathscr{P}'_e(A)$. The extremal vectors of C_η can be found by selecting any three linearly independent equations from the set of four equations

$$\sum_{B'\in\mathscr{P}'_e(A)} \eta_{B,B'}\lambda_{B'}=0, \qquad B\in\mathscr{P}'_e(A)$$

and requiring that the solution satisfies

$$\sum_{B'\in\mathscr{P}'_e(A)} \eta_{B,B'}\lambda_{B'}\geqq 0$$

for the remaining set B. In this way we easily find the following extremal vectors (normalized so that $|\lambda_\emptyset|=1$), with $\lambda_{ij}\equiv\lambda_{\{i,j\}}$:

$$\begin{aligned}&\lambda_\emptyset=-\lambda_{12}=\lambda_{13}=-\lambda_{14}=1,\\&\lambda_\emptyset=-\lambda_{12}=-\lambda_{13}=\lambda_{14}=1,\\&\lambda_\emptyset=\lambda_{12}=-\lambda_{13}=-\lambda_{14}=1,\\&\lambda_\emptyset=-\lambda_{12}=-\lambda_{13}=-\lambda_{14}=-1.\end{aligned} \tag{16}$$

The corresponding extremal Λ-inequalities are

$$(1)(\sigma_1\sigma_2\sigma_3\sigma_4)-(\sigma_1\sigma_2)(\sigma_3\sigma_4)+(\sigma_1\sigma_3)(\sigma_2\sigma_4)-(\sigma_1\sigma_4)(\sigma_2\sigma_3)\geqq 0, \tag{17a}$$

$$(1)(\sigma_1\sigma_2\sigma_3\sigma_4)-(\sigma_1\sigma_2)(\sigma_3\sigma_4)-(\sigma_1\sigma_3)(\sigma_2\sigma_4)+(\sigma_1\sigma_4)(\sigma_2\sigma_3)\geqq 0, \tag{17b}$$

$$(1)(\sigma_1\sigma_2\sigma_3\sigma_4)+(\sigma_1\sigma_2)(\sigma_3\sigma_4)-(\sigma_1\sigma_3)(\sigma_2\sigma_4)-(\sigma_1\sigma_4)(\sigma_2\sigma_3)\geqq 0, \tag{17c}$$

$$-(1)(\sigma_1\sigma_2\sigma_3\sigma_4)+(\sigma_1\sigma_2)(\sigma_3\sigma_4)+(\sigma_1\sigma_3)(\sigma_2\sigma_4)+(\sigma_1\sigma_4)(\sigma_2\sigma_3)\geqq 0. \tag{17d}$$

The inequalities (17a)–(17c) are special cases of inequalities derived by Sherman [3] (see also [4] and [5], Theorem 5). The inequality (17d) is a special case of a set of inequalities due to Newman [5], and is also a consequence of the stronger GHS inequality [6] (see also [7, 8]). By adding up all four Eqs. (17) we obtain

$$(1)(\sigma_1\sigma_2\sigma_3\sigma_4)\geqq 0; \tag{18}$$

by adding up Eqs. (17a) and (17b) we obtain

$$(1)(\sigma_1\sigma_2\sigma_3\sigma_4)\geqq(\sigma_1\sigma_2)(\sigma_3\sigma_4). \tag{19}$$

Inequalities (18) and (19) are examples of the first and second GKS inequality [6], respectively, which are thus seen not to be extremal. We stress the fact that for the given set A the set of inequalities (17) exhausts the class of extremal (i.e. strongest possible) correlationfunction inequalities of the form (4). The example of the GHS inequality shows that there exist stronger inequalities which are not in this class.

To prepare the way for the examples to be discussed in the next section we find it convenient to introduce a change of variables which enables us to write the inequalities in a somewhat simpler form. We define, for $B\in\mathcal{P}_{\mathrm{e}}'(A)$,

$$k_B=\sum_{B'\in\mathcal{P}_{\mathrm{e}}'(A)}\eta_{B,B'}\lambda_{B'}\,. \tag{20}$$

Using the inverse of η it is easily verified that

$$\lambda_B=-\delta_{B,\emptyset}k_\emptyset+2^{-|A|+3}\sum_{B'\in\mathcal{P}_{\mathrm{e}}'(A)}(-1)^{|B\cap B'|}k_{B'}\,;\qquad B\in\mathcal{P}_{\mathrm{e}}'(A)\,. \tag{21}$$

Consider a partition $\pi=\{B_1,\dots,B_k\}\in\Pi_A^{\mathrm{e}}$, with $B_1,\dots,B_k$ nonempty. From the definition of η it follows that for $B\in\mathcal{P}_{\mathrm{e}}'(A)$

$$\eta_\pi(B)=\prod_{m=1}^{k}\{\tfrac{1}{2}(1+(-1)^{|B\cap B_m|})\}\,. \tag{22}$$

Define $K=\{1,\dots,k\}$, and for $L\subset K$ define

$$B_L=\bigcup_{l\in L}B_l \tag{23}$$

(in particular, $B_\emptyset=\emptyset$); $\eta_\pi(B)$ can now be written as

$$\eta_\pi(B)=2^{-k}\sum_{L\subset K}(-1)^{|B\cap B_L|}\,. \tag{24}$$

Using Eqs. (21) and (24) and the fact that

$$\sum_{B\in\mathcal{P}_{\mathrm{e}}'(A)}(-1)^{|B\cap X|}=2^{|A|-2}\{\delta_{X,\emptyset}+\delta_{X,A}\} \tag{25}$$

for all $X\in\mathcal{P}_{\mathrm{e}}(A)$, we find

$$\begin{aligned}\sum_{B\in\mathcal{P}_{\mathrm{e}}'(A)}\eta_\pi(B)\lambda_B&=-2^{-k}\sum_{B\in\mathcal{P}_{\mathrm{e}}'(A)}\sum_{L\subset K}(-1)^{|B\cap B_L|}\delta_{B,\emptyset}k_\emptyset\\&\quad+2^{-k-|A|+3}\sum_{B\in\mathcal{P}_{\mathrm{e}}'(A)}\sum_{B'\in\mathcal{P}_{\mathrm{e}}'(A)}\sum_{L\subset K}(-1)^{|B\cap B'|}(-1)^{|B\cap B_L|}k_{B'}\\&=-k_\emptyset+2^{-k+2}\sum_{\substack{L\subset K\\ B_L\in\mathcal{P}_{\mathrm{e}}'(A)}}k_{B_L}\,.\end{aligned} \tag{26}$$

If we introduce

$$\zeta_\pi(B)=\begin{cases}1 & \text{if } B \text{ is a nonempty union of (nonempty) blocks of } \pi\\ 0 & \text{otherwise}\end{cases}$$

we finally obtain

$$2^{k-2}\sum_{B\in\mathcal{P}_{\mathrm{e}}'(A)}\eta_\pi(B)\lambda_B=-(2^{k-2}-1)k_\emptyset+\sum_{B\in\mathcal{P}_{\mathrm{e}}'(A)}\zeta_\pi(B)k_B\,. \tag{27}$$

In the new variables the set of inequalities (10), with $\mathcal{P}_{\mathrm{e}}(A)$ replaced by $\mathcal{P}_{\mathrm{e}}'(A)$, reads

$$\sum_{B\in\mathcal{P}_{\mathrm{e}}'(A)}\zeta_\pi(B)k_B\geqq(2^{k-2}-1)k_\emptyset\,,\qquad \pi\in\Pi_A^{\mathrm{e}}\,. \tag{28}$$

Note that the set of inequalities (28) includes the set of inequalities $k_B\geqq 0$, for all $B\in\mathcal{P}_{\mathrm{e}}'(A)$.

To find the extremal inequalities from (28), we select a set of $n-1$ independent equations of the form

$$\sum_{B\in\mathscr{P}'_e(A)} \zeta_\pi(B)k_B=(2^{k-2}-1)k_\emptyset\,, \qquad \pi\in\Pi^e_A\,. \tag{29}$$

If the solution of these equations satisfies the inequalities (28) for all remaining π in Π^e_A, then it will be an extremal inequality.

5. Examples of Extremal Λ-Inequalities

In this section we shall give several examples of extremal Λ-inequalities. The examples given do not exhaust the class of all possible extremal Λ-inequalities.

1) We shall first derive four types of extremal Λ-inequalities which are valid for arbitrary sets A with $|A|\geqq 4$. To this end we first select a vertex $v\in A$ and choose for $\mathscr{P}'_e(A)$ the set of all even subsets of A not containing v. As in Sect. 4 we define $n=|\mathscr{P}'_e(A)|=2^{|A|-2}$.

a) Let C be an arbitrary nonempty element of $\mathscr{P}'_e(A)$, and take

$$k_B=1 \quad \text{for} \quad B=C\,, \tag{30a}$$

$$k_B=0 \quad \text{for} \quad B\neq C\,. \tag{30b}$$

Obviously, since $k_\emptyset=0$, all inequalities (28) are satisfied. Using Eq. (21) we see that the Λ-inequality corresponding to the choice (30), multiplied by a factor $2^{|A|-3}$ in order to avoid fractional coefficients, reads

$$\sum_{B\in\mathscr{P}'_e(A)} (-1)^{|B\cap C|}(\sigma_B)(\sigma_{A\setminus B})\geqq 0\,. \tag{31}$$

Since the $n-1$ Eqs. (30b) are manifestly linearly independent, the inequality (31) is an extremal Λ-inequality. Any Λ-inequality with $k_\emptyset=0$ and $k_B\neq 0$ for more than one $B\in\mathscr{P}'_e(A)$ is a positive linear combination of Λ-inequalities of the type (31) with strictly positive coefficients, and hence not extremal; an example is the second GKS inequality $(\sigma_\emptyset)(\sigma_A)-(\sigma_B)(\sigma_{A\setminus B})\geqq 0$.

It is easy to verify that the inequalities (31) are of the type derived by Sherman [3].

b) Select a vertex $v'\in A$, $v'\neq v$, and take

$$k_B=1 \quad \text{if} \quad v'\notin B \quad \text{and} \quad B\neq A\setminus\{v,v'\}\,, \tag{32a}$$

$$k_B=0 \quad \text{otherwise}\,. \tag{32b}$$

Obviously, this set of k_B-values satisfies the inequalities (28) for all π such that $k=|\pi|\leqq 2$. If $|A|\geqq 6$ we further consider a partition $\pi=\{B_1,\ldots,B_k\}$ with $k>2$, where the order of the blocks is chosen so that $v,v'\in B_1\cup B_2$. There are two cases to be distinguished: (α) v and v' are in the same block, say B_1, and (β) v and v' are in different blocks, say v in B_1, and v' in B_2. In case (α), the left-hand side of Eq. (28) is equal to $2^{k-1}-1$ (if $B_1\neq\{v,v'\}$) or equal to $2^{k-1}-2$ (if $B_1=\{v,v'\}$). Since $k_\emptyset=1$ and $k>2$, the inequality (28) is satisfied. In case (β), the left-hand side is equal to $2^{k-2}-1$, and hence the inequality (28) is again satisfied.

We next show that the choice (32) of k_B-values satisfies a set of $n-1$ linearly independent equations of the type (29). This is obvious for $|A|=2$ and $|A|=4$. For $|A|\geqq 6$, we consider the partitions $\pi=\{B_1, B_2, B_3\}$, with $v\in B_1$, $v'\in B_2$. For such a partition Eq. (29) reads

$$k_{B_2\cup B_3}+k_{B_2}+k_{B_3}=k_\emptyset \tag{33}$$

which reduces, by Eq. (32b), to the equation $k_{B_3}=k_\emptyset$. Since for any $B\neq A\backslash\{v,v'\}$ not containing v' such a partition with $B_3=B$ can be found, and since the full set of equations for the k_B thus obtained is linearly independent and has (32) as a solution, the corresponding A-inequality is extremal. By using Eq. (21) one easily verifies that the coefficients λ_B (again multiplied by a factor $2^{|A|-3}$ in order to avoid fractional values) are

$$\lambda_B=\begin{cases} 2^{|A|-3}-1 & \text{if } B=A\backslash\{v,v'\}\,,\\ 1 & \text{if } B \text{ contains } v'\,,\\ -1 & \text{otherwise}\,. \end{cases} \tag{34}$$

c) Take

$$k_B=0 \quad \text{if} \quad |B|>\tfrac{1}{2}|A|-1\,, \tag{35a}$$

$$k_B=1 \quad \text{if} \quad |B|=\tfrac{1}{2}|A|-1\,, \tag{35b}$$

$$k_B=2 \quad \text{if} \quad |B|<\tfrac{1}{2}|A|-1\,. \tag{35c}$$

Again, this set of k_B-values satisfies the inequalities (28) for $k=|\pi|\leqq 2$. If $|A|\geqq 6$ we further consider a partition $\pi=\{B_1,\ldots,B_k\}$ with $k>2$ and $v\in B_1$, and we define $M=\{2,\ldots,k\}$. Using the definition (23) we write Eq. (28) for this partition as

$$k_{B_M}+\sum_{\substack{L\subset M\\ L\neq\emptyset,M}}\tfrac{1}{2}(k_{B_L}+k_{B_{M\backslash L}})\geqq(2^{k-2}-1)k_\emptyset\,. \tag{36}$$

Since for any $L\neq\emptyset$, M we have

$$|B_L|+|B_{M\backslash L}|=|A|-|B_1|\leqq|A|-2\,,$$

$|B_L|$ and $|B_{M\backslash L}|$ cannot be both larger than $\frac{1}{2}|A|-1$. Hence we have, by Eqs. (35a)–(35c) $k_{B_L}+k_{B_{M\backslash L}}\geqq 2$. Since the number of sets $L\neq\emptyset, M$ is $2^{|M|}-2=2^{k-1}-2$, and since $k_\emptyset=2$, the inequality (36) is satisfied.

We shall now show that the set of k_B defined by Eqs. (35a)–(35c) satisfies a set of equations of the form (29) with $k=|\pi|\leqq 3$, among which $n-1$ are linearly independent. First, the Eqs. (35a) are of this form, and they are independent. If $|A|\geqq 6$, we further consider the set of simultaneous equations of the form (29) where $\pi=\{B_1,B_2,B_3\}$, with $B_1=\{v,v'\}$, where v' is an arbitrary vertex not equal to v. They have the form

$$k_{B_2\cup B_3}+k_{B_2}+k_{B_3}=k_\emptyset\,,$$

which reduces to

$$k_{B_2}+k_{B_3}=k_\emptyset\,, \tag{37}$$

since $|B_2 \cup B_3| = |A| - 2 > \frac{1}{2}|A| - 1$. If $|B_2| > |B_3|$, then $k_{B_2} = 0$, and Eq. (37) further reduces to the equation $k_{B_3} = k_\emptyset$. If $|B_2| = |B_3|$ we consider a vertex $v'' \in B_2$ and the sets B_1' and B_2' obtained from B_1 and B_2 by interchanging v' and v''. For the partition $\{B_1', B_2', B_3\}$ Eq. (29) reads

$$k_{B_2'} + k_{B_3} = k_\emptyset . \tag{38}$$

From Eqs. (37) and (38) it follows that $k_{B_2'} = k_{B_2}$. Repeating this argument we find that $k_{B'} = k_B$ for any two sets B, B' with $|B| = |B'|$. In the case $|B_2| = |B_3|$ considered we conclude that $k_{B_2} = k_{B_3} = \frac{1}{2}k_\emptyset$. This shows that if $k_\emptyset$ is fixed, the solution of the set of equations considered is unique. Putting $k_\emptyset = 2$ we obtain Eqs. (35a)–(35c). Consequently, the corresponding Λ-inequality is extremal. The λ_B can be found from Eqs. (21) and (35), but the general expression is not very illuminating.

d) Take

$$k_B = 0 \quad \text{if} \quad |B| \equiv 2 (\mathrm{mod}\, 4) , \tag{39a}$$

$$k_B = 1 \quad \text{if} \quad |B| \equiv 0 (\mathrm{mod}\, 4) . \tag{39b}$$

Consider a partition $\pi = \{B_1, \ldots, B_k\}$ with $k \geqq 1$ and $v \in B_1$. Let k_p, with $p = 0$ or 2, be the number of blocks B_l of π with $l \neq 1$ and $|B_l| \equiv p (\mathrm{mod}\, 4)$. If $M = \{2, \ldots, k\}$, the number of sets $L \subset M$ such that $|B_L| \equiv 0 (\mathrm{mod}\, 4)$ is equal to $2^{k_0 + k_2 - 1} = 2^{k-2}$ if $k_2 > 0$ and equal to $2^{k_0 + k_2} = 2^{k-1}$ if $k_2 = 0$. In both cases, the inequality (28) is satisfied.

As in the examples b) and c), the set of k_B-values defined by Eqs. (39a) and (39b) satisfies a set of $n-1$ linearly independent equations of the form (29) with $k = |\pi| \leqq 3$. This can be seen as follows. In the first place, the Eqs. (39a) are of this form, and they are independent. Consider a set B such that $|B| \equiv 0 (\mathrm{mod}\, 4)$, $B \neq \emptyset$ and $v \notin B$. Obviously $|B| \geqq 4$, and there is a set $B' \subset B$ such that $|B'| = 2$, and hence $|B \backslash B'| \equiv 2 (\mathrm{mod}\, 4)$. Consider Eq. (29) for the partition $\pi = \{B', B \backslash B', A \backslash B\}$:

$$k_{B'} + k_{B \backslash B'} + k_B = k_\emptyset .$$

By (39a) this reduces to $k_B = k_\emptyset$, which determines k_B uniquely in terms of $k_\emptyset$. Therefore, the set of $n-1$ equations thus selected is independent, and the corresponding Λ-inequality is extremal. The Λ-inequality (multiplied by a suitable positive factor) reads

$$c \sum_{B \in \mathscr{P}_e'(A)} (-1)^{|B|/2} (\sigma_B)(\sigma_{A \backslash B}) \geqq 0 , \tag{40}$$

where $c = 1$ if $|A| \equiv 0$ or 2 (mod 8) and $c = -1$ if $|A| \equiv 4$ or 6 (mod 8). The easiest way to see this is by verifying that the substitution of the values $\lambda_B = (-1)^{|B|/2} c$ into Eq. (20) yields for the k_B the values (39). Using the fact that:

$$\begin{aligned} \sum_{Y \in \mathscr{P}_e(X)} (-1)^{|Y|/2} &= \tfrac{1}{2} \sum_l \binom{|X|}{l} (-1)^{l/2} \{1^l + (-1)^l\} \\ &= \tfrac{1}{2}\{(1+\mathrm{i})^{|X|} + (1-\mathrm{i})^{|X|}\} = 2^{|X|/2} \cos \frac{|X|\pi}{4} \end{aligned} \tag{41}$$

we find indeed that

$$\begin{aligned}\sum_{B'\in\mathscr{P}'_{\mathrm{e}}(A)} \eta_{B,B'}\lambda_{B'} &= c \sum_{\substack{B'\in\mathscr{P}'_{\mathrm{e}}(A)\\ B\cap B'\,\mathrm{even}}} (-1)^{|B'|/2}\\ &= c\sum_{B'_1\in\mathscr{P}_{\mathrm{e}}(B)} (-1)^{|B'_1|/2} \sum_{B'_2\in\mathscr{P}'_{\mathrm{e}}(A\setminus B)} (-1)^{|B'_2|/2}\\ &= 2^{(|A|-3)/2} c \cos\frac{(|A|-1)\pi}{4}\{1+(-1)^{|B|/2}\},\end{aligned}$$

which reduces to Eqs. (39a) and (39b) multiplied by $2^{|A|/2-1}$.

Remark. It is easily verified that for $|A|\geqq 4$ the first GKS inequality $(\sigma_\emptyset)(\sigma_A)\geqq 0$ is a positive linear combination, with strictly positive coefficients, of any inequality of type b), c), or d) and some inequalities of type a), and hence not extremal.

2) After having discussed these general types of extremal A-inequalities we now turn to a special case, viz. $|A|=6$. Let $A=\{1,2,3,4,5,6\}$. For this case we will give all extremal A-inequalities. Here it is convenient to abandon the convention for $\mathscr{P}'_{\mathrm{e}}(A)$ followed thus far in this section and to choose for $\mathscr{P}'_{\mathrm{e}}(A)$ the subset of $\mathscr{P}_{\mathrm{e}}(A)$ consisting of all sets B with $|B|\leqq 2$. Using the notation $k_{ij}\equiv k_{\{i,j\}}$ we can write the Eqs. (28) as

$$k_\emptyset \geqq 0, \tag{42a}$$

$$k_{ij}\geqq 0 \quad \text{for all pairs } i,j \text{ such that } 1\leqq i<j\leqq 6, \tag{42b}$$

$$k_{ij}+k_{kl}+k_{mn}\geqq k_\emptyset \quad \text{for all partitions } (ij|kl|mn) \text{ of } A. \tag{42c}$$

To find an extremal A-inequality we select $2^{|A|-2}-1=15$ independent equations from the following set of 31 equations:

$$k_\emptyset = 0, \tag{43a}$$

$$k_{ij}=0, \qquad 1\leqq i<j\leqq 6, \tag{43b}$$

$$k_{ij}+k_{kl}+k_{mn}=k_\emptyset, \qquad (ij|kl|mn)\in\Pi_A^{\mathrm{e}}, \tag{43c}$$

and we verify if the solution of the selected set of equations satisfies the inequalities (42a)–(42c). We denote the set of all solutions which can be obtained in this way by S. For any solution $\{k_B\}_{B\in\mathscr{P}'_{\mathrm{e}}(A)}\in S$ we define $\mathscr{P}=\{B\in\mathscr{P}'_{\mathrm{e}}(A)|B\neq\emptyset,\ k_B>0\}$.

Suppose first that Eq. (43a) is one of the selected equations. From the discussion following Eqs. (30a) and (30b) we conclude that this choice leads to an extremal A-inequality of type a), and we have $|\mathscr{P}|=1$.

Suppose next that $k_\emptyset>0$. In that case it is easily verified that if $|\mathscr{P}|<5$, at least one of the inequalities (42c) is violated. Since further the rank of the set of all Eqs. (43c) is 10, we must have $5\leqq|\mathscr{P}|\leqq 10$.

A straightforward analysis (based on an enumeration of possible cases, which fully exploits the permutation symmetry) shows the following.

α) There are, apart from permutations of the vertices, four solutions in S such that $\mathscr{P}$ does not contain any pair of disjoint sets, viz. one solution with $|\mathscr{P}|=5$, one

Table 1. Values of the k_B, $B \in \mathscr{P}_e'(A)$, for extremal A-inequalities in the case $A = \{1,2,3,4,5,6\}$

	$k_\emptyset$	k_{12}	k_{13}	k_{14}	k_{15}	k_{16}	k_{23}	k_{24}	k_{25}	k_{26}	k_{34}	k_{35}	k_{36}	k_{45}	k_{46}	k_{56}
a	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
b	1	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1
c	2	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1
d	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0
	1	1	0	1	1	1	0	1	1	1	0	0	0	0	0	0
	1	0	0	1	1	1	0	1	1	1	1	1	1	0	0	0

Table 2. Values of the λ_B, $B \in \mathscr{P}_e'(A)$, for extremal A-inequalities in the case $A = \{1,2,3,4,5,6\}$. The last column gives the number N of distinct extremal inequalities obtained from the one represented by a permutation of the numbers 1, 2, 3, 4, 5, 6

	$\lambda_\emptyset$	λ_{12}	λ_{13}	λ_{14}	λ_{15}	λ_{16}	λ_{23}	λ_{24}	λ_{25}	λ_{26}	λ_{34}	λ_{35}	λ_{36}	λ_{45}	λ_{46}	λ_{56}	N
a	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1	1	1	15
b	−1	7	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	15
c	−1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	6
d	−1	−1	−1	−1	−1	−1	1	1	1	1	1	1	1	1	1	1	6
	0	−1	0	0	0	0	0	0	0	0	1	1	1	0	0	0	60
	1	−1	−1	1	1	1	−1	1	1	1	1	1	1	−1	−1	−1	10

with $|\mathscr{P}| = 6$, one with $|\mathscr{P}| = 7$, and one with $|\mathscr{P}| = 9$. The first two are special cases of the examples d) and b), respectively, introduced above, the other two do not belong to the general classes a)–d) discussed under 1).

β) There is, again apart from permutations, exactly one solution in S such that $\mathscr{P}$ contains pairs of disjoint sets; it has $|\mathscr{P}| = 10$, and is a special case of example c).

γ) There is no solution in S such that $\mathscr{P}$ contains a triple of pairwise disjoint sets.

Summing up, we have derived that for $|A| = 6$ there are six extremal inequalities (counting cases which differ by a permutation of the vertices as a single case). They are represented in Tables 1 and 2. Table 1 gives the values of the k_B, $B \in \mathscr{P}_e'(A)$, Table 2 those of the λ_B (multiplied by a common factor in order to avoid fractional values). Observe that the notation for the k_B differs from the one used under 1) as a consequence of the different choice of $\mathscr{P}_e'(A)$. The entry in the first columns indicates the general type of extremal inequality to which the represented inequality belongs. The inequality labelled d) is just the inequality (62) of I. The inequality labelled c) is a special case of Newman's inequalities [5], referred to in Sect. 4, and also mentioned in I, Sect. 6, example (3) (see also the discussion given below).

3) We conclude this section by a discussion of the A-inequalities derived by Newman [5]. Let A be an even set of vertices and X_A a subset of $\mathscr{P}_e'(A)$ such that every partition of A into pairs is a refinement of some two-block partition $\{B, A \setminus B\}$ of A with $B \in X_A$. Newman's inequality reads

$$(\sigma_\emptyset)(\sigma_A) \leqq \sum_{B \in X_A} (\sigma_B)(\sigma_{A \setminus B}). \tag{44}$$

Evidently, this is a Λ-inequality. We consider in particular the case where X_A consists of all sets $B \in \mathscr{P}'_e(A)$ – where $\mathscr{P}'_e(A)$ is chosen as in 1) – such that $|B| = |A| - 2$; the corresponding inequality was derived in Theorem 2 [Eq. (3.4)] of [5]. It is readily verified that X_A satisfies the requirement mentioned above. The corresponding values of the λ_B and the k_B are

$$\lambda_B = \begin{cases} -1 & \text{if} \quad B = \emptyset \\ \ \ 1 & \text{if} \quad |B| = |A| - 2 \\ \ \ 0 & \text{otherwise}, \end{cases} \tag{45}$$

$$k_B = |A \backslash B| - 2. \tag{46}$$

We have seen that for $|A| = 4$ and $|A| = 6$ the corresponding Λ-inequality is extremal. We shall now show that for $|A| > 6$ it is a convex combination of an extremal inequality of type c) and a different inequality (which in general is not extremal).

To this end we consider a set of real numbers k_l (l even, $0 \leqq l \leqq |A| - 2$) satisfying the following inequalities:

$$k_0 \geqq k_2 \geqq \ldots \geqq k_{|A|-2} \geqq 0, \tag{47a}$$

$$k_l + k_{|A|-l-2} \geqq k_0 \quad \text{for} \quad l = 0, 2, \ldots, |A| - 2. \tag{47b}$$

Consider now the family $\{k_B\}_{B \in \mathscr{P}'_e(A)}$ defined by $k_B = k_{|B|}$. We assert that this family satisfies the inequalities (28) and hence corresponds to a Λ-inequality. To show this, we write again $\pi = \{B_1, \ldots, B_k\}$ with $v \in B_1$. The case $k = 1$ is trivial; therefore, let $k \geqq 2$. If $|B_1| = 2$, Eq. (36), and hence Eq. (28), is satisfied in virtue of Eq. (47b). If $|B_1| \geqq 4$ we consider the sets $B'_1 = \{v, v'\}$ with $v' \in B_1$, $v' \neq v$, and $B'_2 = B_2 \cup (B_1 \backslash B'_1)$, and the partition $\pi' = \{B'_1, B'_2, B_3, \ldots, B_k\}$. Since $|B'_1| = 2$, Eq. (28) is satisfied for π'; since $|B_2| < |B'_2|$, Eq. (47a) guarantees that it is also satisfied for the partition π.

Obviously, the special Newman inequality considered above is an example of this class of Λ-inequalities, as is the inequality of type c). Let us denote the corresponding values of the coefficients k_B, given by Eqs. (46) and (35), by $k_l^{(N)}$ and $k_l^{(c)}$, respectively, with $l = |B|$.

It is easily seen that the numbers $k_l^{(0)} = k_l^{(N)} - k_l^{(c)}$ satisfy the inequalities (47a) and (47b) and are not all zero for $|A| > 6$. Hence, $k_l^{(N)}$ is a positive linear combination of $k_l^{(0)}$ and $k_l^{(c)}$, and the corresponding inequality is not extremal.

For $|A| \geqq 6$ there exist other Newman inequalities than the one discussed above. For $|A| = 6$ they are not extremal. We conjecture that this is also true for $|A| > 6$.

Remark. In this paper we have restricted ourselves to graphs G and even sets $A \subset V(G)$ such that $\Pi^e_A(G) = \Pi^e_A$. E.g., G may be a complete graph and A an arbitrary even subset of $V(G)$; for other graphs not every set $A \subset V(G)$ satisfies this condition. The extremal Λ-inequalities valid for a set A in a graph G satisfying the condition are, of course, also valid for the same set A in any spanning subgraph H of G. However, if $\Pi^e_A(H)$ is a proper subset of Π^e_A, they need not be extremal. The extremal inequalities in this case can be determined along the same lines as in the case $\Pi^e_A(G) = \Pi^e_A$; details will be given in a subsequent paper.

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