Energy of a Hypercube and its Complement

Xiaogen Chen

School of Information Science and Technology, Zhanjiang Normal University
Zhanjiang Guangdong, 524048 P.R. China
oamc@163.com

Wanwen Xie

School of Mathematics and Computation Science, Shenzhen University
Shenzhen 518060, P.R. China
xieww@126.com

Abstract

Let $\overline{Q}_n$ denote the complement of $n$-dimensional hypercube $Q_n$, and let $E(G)$ and $LE(G)$ denote, respectively, the (ordinary) energy and Laplacian energy of a graph $G$. We obtain $LE(Q_n)=E(Q_n)=2\left\lceil \frac{n}{2} \right\rceil \binom{n}{\frac{n}{2}}$ and $LE(\overline{Q}_n)=E(\overline{Q}_n)=(n+1)\binom{n}{\frac{n}{2}}+2^n-2n-2$, where $n \geq 1$.

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1 Introduction

Let $G$ be a graph (assumed simple throughout) with $s$ vertices (vertex set denoted by $V(G)$) and $t$ edges (edge set denoted by $e(G)$), and let $A(G)=(a_{ij})$ be the adjacency matrix for $G$. The characteristic polynomial of the adjacency matrix $A(G)$, i.e., $P(G, \lambda) = P(A(G), \lambda) = det(\lambda I - A(G))$ is called the characteristic polynomial of the graph $G$. The eigenvalues of the matrix $A(G)$ are called the eigenvalues of graph $G$. Suppose the distinct eigenvalues of graph $G$ are denoted by $\lambda_1, \lambda_2, \cdots, \lambda_r$ with corresponding multiplicities $m_1, m_2, \cdots, m_r$, where $m_i$ is a nonnegative integer $i = 1, 2, \cdots, r$. The energy of a graph $G$, denoted by $E(G)$, is defined as

$$E(G) = \sum_{i=1}^{r} m_i |\lambda_i|.$$
The energy of $G$ was first defined by Gutman in 1978. This concept arose in chemistry where certain numerical quantities, such as the heat of formation of a hydrocarbon, are related to total $\pi$-electron energy that can be calculated as the energy of an appropriate "molecular" graph[1]. Gutman and Zhou [2] defined the Laplacian energy of a graph $G$ using its Laplacian matrix $D(G) - A(G)$, where $A(G)$ is the adjacency matrix and $D(G)$ is the diagonal matrix of degrees:

$$LE(G) = \sum_{i=1}^{r} m_i \left| \mu_i - \frac{2t}{s} \right|$$

where $\mu_1, \mu_2, \ldots, \mu_r$ are the (Laplacian) eigenvalues of $D(G) - A(G)$. $t$ is the number of edges of $G$, and $2t/s$ is the average degree of a vertex of $G$.

The $n$-dimensional hypercube $Q_n$ is the simple graph whose vertices are the $n$-tuples with entries in $\{0,1\}$ and whose edges are the pairs of $n$-tuples that differ in exactly one position, the number of its vertices and edges are $2^n$ and $n2^{n-1}$ respectively. The complement $\overline{G}$ of a simple graph $G$ is the simple graph with vertex set $V(G)$ defined by $uv \in e(\overline{G})$ if and only if $uv \notin e(G)$. Let $\overline{Q}_n$ denote the complement of $n$-dimensional hypercube $Q_n$, and let $B(Q_n)$ and $B(\overline{Q}_n)$ denote, respectively, the adjacency matrices of $Q_n$ and $\overline{Q}_n$. In [3], we have

$$B(\overline{Q}_n) = J - I - B(Q_n),$$

$$B(Q_1) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, B(Q_{n+1}) = \begin{pmatrix} B(Q_n) & I \\ I & B(Q_n) \end{pmatrix},$$

$$B(\overline{Q}_1) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, B(\overline{Q}_{n+1}) = \begin{pmatrix} B(\overline{Q}_n) & J - I \\ J - I & B(\overline{Q}_n) \end{pmatrix},$$

where $n \geq 1$, $I$ is the identity matrix, $J$ is the matrix of all 1’s.

There are a number of results on the energy of graphs [1,2,4,5,6,7].

In recent years, it is found that hypercubes are becoming a fundamental tool in computer science, coding and cryptography, genetic algorithms and discrete neural network etc[8]. In this paper, we have solved the problem for $E(Q_n)$, $E(\overline{Q}_n)$, $LE(Q_n)$ and $LE(\overline{Q}_n)$.

2 The (ordinary) energy of hypercubes

Let $P(Q_n, \lambda) = \text{det}(\lambda I - B(Q_n))$ be the characteristic polynomial of $Q_n$. It is easy to verify that $P(Q_1, \lambda) = \text{det}(\lambda I - B(Q_1)) = (\lambda + 1)(\lambda - 1)$, and $P(Q_{n+1}, \lambda) = P(Q_n, \lambda + 1)P(Q_n, \lambda - 1)$, where $n \geq 1$. We have the following.

**Lemma 2.1** ([3]) Let $Q_n$ be an $n$-dimensional hypercube. Then $Q_n$ has $n + 1$ distinct eigenvalues. They are given by $q_k = -n + 2k$, and the eigenvalue $q_k$ has multiplicity $\left(\binom{n}{k}\right)$, $k = 0, 1, 2, \cdots, n$, where $n \geq 1,$ $\binom{n}{k}$ is binomial coefficient.

One can easily prove the following.
Lemma 2.2 Let $n$ be a nonnegative integer. Then
(1) $\sum_{k=0}^{n} \binom{n}{k} = 2^n$;
(2) $\sum_{k=0}^{n} k \binom{n}{k} = n2^{n-1}$;
(3) $\sum_{k=0}^{n} k \binom{2n}{k} = n2^{2n-1}$;
(4) $\sum_{k=0}^{n} k \binom{2n+1}{k} = (2n+1)2^{2n-1} - \frac{2n+1}{2}(2n)$;
(5) $\sum_{j=0}^{n} \binom{j}{k} = \binom{n+1}{k+1}$.

Theorem 2.3 Let $E(Q_n)$ be the (ordinary) energy of $n$-dimensional hypercube $Q_n$. Then $E(Q_n) = 2\lceil \frac{n}{2} \rceil \binom{n}{\lceil \frac{n}{2} \rceil}$, where $n \geq 1$, $\lceil a \rceil$ is the ceiling of number $a$.

Proof By Lemma 2.1 and Lemma 2.2, we have
$E(Q_n) = \sum_{k=0}^{n} \left| q_k \right| \binom{n}{k}$
$= \sum_{k=0}^{\frac{n}{2}} (n-2k) \binom{n}{k} + \sum_{k=\frac{n}{2}+1}^{n} (2k-n) \binom{n}{k}$
$= n \sum_{k=0}^{\frac{n}{2}} \binom{n}{k} - 2 \sum_{k=\frac{n}{2}+1}^{n} \binom{n}{k} + 2 \sum_{k=\frac{n}{2}+1}^{n} k \binom{n}{k} - n \sum_{k=\frac{n}{2}+1}^{n} \binom{n}{k}$
$= 2 \sum_{k=0}^{\frac{n}{2}} (n-2k) \binom{n}{k} + 2 \sum_{k=0}^{\frac{n}{2}} k \binom{n}{k} - n \sum_{k=0}^{n} \binom{n}{k}$
$= 2 \sum_{k=0}^{\frac{n}{2}} (n-2k) \binom{n}{k} + 2n2^{n-1} - n2^n$
$= 2 \sum_{k=0}^{\frac{n}{2}} (n-2k) \binom{n}{k}$, where $\lfloor a \rfloor$ is the floor of number $a$.

Case 1. If $n$ is even, then $\sum_{k=0}^{\frac{n}{2}} \binom{n}{k} = 2^{n-1} + \frac{1}{2} \binom{n}{\frac{n}{2}}$.

Case 2. If $n$ is odd, then $\sum_{k=0}^{\frac{n}{2}} \binom{n}{k} = 2^{n-1} - \frac{1}{2} \binom{n-1}{\frac{n-1}{2}}$.

Hence $E(Q_n) = 2 \sum_{k=0}^{\frac{n}{2}} (n-2k) \binom{n}{k}$
$= 2n \binom{n-1}{\frac{n}{2}} = 2n \binom{n+1}{\frac{n}{2}+1}$
$= 2n \binom{n}{\frac{n}{2}+1}$

Combining above all cases we complete the proof.

3 The (ordinary) energy of the complement of hypercubes

Let $P(Q_n, \lambda) = \det(\lambda I - B(Q_n))$ be the characteristic polynomial of $Q_n$.

Clearly, $P(\overline{Q}_1, \lambda) = \det(\lambda I - B(\overline{Q}_1)) = \lambda^2$. For $P(Q_n, \lambda), n \geq 2$, we have the following.
Lemma 3.1 Let \( P(\bar{Q}, \lambda) = \det(\lambda I - B(\bar{Q})) \) be the characteristic polynomial of \( \bar{Q} \), then
\[
P(\bar{Q}, \lambda) = \prod_{k=0}^{n-2} P(-B(Q_{n-k-1}), \lambda + k)P((2^{n-1} - 1)J_2, \lambda + n - 1)
\]
where \( n \geq 2 \), \( J_2 \) is a 2 \times 2 matrix of all 1’s.

Proof It is easy to check that If \( A \) and \( C \) are square matrices of the same order, and \( AC = CA \), then
\[
\det \begin{pmatrix} \lambda I - A & C \\ C & \lambda I - A \end{pmatrix} = \det(\lambda I - A - C)\det(\lambda I - A + C),
\]
where \( I \) is the identity matrix. Hence
\[
P(\bar{Q}, \lambda) = \det(\lambda I - B(\bar{Q})) = \det(\begin{pmatrix} \lambda I & 0 \\ 0 & \lambda I \end{pmatrix} - \begin{pmatrix} B(Q_{n-1}) & J - I \\ J - I & B(\bar{Q}_{n-1}) \end{pmatrix})
\]
\[
= \det(\begin{pmatrix} \lambda I - B(\bar{Q}_{n-1}) & -J + I \\ -J + I & \lambda I - B(\bar{Q}_{n-1}) \end{pmatrix})
\]
\[
= \det(\lambda I - B(\bar{Q}_{n-1}) + J - I) \det(\lambda I - B(\bar{Q}_{n-1}) - J + I)
\]
\[
= \det(\lambda I + B(Q_{n-1})) \det((\lambda + 1)I - (J + B(Q_{n-1}))).
\]
In a similar manner we arrive at
\[
\det((\lambda + k)I - ((2^{k-1} - 1)J + B(\bar{Q}_{n-k})))
\]
\[
= \det((\lambda + k)I + B(Q_{n-k-1})) \det((\lambda + k + 1)I - ((2^{k+1} - 1)J + B(\bar{Q}_{n-k-1}))),
\]
k = 1, 2, \ldots, n - 2.

If \( k = n - 2 \), then
\[
\det((\lambda + k + 1)I - ((2^{k+1} - 1)J + B(\bar{Q}_{n-k-1})))
\]
\[
= \det((\lambda + n - 2 + 1)I - (2^{n-2+1} - 1)J_2 + B(\bar{Q}_{n-(n-2)-1}))
\]
\[
= \det((\lambda + n - 1)I - (2^{n-1} - 1)J_2 + B(\bar{Q}_1))
\]
\[
= \det((\lambda + n - 1)I - (2^{n-1} - 1)J_2)
\]
\[
= P((2^{n-1} - 1)J_2, \lambda + n - 1).
\]
Thus we arrive at the conclusion that \( P(\bar{Q}, \lambda) = \prod_{k=0}^{n-2} (-B(Q_{n-k-1}), \lambda + k)P((2^{n-1} - 1)J_2, \lambda + n - 1) \), where \( n \geq 2 \).

Let \( E(\bar{Q}) \) is the (ordinary) energy of \( \bar{Q} \). Obviously, \( E(\bar{Q}_1) = 0 \), and \( E(\bar{Q}_2) = 4 \), for \( n > 2 \), we have

Theorem 3.2 Let \( \bar{Q} \) be the complement of \( n \)-dimensional hypercube \( Q_n \). Then \( E(\bar{Q}_n) = (n + 1)\binom{n}{2} + 2^n - 2n - 2 \), where \( n \geq 2 \).

Proof Let \( Q_j \) be \( j \)-dimensional hypercube, and \( q_{k,j} \) be the eigenvalue of \( B(Q_j) \), where \( j = 1, 2, \ldots, n - 1, k = 0, 1, 2, \ldots, j \). By Lemma 2.1, \( q_{k,j} = -j + 2k \) is the eigenvalue of \( -B(Q_j) \) too, and the eigenvalue \( q_{k,j} \) (of \( B(Q_j) \)) has multiplicity \( \binom{j}{k} \), \( k = 0, 1, 2, \ldots, j \). The eigenvalues of \( (2^{n-1} - 1)J_2 \) are 0 and \( 2^n - 2 \). By Lemma 2.2 and Lemma 3.1, The eigenvalues of \( \bar{Q} \) are
\[
0 - (n - 1), 2^n - 2 - (n - 1), -j + 2k - (n - 1 - j), \ j = 1, 2, \ldots, n - 1, k = 0, 1, 2, \ldots, j.
\]
i.e. \(-n + 1, 2^n - n - 1, -n + 1 + 2k, j = 1, 2, \cdots, n - 1, k = 0, 1, 2, \cdots, j\).

Hence \(E(Q_n) = \sum_{j=1}^{n-1} \sum_{k=0}^{j} |n - 1 + 2k| j \binom{j}{k} + |n - 1| + 2^n - n - 1|\)
\(= \sum_{k=0}^{n-1} \sum_{j=1}^{n-1} \binom{n}{k} + 2^n - 2\)
\(= \sum_{k=1}^{n-1} \sum_{j=1}^{n-1} \binom{n}{j+1} - \binom{n}{j} + 2^n - 2\)
\(= \sum_{k=0}^{n-1} \sum_{j=1}^{n-1} \binom{n}{k+1} + (n - 1)^2 + 2^n - 2\)
\(= \sum_{k=0}^{n-1} \sum_{j=1}^{n-1} \binom{n}{k+1} + 2^n - n - 1\)
\(= \sum_{k=0}^{n-1} \sum_{j=1}^{n-1} \binom{n}{k} + 2^n - 2n - 2\)
\(= \sum_{k=0}^{n-1} \binom{n}{k} + 2^n - n - 1\)
\(= \sum_{k=0}^{n-1} \binom{n}{k} + 2^n - n - 2\)
\(= 2(2^n - 1) + 2^n - n - 2\)

**Case 1.** If \(n\) is even, By Lemma 2.2(1), (3), we have
\(\sum_{k=0}^{n-1} \binom{n}{k} = 2^{n-1} + \frac{1}{2} \binom{n}{2}\),
\(\sum_{k=0}^{n-1} \binom{n}{k} = \sum_{k=0}^{n} k \binom{n}{k} = n2^{n-2}\).

Hence \(E(Q_n) = 2(2^n - 1) + 2^n - n - 2\)
\(= 2(2^n - 1) + 2^n - n - 2\)
\(= (n + 1) \binom{n}{2} + 2^n - n - 2\)

**Case 2.** If \(n\) is odd, By Lemma 2.2(1), (4), we have
\(\sum_{k=0}^{n-1} \binom{n}{k} = \sum_{k=0}^{n} k \binom{n}{k} = n2^{n-2} + \frac{n-1}{2} \binom{n}{2}\)
\(= n2^{n-2} + \frac{n-1}{2} \binom{n}{2}\). Hence
\(E(Q_n) = 2(2^n - 1) + 2^n - n - 2\)
\(= 2(2^n - 1) + 2^n - n - 2\)
\(= (n + 1) \binom{n}{2} + 2^n - n - 2\).

Combining above all cases we complete the proof.
Clearly, if \(n = 1\), then the theorem holds too.

4. The Laplacian energy of hypercubes and its complement

The simple graph \(G\) is \(k\)-regular if its each vertex degree is \(k\). Let \(G\) be an \(k\)-regular, and let \(s\) and \(t\) denote, respectively, the number of its vertices and edges. It is to show that if \(\lambda_1, \lambda_2, \cdots, \lambda_n\) are the eigenvalue of \(k\)-regular graph \(G\), then \(k - \lambda_1, k - \lambda_2, \cdots, k - \lambda_n\) are the (Laplacian) eigenvalues of \(D(G) - A(G)\).

Hence \(LE(G) = \sum_{j=1}^{s-1} |k - \lambda_j - \frac{\lambda_1}{s}| = \sum_{j=1}^{s} |k - \lambda_j - k| = \sum_{j=1}^{s} |\lambda_j| = E(G)\).

We have
Lemma 4.1  Let $G$ be an $k$-regular graph. Then $LE(G) = E(G)$.

Theorem 4.2 Let $n$ be an integer, $n \geq 1$. Then

1. $LE(Q_n) = E(Q_n) = 2\left\lceil \frac{n}{2} \right\rceil \left(\frac{n}{2}\right)$;
2. $LE(\bar{Q}_n) = E(\bar{Q}_n) = (n + 1)\left(\frac{n}{2}\right) + 2^n - 2n - 2$;
3. $E(Q_n) + E(\bar{Q}_n) = LE(Q_n) + LE(\bar{Q}_n)$
   $= (n + 2\left\lceil \frac{n}{2} \right\rceil + 1)\left(\frac{n}{2}\right) + 2^n - 2n - 2$.

Proof  Obviously, $Q_n$ and $\bar{Q}_n$ are $n$-regular and $(2^n - n - 1)$-regular respectively. From Theorem 2.3, Theorem 3.2 and Lemma 4.1, it is evident to see that the theorem holds.

Remark 4.3  A graph is called integral if its spectrum consists entirely of integers. By Lemma 2.1 and Lemma 3.1, we have that $Q_n$ and $\bar{Q}_n$ are integral.

Remark 4.4  Suppose $G$ is a graph of order $n$. $G$ is called hyperenergetic if the energy $E(G)$ of $G$ satisfies $E(G) > 2(n - 1)$ . It is easy to prove that $E(Q_n) = 2\left\lceil \frac{n}{2} \right\rceil \left(\frac{n}{2}\right) > 2(2^n - 1)$, where $n \geq 7$ , and $E(\bar{Q}_n) = (n + 1)\left(\frac{n}{2}\right) + 2^n - 2n - 2 > 2(2^n - 1)$, where $n \geq 5$. Clearly, $Q_n$ and $\bar{Q}_n$ are hyperenergetic.

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References


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