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Various energies of random graphs[1]

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Abstract

In 1970s, Gutman introduced the concept of energy $E(G)$ for a simple graph G, which is defined as the sum of the absolute values of the eigenvalues of G and can be used to estimate the total π-electron energy in conjugated hydrocarbons. The concept attracted lots of attention and furthermore, some other similar notions were also considered such as Laplacian energy $LE(G)$, signless Laplacian energy $LE^+(G)$, incidence energy $IE(G)$, distance energy $DE(G)$ and Lapacian-energy like invariant $LEL(G)$. Moreover, many researchers established a large number of upper and lower bounds for those invariants. But there are only a few graphs attaining the equalities of those bounds. In the present paper, however, we present exact estimates of $LEL(G)$, $IE(G)$, and $DE(G)$, and a tight bound of $LE^+(G)$ for almost all graphs by probabilistic and algebraic approaches.

1 Introduction

Throughout this paper, G stands for a simple graph on vertex set $[n] = \{1, \ldots, n\}$. The eigenvalues $\lambda_1, \ldots, \lambda_n$ of the adjacency matrix $\mathbf{A}(G) = (a_{ij})_{n\times n}$ (or $\mathbf{A}$ for short) are said to be the *eigenvalues of* G. In chemistry, there is a closed relation between the molecular orbital energy levels of π-electrons in conjugated hydrocarbons and the eigenvalues of the corresponding molecular graph. For the Hückel molecular orbital approximation, the total π-electron energy in conjugated hydrocarbons is given by

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the sum of absolute values of the eigenvalues corresponding to the molecular graph G in which the maximum degree is not more than three in general. In 1970s, Gutman [6] extended the concept of energy to all simple graphs G, and defined the *energy of* G as

$$E(G) = \sum_{i=0}^{n} |\lambda_i| \tag{1}$$

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of G. Evidently, one can immediately get the energy of a graph by computing the eigenvalues of the graph. Unfortunately, it is rather hard to deal directly with even the special case, $(0,1)$-matrix $\mathbf{A}$. So, many researchers established a lot of lower and upper bounds to estimate the invariant for some classes of graphs. For further details, we refer readers to the comprehensive survey [9]. But there is a common flaw of those inequalities that only a few graphs attain the equalities of those bounds. Consequently one can hardly see the major behavior of the invariant $E(G)$ for most graphs with respect to other graph parameters ($|V(G)|$, for instance). However, it is surprising that one can employ probabilistic and algebraic approaches to obtain an exact estimate of energy for almost all graphs. For instance, it was shown in [4] that almost every graph $G_n(p)$ in $\mathcal{G}_n(p)$ satisfies

$$E(G_n(p)) = \left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right) \cdot n^{3/2} \tag{2}$$

where $\mathcal{G}_n(p)$ stands for the Erdős–Rényi random graph model and p is a constant with $0 < p < 1$.

Recently, several other energy-like quantities to be presented below, such as Laplacian energy, signless Laplacian energy, Laplacian-energy like invariant, incidence energy, and distance energy, have been proposed and studied in the mathematical and mathematico-chemical literature.

For the convenience of description, we first present the notion of energy of a matrix. Let $\mathbf{X}$ be a real symmetric matrix of order n, and $\lambda_1(\mathbf{X}), \ldots, \lambda_n(\mathbf{X})$ the eigenvalues of $\mathbf{X}$. We define the *energy of* $\mathbf{X}$ as

$$E(\mathbf{X}) = \sum_{i=1}^{n} |\lambda_i(\mathbf{X})| \,.$$

Accordingly, $E(G) = E(\mathbf{A})$. The *Laplacian matrix of* G is defined as $\mathbf{L}(G) = \mathbf{\Delta}(G) - \mathbf{A}(G)$, where $\mathbf{\Delta}(G)$ is the diagonal matrix in which every diagonal entry is equal to the degree of the corresponding vertex. In what follows, we shall sometimes use $\mathbf{L}$ and $\mathbf{\Delta}$ to denote $\mathbf{L}(G)$ and $\mathbf{\Delta}(G)$, respectively. Supposing that $\lambda_1(\mathbf{L}), \ldots, \lambda_n(\mathbf{L})$ are the eigenvalues of $\mathbf{L}$, Gutman and Zhou [10] defined the *Laplacian energy of* G as

$$LE = LE(G) = E\left(\mathbf{\Delta} - \mathbf{A} - \frac{2m}{n}\mathbf{I}\right) = \sum_{i=1}^{n} \left|\lambda_i(\mathbf{L}) - \frac{2m}{n}\right|$$

where m is the number of edges of G and $\mathbf{I}$ is the unit matrix of order n. It was shown in [4] that for almost every graph $G_n(p) \in \mathcal{G}_n(p)$, the Laplacian energy of $G_n(p)$ satisfies the following bounds

$$\left(\frac{2\sqrt{2}}{3}\sqrt{p(1-p)} + o(1)\right) \cdot n^{3/2} \le LE(G_n(p)) \le \left(\sqrt{2} \cdot \sqrt{p(1-p)} + o(1)\right) \cdot n^{3/2}\ . \quad (3)$$

The signless Lapacian energy of G is directly relevant to the *signless Lapacian matrix of* G, which is defined as $\mathbf{L}^+ = \mathbf{L}^+(G) = \mathbf{\Delta}(G) + \mathbf{A}(G)$. Supposing that $\lambda_1(\mathbf{L}^+), \ldots, \lambda_n(\mathbf{L}^+)$ are the eigenvalues of $\mathbf{L}^+$, So *et al.* [18] defined the *signless Lapacian energy of* G as

$$LE^+ = LE^+(G) = E\left(\mathbf{\Delta} + \mathbf{A} - \frac{2m}{n}\mathbf{I}\right) = \sum_{i=1}^{n} \left|\lambda_i(\mathbf{L}^+) - \frac{2m}{n}\right|$$

where m is the number of edges of G. Furthermore, Liu *et al.* [12] proposed a *Laplacian-energy-like invariant*, which is defined as

$$LEL = LEL(G) = \sum_{i=1}^{n} \sqrt{\lambda_i(\mathbf{L})}\ .$$

Gutman *et al.* pointed out in [11] that LEL is more similar to E than to LE.

Moreover, Jooyandeh *et al.* [15] introduced the *incidence energy* IE *of* G, which is defined as the sum of the singular values of the incidence matrix of G. Gutman *et al.* [7] showed that

$$IE = IE(G) = \sum_{i=1}^{n} \sqrt{\lambda_i(\mathbf{L}^+)}\ .$$

Finally, we present the concept of distance energy of G. Let $\mathbf{D} = \mathbf{D}(G)$ be the *distance matrix of* G in which the entry $\mathbf{D}(i,j)$ is equal to the distance between vertices i and j. Indulal *et al.* [14] defined the *distance energy of* G as

$$DE = DE(G) = E(\mathbf{D}) = \sum_{i=1}^{n} |\lambda_i(\mathbf{D})|\ .$$

Some upper and lower bounds were established for those energy-like quantities so far. For instance, we refer readers to [8, 13, 16, 17] for further details. Those inequalities, however, have a common flaw similar to $E(G)$ that only a few graphs attain the equalities of the bounds. In this paper, we employ probabilistic and algebraic approaches to investigate those energy-like quantities, and present exact estimates of LEL, IE and DE, and a tight bound of LE^+ like (3) for almost all graphs.

2 The estimates of LE^+, LEL, IE, and DE for random graphs

In this section, we shall present the estimates of LE^+, LEL, IE, and DE for random graphs. Let us begin with the Erdős–Rényi model $\mathcal{G}_n(p)$ of random graphs, which consists of all simple graphs with vertex set $[n]$ in which the edges are chosen independently with probability p. Throughout this paper, we assume p is a constant with $0 < p < 1$ for the convenience of description. In fact, one can obtain similar results to be formulated below for a larger range of p (for instance, $p = p(n) \to c$, $n \to \infty$ and $0 < c < 1$). Evidently, the adjacency matrix $\mathbf{A}(G_n(p))$ (we still abbreviate it to $\mathbf{A}$) of a random graph $G_n(p) \in \mathcal{G}_n(p)$ is a random matrix whose entries are i.i.d random variables with Bernoulli distribution. For the model $\mathcal{G}_n(p)$, we shall estimate those energy-like quantities by using probabilistic and algebraic approaches to be presented below.

Throughout this paper, following the term introduced in Bollobás's book [2], we say that *almost every* (a.e.) graph $G_n(p)$ in $\mathcal{G}_n(p)$ has a certain property Q if the probability that $G_n(p)$ has Q converges to 1 as n tends to infinity. Sometimes, we may use *"almost all"* instead of "almost every". Evidently, if the probability of random graphs satisfying Q converges almost surely (a.s.), we can deduce that almost every graph in $\mathcal{G}_n(p)$ has Q.

First, we estimate LE^+ for random graphs $G_n(p)$ in $\mathcal{G}_n(p)$ by virtue of (2), (3) and the following lemma.

Lemma 1 (Fan Ky's inequality [5]). *Let $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ be real symmetric matrices of order n such that $\mathbf{X} + \mathbf{Y} = \mathbf{Z}$. Then*

$$E(\mathbf{X}) + E(\mathbf{Y}) \geq E(\mathbf{Z}) \ .$$

Set $\widehat{\mathbf{L}}^+ = \mathbf{\Delta} + \mathbf{A} - \frac{2m}{n}\mathbf{I}$ and $\widehat{\mathbf{L}} = \mathbf{\Delta} - \mathbf{A} - \frac{2m}{n}\mathbf{I}$. In accordance with the definitions of LE^+ and LE, one can readily see that $LE^+ = E(\widehat{\mathbf{L}}^+)$ and $LE = E(\widehat{\mathbf{L}})$. Applying Lemma 1 to $\widehat{\mathbf{L}}^+ = \widehat{\mathbf{L}} + 2\mathbf{A}$ and $\widehat{\mathbf{L}}^+ + (-\widehat{\mathbf{L}}) = 2\mathbf{A}$, we have

$$2E(\mathbf{A}) - E(\widehat{\mathbf{L}}) \leq E(\widehat{\mathbf{L}}^+) \leq 2E(\mathbf{A}) + E(\widehat{\mathbf{L}}) \; .$$

According to the inequality (3), a.e. graph $G_n(p)$ in $\mathcal{G}_n(p)$ satisfies

$$LE(G_n(p)) = E(\widehat{\mathbf{L}}) \leq \left(\sqrt{2} \cdot \sqrt{p(1-p)} + o(1)\right) \cdot n^{3/2} \; .$$

Using the equation (2), we thus obtain that for a.e. graph $G_n(p)$, the following inequalities hold

$$\left[\left(\frac{16}{3\pi} - \sqrt{2}\right) \cdot \sqrt{p(1-p)} + o(1)\right] \cdot n^{3/2} \leq E\left(\widehat{\mathbf{L}}^+[G_n(p)]\right) \leq$$
$$\left[\left(\frac{16}{3\pi} + \sqrt{2}\right) \cdot \sqrt{p(1-p)} + o(1)\right] \cdot n^{3/2} \; .$$

Consequently, the following theorem is relevant.

Theorem 2. *A.e. graph $G_n(p)$ in $\mathcal{G}_n(p)$ satisfies the following inequalities*

$$\left[\left(\frac{16}{3\pi} - \sqrt{2}\right) \cdot \sqrt{p(1-p)} + o(1)\right] \cdot n^{3/2} \leq LE^+(G_n(p)) \leq$$
$$\left[\left(\frac{16}{3\pi} + \sqrt{2}\right) \cdot \sqrt{p(1-p)} + o(1)\right] \cdot n^{3/2} \; .$$

Next, we explore LEL and IE for random graphs $G_n(p)$ in $\mathcal{G}_n(p)$. In fact, we shall present the explicit information about the eigenvalues of the corresponding matrices. We start with a useful lemma concerning the asymptotic of the spectral radius $||\mathbf{M}||$ of a random matrix $\mathbf{M}$.

Lemma 3 (**Bryc** *et al.* **[3]).** *Suppose $\mathbf{X}$ is a real symmetric random matrix of order n in which the entries on the diagonal are zeros and $\mathbf{X}(ij)$, $1 \leq i < j$, are i.i.d random variables with mean zero and variance one. Furthermore, we assume that the fourth moments of $\mathbf{X}(ij)$, $1 \leq i < j$, are finite. Set $\mathbf{S} = diag(\sum_{i \neq j} \mathbf{X}(ij))_{1 \leq i \leq n}$ and $\mathbf{M} = \mathbf{S} - \mathbf{X}$. Then*

$$\lim_{n \to \infty} \frac{||\mathbf{M}||}{\sqrt{2n \log n}} = 1 \;\; a.s.$$

Let $\mathbf{L} = \mathbf{L}(G_n(p))$ be the Laplacian matrix of a random graph $G_n(p)$. Setting $\mathbf{R} = p(n-1)\mathbf{I} - p(\mathbf{J} - \mathbf{I})$ where $\mathbf{J}$ is the matrix of order n in which all entries equal 1, we define an auxiliary matrix $\overline{\mathbf{L}}$ as

$$\overline{\mathbf{L}} = \mathbf{L} - \mathbf{R}$$

i. e., $\overline{\mathbf{L}} = \left(\mathbf{\Delta} - p(n-1)\mathbf{I}\right) - \left(\mathbf{A} - p(\mathbf{J} - \mathbf{I})\right)$. It is not difficult to verify that the random matrix $\left(p(1-p)\right)^{-1/2}\overline{\mathbf{L}}$ satisfies the conditions of Lemma 3. Consequently,

$$\lim_{n\to\infty} \frac{||\overline{\mathbf{L}}||}{\sqrt{2p(1-p)n\log n}} = 1 \text{ a.s.}$$

and thus,

$$\lim_{n\to\infty} \frac{||\overline{\mathbf{L}}||}{n} = 0 \text{ a.s.}$$

i. e., $||\overline{\mathbf{L}}|| = o(1)n$ a.s. In order to estimate the eigenvalues of $\mathbf{L}$, we need the famous result below.

Lemma 4 (**Weyl's Inequality** [19])**.** *If* $\mathbf{X}$, $\mathbf{Y}$, *and* $\mathbf{Z}$ *are all* $n \times n$ *real symmetric matrices, and* $\mathbf{X} = \mathbf{Y} + \mathbf{Z}$ *where* $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ *have eigenvalues, respectively,* $\lambda_1(\mathbf{X}) \geq \cdots \geq \lambda_n(\mathbf{X})$, $\lambda_1(\mathbf{Y}) \geq \cdots \geq \lambda_n(\mathbf{Y})$, $\lambda_1(\mathbf{Z}) \geq \cdots \geq \lambda_n(\mathbf{Z})$, *then*

$$\lambda_i(\mathbf{Y}) + \lambda_n(\mathbf{Z}) \leq \lambda_i(\mathbf{X}) \leq \lambda_i(\mathbf{Y}) + \lambda_1(\mathbf{Z}) \ .$$

Since $\overline{\mathbf{L}} + \mathbf{R} = \mathbf{L}$, it follows from Lemma 4 that

$$\lambda_i(\mathbf{R}) + \lambda_n(\overline{\mathbf{L}}) \leq \lambda_i(\mathbf{L}) \leq \lambda_i(\mathbf{R}) + \lambda_1(\overline{\mathbf{L}}) \ .$$

Moreover, it is easy to see that the eigenvalues of $\mathbf{R}$ are pn (with multiplicity $n-1$) and 0 (with multiplicity 1). Therefore, by the fact that $||\overline{\mathbf{L}}|| = o(1)n$ a.s., the eigenvalues of $\mathbf{L}$ satisfy a.s. the following

$$\lambda_i(\mathbf{L}) = (p + o(1))n, \ 1 \leq i \leq n-1, \text{ and } \lambda_n(\mathbf{L}) = o(1)n \ .$$

Consequently, by the definition of LEL, a.e. random graph $G_n(p)$ satisfies

$$LEL(G_n(p)) = \sum_{i=1}^{n-1} \sqrt{(p + o(1))n} + \sqrt{o(1)n} = (\sqrt{p} + o(1))n^{3/2} \ .$$

We thus obtain the result below.

Theorem 5. *A.e. graph* $G_n(p)$ *in* $\mathcal{G}_n(p)$ *satisfies the relation*

$$LEL(G_n(p)) = (\sqrt{p} + o(1))n^{3/2} \ .$$

In accordance with the definition of $\mathbf{L}^+$, we have $\mathbf{L}^+ = \mathbf{L} + 2\mathbf{A}$. We shall estimate $E(\mathbf{L}^+)$ by the relation between the eigenvalues of $\mathbf{L}$ and $\mathbf{L}^+$.

Lemma 6 (**Bai** [1])**.** *Let* $\mathbf{A}$ *be the adjacency matrix of a random graph* $G_n(p)$*, and let* $\mathbf{A}' = \mathbf{A} - p(\mathbf{J} - \mathbf{I})$ *. Then*

$$\lim_{n\to\infty} ||n^{-1/2}\mathbf{A}'|| = 2\sqrt{p(1-p)} \ a.s.$$

Since $\mathbf{A} = \mathbf{A}' + p(\mathbf{J} - \mathbf{I})$, it follows from Lemma 4 that

$$p\lambda_i(\mathbf{J} - \mathbf{I}) + \lambda_n(\mathbf{A}') \leq \lambda_i(\mathbf{A}) \leq p\lambda_i(\mathbf{J} - \mathbf{I}) + \lambda_1(\mathbf{A}') \ .$$

It is easy to get that $\lambda_1(\mathbf{J}-\mathbf{I}) = n-1$, $\lambda_2(\mathbf{J}-\mathbf{I}) = \cdots = \lambda_n(\mathbf{J}-\mathbf{I}) = -1$. Moreover, by Lemma 6, we have $||\mathbf{A}'|| = O(n^{1/2})$ a.s. Thus, the eigenvalues of $\mathbf{A}$ satisfy a.s. the following

$$\lambda_1(\mathbf{A}) = O(n) \text{ and } \lambda_i(\mathbf{A}) = O(n^{1/2}) \ , \ 2 \leq i \leq n \ .$$

Since $\mathbf{L}^+ = \mathbf{L} + 2\mathbf{A}$, it follows again from Lemma 4 that

$$\lambda_i(\mathbf{L}^+) \leq 2\lambda_i(\mathbf{A}) + \lambda_1(\mathbf{L})$$

and

$$\lambda_i(\mathbf{L}^+) \geq \lambda_i(\mathbf{L}) + 2\lambda_n(\mathbf{A}) \ .$$

Consequently, together with the estimates of the eigenvalues of $\mathbf{L}$ and $\mathbf{A}$, the following relation holds a.s.

$$\lambda_1(\mathbf{L}^+) = O(n)$$

$$\lambda_i(\mathbf{L}^+) = (p + o(1))n, 1 < i < n$$

and

$$\lambda_n(\mathbf{L}^+) = O(n^{1/2}) \ .$$

Therefore, it follows that

$$\begin{aligned} IE(G_n(p)) &= \sqrt{(p+o(1))n} \cdot (n-2) + \sqrt{\lambda_1(\mathbf{L}^+)} + \sqrt{\lambda_n(\mathbf{L}^+)} \\ &= (\sqrt{p} + o(1))n^{3/2} \text{ a.s.} \end{aligned}$$

Hence, the following result is relevant.

Theorem 7. *A.e. graph* $G_n(p)$ *in* $\mathcal{G}_n(p)$ *satisfies the relationj*

$$IE(G_n(p)) = (\sqrt{p} + o(1))n^{3/2} \ .$$

Finally, we investigate the distance energy DE for random graphs in $\mathcal{G}_n(p)$, and use $\mathbf{D} = \mathbf{D}(G_n(p))$ to denote the distance matrix of a random graph $G_n(p)$. Recall that the diameter of a graph G is the greatest distance between two vertices of G. In order to estimate $DE(G_n(p))$, we first present a result due to Bollobás [2]:

Lemma 8. *Suppose $p^2n - 2\log n \to \infty$ and $n^2(1-p) \to \infty$. Then a.e. graph $G_n(p)$ in $\mathcal{G}_n(p)$ has diameter 2.*

Since p is a constant with $0 < p < 1$ in this paper, it follows from Lemma 8 that a.e. graph $G_n(p)$ has diameter 2. Let $\mathcal{D}_n(p)$ be a subset of $\mathcal{G}_n(p)$ consisting of graphs with diameter 2. By virtue of Lemma 8, we have

$$\lim_{n\to\infty} \frac{|\mathcal{D}_n(p)|}{|\mathcal{G}_n(p)|} = 1 \,. \tag{4}$$

In accordance with the definition of the term "almost every", if we prove that a.e. graph $G_n(p)$ in $\mathcal{D}_n(p)$ has a certain property Q, then so is in $\mathcal{G}_n(p)$. Thus, to estimate $DE(G_n(p))$ for graphs $G_n(p) \in \mathcal{G}_n(p)$, it suffices to do it for $\mathcal{D}_n(p)$.

Let $G_n(p)$ be a random graph in $\mathcal{D}_n(p)$. Evidently, the entries of $\mathbf{D}(G_n(p))$ satisfy the following

$$\mathbf{D}(ij) = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if } i \text{ and } j \text{ are adjacent} \\ 2 & \text{if } i \text{ and } j \text{ are nonadjacent.} \end{cases}$$

Consequently,

$$\mathbf{D} = 2(\mathbf{J} - \mathbf{I}) - \mathbf{A} \,. \tag{5}$$

According to relations (2) and (4), a.e. graph $G_n(p)$ in $\mathcal{D}_n(p)$ satisfies the relation

$$E(G_n(p)) = E(\mathbf{A}) = \left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1) \right) n^{3/2} \,.$$

Furthermore, applying Lemma 1 to $\mathbf{D} = 2(\mathbf{J}-\mathbf{I}) - \mathbf{A}$ and $\mathbf{A} = 2(\mathbf{J}-\mathbf{I}) - \mathbf{D}$, we have $E(\mathbf{D}) \le 2E(\mathbf{J}-\mathbf{I}) + E(-\mathbf{A})$ and $E(\mathbf{A}) \le 2E(\mathbf{J}-\mathbf{I}) + E(-\mathbf{D})$. Thus,

$$E(\mathbf{A}) - 2E(\mathbf{J}-\mathbf{I}) \le E(\mathbf{D}) \le E(\mathbf{A}) + 2E(\mathbf{J}-\mathbf{I}) \,.$$

It is easy to see that $E(\mathbf{J}-\mathbf{I}) = 2(n-1)$. Consequently, a.e. graph $G_n(p)$ in $\mathcal{D}_n(p)$ satisfies

$$DE(G_n(p)) = E(\mathbf{D}) = \left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1) \right) n^{3/2} \,.$$

Therefore, we obtain the result below.

Theorem 9. *A.e. graph $G_n(p)$ in $\mathcal{G}_n(p)$ obeys the relation*

$$DE(G_n(p)) = \left(\frac{8}{3\pi}\sqrt{p(1-p)} + o(1)\right) n^{3/2} \ .$$

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