

The Laplacian energy of random graphs*

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Abstract

Gutman *et al.* introduced the concepts of energy $\mathcal{E}(G)$ and Laplacian energy $\mathcal{E}_L(G)$ for a simple graph G , and furthermore, they proposed a conjecture that for every graph G , $\mathcal{E}(G)$ is not more than $\mathcal{E}_L(G)$. Unfortunately, the conjecture turns out to be incorrect since Liu *et al.* and Stevanović *et al.* constructed counterexamples. However, So *et al.* verified the conjecture for bipartite graphs. In the present paper, we obtain, for a random graph, the lower and upper bounds of the Laplacian energy, and show that the conjecture is true for almost all graphs.

Keywords: eigenvalues, graph energy, Laplacian energy, random graph, random matrices, empirical spectral distribution, limiting spectral distribution.

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1 Introduction

Throughout this paper, G denotes a simple graph of order n . The eigenvalues $\lambda_1, \dots, \lambda_n$ of the adjacency matrix $\mathbf{A}(G) = (a_{ij})_{n \times n}$ 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 the sum of absolute values of the eigenvalues corresponding to the molecular graph G in which the maximum degree is not more than 4 in general. In 1970s, Gutman [9] extended the concept of energy to all simple graphs G , and defined that

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

where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of G . Evidently, one can immediately get the energy of a graph by computing the eigenvalues of the graph. It is rather hard, however, to compute the eigenvalues for a large matrix, even for a large symmetric (0,1)-matrix like

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$\mathbf{A}(G)$. 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 [11]. But there is a common flaw for those inequalities that only a few graphs attain the equalities of those bounds. Consequently we can hardly see the major behavior of the invariant $\mathcal{E}(G)$ for most graphs with respect to other graph parameters ($|V(G)|$, for instance). In the next section, however, we shall present an exact estimate of the energy for almost all graphs by Wigner's semi-circle law.

In spectral graph theory, the matrix $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$ is called *Laplacian matrix of G* , where $\mathbf{D}(G)$ is a diagonal matrix in which d_{ii} equals the degree $d_G(v_i)$ of the vertex v_i , $i = 1, \dots, n$. Gutman *et al.* [12] introduced a new matrix $\bar{\mathbf{L}}(G)$ for a simple graph G , *i.e.*,

$$\bar{\mathbf{L}}(G) = \mathbf{L}(G) - \sum_{i=1}^n d_G(v_i)/n \mathbf{I}_n = \mathbf{L}(G) - 2 \sum_{i=1}^n \sum_{j>i} a_{ij}/n \mathbf{I}_n,$$

where \mathbf{I}_n is the unit matrix of order n , and defined the *Laplacian energy $\mathcal{E}_L(G)$ of G* , *i.e.*,

$$\mathcal{E}_L(G) = \sum_{i=1}^n |\zeta_i|,$$

where ζ_1, \dots, ζ_n are the eigenvalues of $\bar{\mathbf{L}}(G)$. Obviously, we can easily evaluate the Laplacian energy $\mathcal{E}_L(G)$ if we could obtain the eigenvalues of $\bar{\mathbf{L}}(G)$. In Section 3 we shall establish the lower and upper bounds of the Laplacian energy for almost all graphs by exploring the spectral distribution of the matrix $\bar{\mathbf{L}}(G_n(p))$ for a random graph $G_n(p)$ constructed from the classical Erdős–Rényi model (see [3]).

In a recent paper [10], Gutman *et al.* proposed the following conjecture concerning the relation between the energy and the Laplacian energy of a graph.

Conjecture 1. *Let G be a simple graph. Then $\mathcal{E}(G) \leq \mathcal{E}_L(G)$.*

Unfortunately, the conjecture turns out to be incorrect. In fact, Liu *et al.* [14] and Stevanović *et al.* [19] constructed two classes of graphs violating the assertion. However, So *et al.* [17] proved that the conjecture is true for bipartite graphs. We shall show that the conjecture above is true for almost all graphs by comparing the energy with the Laplacian energy of a random graph in the third section.

2 The energy of $G_n(p)$

In this section, we shall formulate an exact estimate of the energy for almost all graphs by Wigner's semi-circle law.

We start by recalling the Erdős–Rényi model $\mathcal{G}_n(p)$ (see [3]), which consists of all graphs with vertex set $[n] = \{1, 2, \dots, n\}$ in which the edges are chosen independently with probability $p = p(n)$. Apparently, the adjacency matrix $\mathbf{A}(G_n(p))$ of the random graph $G_n(p) \in \mathcal{G}_n(p)$ is a random matrix, and thus one can readily evaluate the energy of $G_n(p)$ once the spectral distribution of the random matrix $\mathbf{A}(G_n(p))$ is known.

In fact, the research on the spectral distributions of random matrices is rather abundant and active, which can be traced back to [24]. We refer readers to [1, 6, 15] for an

overview and some spectacular progress in this field. One important achievement in that field is Wigner's semi-circle law which characterizes the limiting spectral distribution of the empirical spectral distribution of eigenvalues for a sort of random matrix.

In order to characterize the statistical properties of the wave functions of quantum mechanical systems, Wigner in 1950s investigated the spectral distribution for a sort of random matrix, so-called *Wigner matrix*,

$$\mathbf{X}_n := (x_{ij}), \quad 1 \leq i, j \leq n,$$

which satisfies the following properties:

- x_{ij} 's are independent random variables with $x_{ij} = x_{ji}$;
- the x_{ii} 's have the same distribution F_1 , while the x_{ij} 's ($i \neq j$) are to possess the same distribution F_2 ;
- $\text{Var}(x_{ij}) = \sigma_2^2 < \infty$ for all $1 \leq i < j \leq n$.

We denote the eigenvalues of \mathbf{X}_n by $\lambda_{1,n}, \lambda_{2,n}, \dots, \lambda_{n,n}$, and their empirical spectral distribution (ESD) by

$$\Phi_{\mathbf{X}_n}(x) = \frac{1}{n} \cdot \#\{\lambda_{i,n} \mid \lambda_{i,n} \leq x, i = 1, 2, \dots, n\}.$$

Wigner [22, 23] considered the limiting spectral distribution (LSD) of \mathbf{X}_n , and obtained the semi-circle law.

Theorem 1. *Let \mathbf{X}_n be a Wigner matrix. Then*

$$\lim_{n \rightarrow \infty} \Phi_{n^{-1/2}\mathbf{X}_n}(x) = \Phi(x) \text{ a.s.}$$

i.e., with probability 1, the ESD $\Phi_{n^{-1/2}\mathbf{X}_n}(x)$ converges weakly to a distribution $\Phi(x)$ as n tends to infinity, where $\Phi(x)$ has the density

$$\phi(x) = \frac{1}{2\pi\sigma_2^2} \sqrt{4\sigma_2^2 - x^2} \mathbf{1}_{|x| \leq 2\sigma_2}.$$

Remark. It is interesting that the existence of the second moment of the off-diagonal entries is the necessary and sufficient condition for the semi-circle law, and there is no moment requirement on the diagonal elements. Furthermore, we can get more information about spectra of Wigner matrices. Set $\mu_i = \int x dF_i$ ($i = 1, 2$) and

$$\bar{\mathbf{X}}_n = \mathbf{X}_n - \mu_1 \mathbf{I}_n - \mu_2 (\mathbf{J}_n - \mathbf{I}_n),$$

where \mathbf{J}_n is the all 1's matrix. One can easily check that each entry of $\bar{\mathbf{X}}_n$ has mean 0. By means of Wigner's trace method, one can show that the spectral radius $\rho(n^{-1/2}\bar{\mathbf{X}}_n)$ converges to $2\sigma_2$ with probability 1 as n tends to infinity (see Theorem 2 in [8], for instance). For further comments on Wigner's semi-circle law, we refer readers to the extraordinary survey by Bai [1].

Following the book [3], we will say that *almost every* (a.e.) graph in $\mathcal{G}_n(p)$ has a certain property Q if the probability that a random graph $G_n(p)$ has the property Q converges to 1 as n tends to infinity. Occasionally, we shall write *almost all* instead of almost every. It is easy to see that if F_1 is a *pointmass at 0*, i.e., $F_1(x) = 1$ for $x \geq 0$ and $F_1(x) = 0$ for $x < 0$, and F_2 is the *Bernoulli distribution with mean p* , then the Wigner matrix \mathbf{X}_n coincides with the adjacency matrix of $G_n(p)$. Obviously, $\sigma_2 = \sqrt{p(1-p)}$ in this case.

To establish the exact estimate of the energy $\mathcal{E}(G_n(p))$ for a.e. graph $G_n(p)$, we first present some notions and assertions. In what follows, we shall use \mathbf{A} to denote the adjacency matrix $\mathbf{A}(G_n(p))$ for convenience. Set

$$\overline{\mathbf{A}} = \mathbf{A} - p(\mathbf{J}_n - \mathbf{I}_n).$$

Evidently, $\overline{\mathbf{A}}$ is a Wigner matrix. By means of Theorem 1, we have

$$\lim_{n \rightarrow \infty} \Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) = \Phi(x) \text{ a.s.} \quad (1)$$

It is easy to check that each entry of $\overline{\mathbf{A}}$ has mean 0. According to the remark above,

$$\lim_{n \rightarrow \infty} \rho(n^{-1/2}\overline{\mathbf{A}}) = 2\sigma_2 \text{ a.s.} \quad (2)$$

We further define the *energy* $\mathcal{E}(\mathbf{M})$ of a matrix \mathbf{M} as the sum of absolute values of the eigenvalues of \mathbf{M} . By virtue of Equation (1) and (2), we shall formulate an estimate of the energy $\mathcal{E}(\overline{\mathbf{A}})$, and then establish the exact estimate of $\mathcal{E}(\mathbf{A}) = \mathcal{E}(G_n(p))$ using Lemma 2.

According to Equation (2), for any given $\epsilon > 0$, there exists an integer N such that with probability 1, for all $n > N$ the spectral radius $\rho(n^{-1/2}\overline{\mathbf{A}})$ is not more than $2\sigma_2 + \epsilon$. Since the density $\phi(x)$ of $\Phi(x)$ is bounded on \mathbb{R} , invoking Equation (1) and bounded convergence theorem yields that for all $n > N$,

$$\begin{aligned} \lim_{n \rightarrow \infty} \int |x| d\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) &= \lim_{n \rightarrow \infty} \int_{-2\sigma_2 - \epsilon}^{2\sigma_2 + \epsilon} |x| d\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) \text{ a.s.} \\ &= \int_{-2\sigma_2 - \epsilon}^{2\sigma_2 + \epsilon} |x| d\Phi(x) \text{ a.s.} \\ &= \int |x| d\Phi(x). \end{aligned} \quad (3)$$

We now turn to the estimate of the energy $\mathcal{E}(\overline{\mathbf{A}})$. Suppose $\overline{\lambda}_1, \dots, \overline{\lambda}_n$ and $\overline{\lambda}'_1, \dots, \overline{\lambda}'_n$ are the eigenvalues of $\overline{\mathbf{A}}$ and $n^{-1/2}\overline{\mathbf{A}}$, respectively. Clearly, $\sum_{i=1}^n |\overline{\lambda}_i| = n^{1/2} \sum_{i=1}^n |\overline{\lambda}'_i|$. By

Equation (3), we can deduce that

$$\begin{aligned}
\mathcal{E}(\overline{\mathbf{A}})/n^{3/2} &= \frac{1}{n^{3/2}} \sum_{i=1}^n |\overline{\lambda}_i| \\
&= \frac{1}{n} \sum_{i=1}^n |\overline{\lambda}'_i| \\
&= \int |x| d\Phi_{n^{-1/2}\overline{\mathbf{A}}}(x) \\
&\rightarrow \int |x| d\Phi(x) \text{ a.s. } (n \rightarrow \infty) \\
&= \frac{1}{2\pi\sigma_2^2} \int_{-2\sigma_2}^{2\sigma_2} |x| \sqrt{4\sigma_2^2 - x^2} dx \\
&= \frac{8}{3\pi}\sigma_2 = \frac{8}{3\pi}\sqrt{p(1-p)}.
\end{aligned}$$

Therefore, with probability 1, the energy $\mathcal{E}(\overline{\mathbf{A}})$ enjoys the equation as follows:

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

We proceed to investigate $\mathcal{E}(\mathbf{A}) = \mathcal{E}(G_n(p))$ and present the following result due to Fan.

Lemma 2 (Fan [7]). *Let $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ be real symmetric matrices of order n such that $\mathbf{X} + \mathbf{Y} = \mathbf{Z}$, then*

$$\sum_{i=1}^n |\lambda_i(\mathbf{X})| + \sum_{i=1}^n |\lambda_i(\mathbf{Y})| \geq \sum_{i=1}^n |\lambda_i(\mathbf{Z})|$$

where $\lambda_i(\mathbf{M})$ ($i = 1, \dots, n$) is an eigenvalue of the matrix \mathbf{M} .

It is not difficult to verify that the eigenvalues of the matrix $\mathbf{J}_n - \mathbf{I}_n$ are $n - 1$ and -1 of $n - 1$ times. Consequently $\mathcal{E}(\mathbf{J}_n - \mathbf{I}_n) = 2(n - 1)$. One can readily see that $\mathcal{E}(p(\mathbf{J}_n - \mathbf{I}_n)) = p\mathcal{E}(\mathbf{J}_n - \mathbf{I}_n)$. Thus,

$$\mathcal{E}(p(\mathbf{J}_n - \mathbf{I}_n)) = 2p(n - 1).$$

Since $\mathbf{A} = \overline{\mathbf{A}} + p(\mathbf{J}_n - \mathbf{I}_n)$, it follows from Lemma 2 that with probability 1,

$$\begin{aligned}
\mathcal{E}(\mathbf{A}) &\leq \mathcal{E}(\overline{\mathbf{A}}) + \mathcal{E}(p(\mathbf{J}_n - \mathbf{I}_n)) \\
&= n^{3/2} \left(\frac{8}{3\pi} \sqrt{p(1-p)} + o(1) \right) + 2p(n - 1).
\end{aligned}$$

Consequently,

$$\lim_{n \rightarrow \infty} \mathcal{E}(\mathbf{A})/n^{3/2} \leq \frac{8}{3\pi} \sqrt{p(1-p)} \text{ a.s.} \quad (4)$$

On the other hand, since $\bar{\mathbf{A}} = \mathbf{A} + p(-(\mathbf{J}_n - \mathbf{I}_n))$, we can deduce by Lemma 2 that with probability 1,

$$\begin{aligned} \mathcal{E}(\mathbf{A}) &\geq \mathcal{E}(\bar{\mathbf{A}}) - \mathcal{E}(p(-(\mathbf{J}_n - \mathbf{I}_n))) \\ &= \mathcal{E}(\bar{\mathbf{A}}) - \mathcal{E}(p(\mathbf{J}_n - \mathbf{I}_n)) \\ &= n^{3/2} \left(\frac{8}{3\pi} \sqrt{p(1-p)} + o(1) \right) - 2p(n-1). \end{aligned}$$

Consequently,

$$\lim_{n \rightarrow \infty} \mathcal{E}(\mathbf{A})/n^{3/2} \geq \frac{8}{3\pi} \sqrt{p(1-p)} \text{ a.s.} \quad (5)$$

Combining equations (4) with (5), we have

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

Recalling that \mathbf{A} is the adjacency matrix of $G_n(p)$, we thus obtain that a.e. random graph $G_n(p)$ enjoys the equation as follows:

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

Note that for $p = \frac{1}{2}$, Nikiforov in [16] got the above equation. Here, our result is for any probability p , which could be seen as a generalization of his result.

3 The Laplacian energy of $G_n(p)$

In this section, we shall establish the lower and upper bounds of the Laplacian energy of $G_n(p)$ by employing the LSD of Markov matrix. Finally, we shall show that Conjecture 1 is true for almost all graphs by comparing the energy with the Laplacian energy of a random graph.

3.1 The limiting spectral distribution

We begin with another random matrix we are interested in. Define a random matrix $\mathbf{M}_n = \mathbf{X}_n - \mathbf{D}_n$ to be a *Markov matrix* if \mathbf{X}_n is a Wigner matrix such that F_1 is the pointmass at zero, and \mathbf{D}_n is a diagonal matrix in which $d_{ii} = \sum_{j \neq i} x_{ij}$, $i = 1, \dots, n$. The matrix is introduced as the derivative of a transition matrix in a Markov process. Bryc *et al.* in [5] obtained the LSD of Markov matrix. Define the standard semi-circle distribution $\Phi_{0,1}(x)$ of zero mean and unit variance to be the measure on the real set of compact support with density $\phi_{0,1}(x) = \frac{1}{2\pi} \sqrt{4-x^2} \mathbf{1}_{|x| \leq 2}$.

Theorem 3 (Bryc *et al.* [5]). *Let \mathbf{M}_n be a markov matrix such that $\int x dF_2(x) = 0$ and $\sigma_2 = 1$. Then*

$$\lim_{n \rightarrow \infty} \Phi_{n^{-1/2}\mathbf{M}_n}(x) = \Psi(x) \text{ a.s.}$$

where $\Psi(x)$ is the free convolution of the standard semi-circle distribution $\Phi_{0,1}(x)$ and the standard normal measures. Moreover, this measure $\Psi(x)$ is a non-random symmetric probability measure with smooth bounded density, and does not depend on the distribution of the random variable x_{ij} .

Remark. To prove the theorem above, Bryc *et al.* employ the moment approach. In fact, they show that for each positive integer k ,

$$\lim_{n \rightarrow \infty} \int x^k d\Phi_{n^{-1/2}\mathbf{M}_n}(x) = \int x^k d\Psi(x) \text{ a.s.} \quad (6)$$

For two probability measures μ and ν , there exists a unique probability measure $\mu \boxplus \nu$ called the *free convolution* of μ and ν . This concept introduced by Voiculescu [20] via C^* -algebraic will be discussed in detail in the second part of this section.

Let $G_n(p)$ be a random graph of $\mathcal{G}_n(p)$. Set $\sigma = \sqrt{p(1-p)}$. One can easily see that σ^2 is the variance of the random variable a_{ij} ($i > j$) in $\mathbf{A}(G_n(p))$. To state the main result of this part, we present a new matrix \mathbf{L}_1 as follows:

$$\begin{aligned} \mathbf{L}_1 = \mathbf{L}_1(G_n(p)) &= \bar{\mathbf{L}}(G_n(p)) + p(\mathbf{J}_n - \mathbf{I}_n) \\ &= \left(\mathbf{D}(G_n(p)) - 2 \sum_{i=1}^n \sum_{j>i} a_{ij}/n \mathbf{I}_n \right) - (\mathbf{A}(G_n(p)) - p(\mathbf{J}_n - \mathbf{I}_n)). \end{aligned} \quad (7)$$

The following result is concerned with the LSD of \mathbf{L}_1 .

Theorem 4. *Let $G_n(p)$ be a random graph of $\mathcal{G}_n(p)$. Then*

$$\lim_{n \rightarrow \infty} \Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) = \Psi(x) \text{ a.s.}$$

To prove the theorem above, we introduce an auxiliary matrix as follows:

$$\begin{aligned} \mathbf{L}_2 = \mathbf{L}_2(G_n(p)) &= \mathbf{L}(G_n(p)) - (n-1)p\mathbf{I}_n + p(\mathbf{J}_n - \mathbf{I}_n) \\ &= (\mathbf{D}(G_n(p)) - (n-1)p\mathbf{I}_n) - (\mathbf{A}(G_n(p)) - p(\mathbf{J}_n - \mathbf{I}_n)). \end{aligned}$$

First of all, one can readily see that \mathbf{L}_2 is a Markov matrix in which the Wigner matrix is $-\mathbf{A}(G_n(p)) + p(\mathbf{J}_n - \mathbf{I}_n)$ and the diagonal matrix is $-\mathbf{D}(G_n(p)) + (n-1)p\mathbf{I}_n$. Furthermore, the off-diagonal entries of $\sigma^{-1}\mathbf{L}_2$ have mean 0 and variance 1. Since the LSD $\Psi(x)$ does not depend on the random variables x_{ij} , Theorem 3 yields

$$\lim_{n \rightarrow \infty} \Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x) = \Psi(x) \text{ a.s.}$$

In what follows, we shall show that $(\sigma\sqrt{n})^{-1}\mathbf{L}_1$ and $(\sigma\sqrt{n})^{-1}\mathbf{L}_2$ have the same LSD $\Psi(x)$, by which Theorem 4 follows. To this end, we first estimate the difference $(\sigma\sqrt{n})^{-1}(\mathbf{L}_1 - \mathbf{L}_2)$ by Chernoff's inequality (see [13], pp. 26 for instance).

Lemma 5 (Chernoff's Inequality). *Let X be a random variable with binomial distribution $Bi(n, p)$. Then, for any $\epsilon > 0$,*

$$\mathbb{P}(|X - \mathbb{E}(X)| \geq \epsilon) \leq \exp \left\{ -\frac{\epsilon^2}{2(np - \epsilon/3)} \right\}.$$

Apparently,

$$(\sigma\sqrt{n})^{-1}\mathbf{L}_2 - (\sigma\sqrt{n})^{-1}\mathbf{L}_1 = (\sigma\sqrt{n})^{-1} \left(2 \sum_{i=1}^n \sum_{j>i} a_{ij}/n - (n-1)p \right) \mathbf{I}_n.$$

Denote $(\sigma\sqrt{n})^{-1}(2 \sum_{i=1}^n \sum_{j>i} a_{ij}/n - (n-1)p)$ by Δ_n for convenience. By means of Lemma 5, for any given $\epsilon > 0$, we have

$$\begin{aligned} & \mathbb{P} \left((\sigma\sqrt{n})^{-1} \left| 2 \sum_{i=1}^n \sum_{j>i} a_{ij}/n - (n-1)p \right| \geq \epsilon \right) \\ &= \mathbb{P} \left(\left| \sum_{i=1}^n \sum_{j>i} a_{ij} - \frac{n(n-1)p}{2} \right| \geq \frac{\epsilon \cdot \sigma n^{3/2}}{2} \right) \\ &\leq \exp \left\{ -\frac{2^{-2}(\epsilon\sigma)^2 n^3}{2(n(n-1)p + \epsilon\sigma n^{3/2}/6)} \right\} \\ &< \exp \left\{ -\frac{(\epsilon\sigma)^2 \cdot n^3}{8(p + \epsilon\sigma/6) \cdot n^2} \right\} \\ &= \exp \left\{ -\frac{(\epsilon\sigma)^2}{8(p + \epsilon\sigma/6)} \cdot n \right\}. \end{aligned}$$

Therefore, by the first Borel-Cantelli lemma (see [2], pp. 59 for instance), we can deduce

$$|\Delta_n| = (\sigma\sqrt{n})^{-1} \left| 2 \sum_{i=1}^n \sum_{j>i} a_{ij}/n - (n-1)p \right| \rightarrow 0 \text{ a.s. } (n \rightarrow \infty).$$

Furthermore, it is easy to see that λ is an eigenvalue of $(\sigma\sqrt{n})^{-1}\mathbf{L}_1$ if and only if $\lambda + \Delta_n$ is an eigenvalue of $(\sigma\sqrt{n})^{-1}\mathbf{L}_2$. By the definition of the ESD, it follows that

$$\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) = \Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x + \Delta_n). \quad (8)$$

Clearly, for any $\epsilon > 0$, there exists N such that $|\Delta_n| < \epsilon$ a.s. for all $n > N$. Noting that $\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x)$ is an increasing function, for all $n > N$, we have

$$\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x - \epsilon) \leq \Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x + \Delta_n) \leq \Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x + \epsilon) \text{ a.s.}$$

Consequently,

$$\begin{aligned} \Psi(x - \epsilon) &= \lim_{n \rightarrow \infty} \Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x - \epsilon) \\ &\leq \lim_{n \rightarrow \infty} \Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x + \Delta_n) \\ &\leq \lim_{n \rightarrow \infty} \Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x + \epsilon) = \Psi(x + \epsilon) \text{ a.s.} \end{aligned}$$

Moreover, since the density of $\Psi(x)$ is smooth bounded, $\Psi(x)$ is continuous. Together with the fact that ϵ is arbitrary, we conclude

$$\lim_{n \rightarrow \infty} \Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) = \lim_{n \rightarrow \infty} \Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x + \Delta_n) = \Psi(x) \text{ a.s.,}$$

which completes the proof of Theorem 4.

3.2 The bounds of $\mathcal{E}_L(G_n(p))$

In this part, we shall establish the lower and upper bounds of $\mathcal{E}_L(G_n(p))$ by employing Theorem 4, and then show that Conjecture 1 is true for almost all graphs at last.

Let X be a random variable with the distribution $\Psi(x)$. We start with an estimate of $\mathbb{E}|X| = \int |x|d\Psi(x)$. Since $\Psi(x)$ is the free convolution of the standard semi-circle distribution $\Phi_{0,1}(x)$ and the standard normal measure, let us investigate the free convolution in depth. Here, we follow the notation given by Voiculescu [21]. The Cauchy-Stieltjes transform of a probability measure μ is

$$G_\mu(z) = \int_{-\infty}^{\infty} \frac{\mu(dx)}{z-x}$$

which is analytic on the complex upper half plane. For some $\alpha, \beta > 0$, there exists a domain $D_{\alpha,\beta} = \{u+iv \mid |u| < \alpha v, v > \beta\}$ on which G_μ is univalent. For the image $G_\mu(D_{\alpha,\beta})$, we can define the inverse function K_μ of G_μ in the area $\Gamma_{a,b} = \{u+iv \mid |u| < -av, -b < v < 0\}$. And let $R_\mu(z) = K_\mu(z) - 1/z$. Then for probability measures μ and ν , there exists a unique probability measure, denoted by $\mu \boxplus \nu$, on $\Gamma_{a,b}$ such that

$$R_{\mu \boxplus \nu} = R_\mu + R_\nu.$$

The measure $\mu \boxplus \nu$ is said to be the free convolution of μ and ν .

In the above definition, the Cauchy-Stieltjes transform and inverse function may be difficult to compute in practice. Consequently, we do not compute $\mathbb{E}|X|$ directly. In what follows, we employ another definition of free convolution via combinatorial way (see [4, 18]) applicable only to probability measures with all moments.

For probability measure μ , set $m_k = \int x^k \mu(dx)$ and

$$M_\mu(z) = 1 + \sum_{k=1}^{\infty} m_k z^k.$$

Define a formal power series

$$T_\mu(z) = \sum_{k=1}^{\infty} c_k z^{k-1}$$

such that

$$M_\mu(z) = 1 + zM_\mu(z)T_\mu(zM_\mu(z)).$$

Then, the free convolution of μ, ν is the probability measure $\mu \boxplus \nu$ satisfying

$$T_{\mu \boxplus \nu}(z) = T_\mu(z) + T_\nu(z). \tag{9}$$

It is not difficult to see that this definition is coincident with the analytical one (see [18]).

Next, we calculate $\mathbb{E}|X|$ by the following result due to Bryc [4]. Let $M_{\mu,n} \equiv M_\mu(z) \bmod z^{n+1}$, $T_{\mu,n}(z) \equiv T_\mu(z) \bmod z^{n+1}$ be the n -th truncations, *i.e.*, $M_{\mu,n} = 1 + \sum_{k=1}^n m_k z^k$ and $T_{\mu,n}(z) = \sum_{k=1}^{n+1} c_k z^{k-1}$.

Lemma 6 (Bryc [4]). *With $M_{\mu,0}(z) = 1$ and $c_1 = M'_{\mu,1}(0)$, we have*

$$M_{\mu,n}(z) \equiv 1 + zM_{\mu,n-1}(z)T_{\mu,n-1}(zM_{\mu,n-1}(z)) \pmod{z^{n+1}}, n \geq 1,$$

and

$$c_k = -\frac{1}{k-1} \frac{1}{k!} \frac{d^k}{dz^k} \frac{1}{M_{\mu,n}^{k-1}(z)} \Big|_{z=0}.$$

Therefore, combining with the formula (9), we can calculate the moments of $\mu \boxplus \nu$ by the moments of μ, ν in recurrence. It is not difficult to verify that $\mathbb{E} X^2 = 2$ and $\mathbb{E} X^4 = 9$ (see [4] for details). Employing Cauchy-Schwartz inequality

$$|\mathbb{E}(XY)|^2 \leq \mathbb{E} X^2 \cdot \mathbb{E} Y^2,$$

we have

$$\mathbb{E} |X| \leq \sqrt{\mathbb{E} X^2}$$

and

$$(\mathbb{E} X^2)^2 \leq \mathbb{E} |X| \cdot \mathbb{E} |X|^3 \leq \mathbb{E} |X| \cdot \sqrt{\mathbb{E} X^2 \cdot \mathbb{E} X^4}.$$

Therefore,

$$\frac{2\sqrt{2}}{3} \leq \mathbb{E} |X| \leq \sqrt{2}.$$

In what follows, we shall establish the lower and upper bounds of $\mathcal{E}_L(G_n(p))$ by employing an estimate of the energy $\mathcal{E}(\mathbf{L}_1)$. We first investigate the convergence of $\int |x| d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x)$. Let I be the interval $[-1, 1]$. By Theorem 4 and the bounded convergence theorem, one can easily see that

$$\lim_{n \rightarrow \infty} \int_I |x| d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) = \int_I |x| d\Psi(x) \text{ a.s.} \quad (10)$$

We proceed to prove that

$$\lim_{n \rightarrow \infty} \int_{I^c} |x| d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) = \int_{I^c} |x| d\Psi(x) \text{ a.s.}$$

where $I^c = \mathbb{R} \setminus I$. Since $\sigma^{-1}\mathbf{L}_2$ is the Markov matrix such that the off-diagonal entries have mean 0 and variance 1, we can deduce, by Equation (6), that

$$\lim_{n \rightarrow \infty} \int x^2 d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x) = \int x^2 d\Psi(x) \text{ a.s.} \quad (11)$$

According to the relation (8), we have

$$\begin{aligned} \int x^2 d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) &= \int x^2 d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x + \Delta_n) \\ &= \int (x - \Delta_n)^2 d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x) \\ &= \int x^2 d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x) - 2\Delta_n \int x d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x) \\ &\quad + \Delta_n^2 \int d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x). \end{aligned}$$

Since $\lim_{n \rightarrow \infty} \Delta_n = 0$ a.s., Equation (11) implies that

$$\lim_{n \rightarrow \infty} \int x^2 d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) = \lim_{n \rightarrow \infty} \int x^2 d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x) = \int x^2 d\Psi(x) \text{ a.s.} \quad (12)$$

Consequently,

$$\begin{aligned} \lim_{n \rightarrow \infty} \int_{I^c} x^2 d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) &= \lim_{n \rightarrow \infty} \left(\int x^2 d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) - \int_I x^2 d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) \right) \\ &= \int_{I^c} x^2 d\Psi(x) \text{ a.s.} \end{aligned}$$

Lemma 7 (Billingsley [2] pp. 219). *Let μ be a measure. Suppose that functions a_n, b_n, f_n converges almost everywhere to functions a, b, f , respectively, and that $a_n \leq f_n \leq b_n$ almost everywhere. If $\int a_n d\mu \rightarrow \int a d\mu$ and $\int b_n d\mu \rightarrow \int b d\mu$, then $\int f_n d\mu \rightarrow \int f d\mu$.*

Suppose that $\phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x)$ is the density of $\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x)$. By virtue of Theorem 4 and Lemma 7, we can deduce by setting $a_n(x) = 0$, $b_n(x) = x^2 \phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x)$ and $f_n(x) = |x| \phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x)$ that

$$\lim_{n \rightarrow \infty} \int_{I^c} |x| d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) = \int_{I^c} |x| d\Psi(x) \text{ a.s.}$$

Combining the above equation with Equation (10), we have

$$\lim_{n \rightarrow \infty} \int |x| d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) = \int |x| d\Psi(x) \text{ a.s.}$$

We are now ready to present an estimate of the energy $\mathcal{E}(\mathbf{L}_1)$. By an argument similar to evaluate the energy $\mathcal{E}(\overline{\mathbf{A}})$, we have

$$\begin{aligned} \mathcal{E}(\mathbf{L}_1)/\sigma n^{3/2} &= \int |x| d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) \\ &\rightarrow \int |x| d\Psi(x) \text{ a.s. } (n \rightarrow \infty). \end{aligned}$$

Since $2\sqrt{2}/3 \leq \mathbb{E}|X| \leq \sqrt{2}$,

$$\frac{2\sqrt{2}}{3} \leq \frac{\mathcal{E}(\mathbf{L}_1)}{\sigma n^{3/2}} \leq \sqrt{2} \text{ a.s. } (n \rightarrow \infty).$$

Consequently,

$$\left(\frac{2\sqrt{2}}{3} \sigma + o(1) \right) n^{3/2} \leq \mathcal{E}(\mathbf{L}_1) \leq \left(\sqrt{2} \sigma + o(1) \right) n^{3/2} \text{ a.s.} \quad (13)$$

Employing the equation above, we can establish the lower and upper bounds of $\mathcal{E}_L(G_n(p))$. Note that $\mathcal{E}_L(G_n(p)) = \mathcal{E}(\overline{\mathbf{L}})$ according to the definition of the energy of

a matrix. So we turn our attention to the bounds of $\mathcal{E}(\bar{\mathbf{L}})$. By means of Equation (7), we have

$$\mathbf{L}_1 = \bar{\mathbf{L}} + p(\mathbf{J}_n - \mathbf{I}_n) \text{ and } \bar{\mathbf{L}} = \mathbf{L}_1 + p(\mathbf{I}_n - \mathbf{J}_n).$$

Thus, Lemma 2 yields that

$$\mathcal{E}(\mathbf{L}_1) - \mathcal{E}(p(\mathbf{J}_n - \mathbf{I}_n)) \leq \mathcal{E}(\bar{\mathbf{L}}) \leq \mathcal{E}(\mathbf{L}_1) + \mathcal{E}(p(\mathbf{I}_n - \mathbf{J}_n)).$$

Recalling the fact that $\mathcal{E}(p(\mathbf{J}_n - \mathbf{I}_n)) = \mathcal{E}(p(\mathbf{I}_n - \mathbf{J}_n)) = 2p(n-1)$, Equation (13) implies that

$$\left(\frac{2\sqrt{2}}{3}\sigma + o(1) \right) n^{3/2} - 2p(n-1) \leq \mathcal{E}(\bar{\mathbf{L}}) \leq \left(\sqrt{2}\sigma + o(1) \right) n^{3/2} + 2p(n-1) \text{ a.s.}$$

Therefore, we obtain the the lower and upper bounds of the Laplacian energy for almost all graphs.

Theorem 8. *Almost every random graph $G_n(p)$ satisfies*

$$\left(\frac{2\sqrt{2}}{3}\sigma + o(1) \right) \cdot n^{3/2} \leq \mathcal{E}_L(G_n(p)) \leq \left(\sqrt{2}\sigma + o(1) \right) \cdot n^{3/2}.$$

Since a.e. random graph $G_n(p)$ satisfies

$$\lim_{n \rightarrow \infty} \frac{\mathcal{E}(G_n(p))}{n^{3/2}} = \frac{8}{3\pi}\sigma < \frac{2\sqrt{2}}{3}\sigma \leq \lim_{n \rightarrow \infty} \frac{\mathcal{E}_L(G_n(p))}{n^{3/2}},$$

we thus establish the result below.

Theorem 9. *For almost every random graph $G_n(p)$, $\mathcal{E}(G_n(p)) < \mathcal{E}_L(G_n(p))$.*

By virtue of the theorem above, Conjecture 1 is true for almost all graphs.

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References

- [1] Z.D. Bai, Methodologies in spectral analysis of large dimensional random matrices, a review, *Statistica Sinica* **9**(1999), 611–677.
- [2] P. Billingsley, *Probability and Measure* 3rd ed., John Wiley & Sons, Inc. 1995.
- [3] B. Bollobás, *Random Graphs (2nd Ed.)*, Cambridge Studies in Advanced Math., Vol.73, Cambridge University Press, Cambridge, 2001.
- [4] W. Bryc, Computing moments of free additive convloution of measures, *Appl. Math. Comput.* **194**(2007), 561-567.

- [5] W. Bryc, A. Dembo, T. Jiang, Spectral measure of large random Hankel, Markov and Toeplitz Matrices, *Ann. Probab.* **34**(2006), 1–38.
- [6] P. Deift, Orthogonal Polynomials and Random Matrices: A Riemann-Hilbert Approach. New York University-Courant Institute of Mathematical Sciences, AMS, 2000.
- [7] K. Fan, Maximum properties and inequalities for the eigenvalues of completely continuous operators, *Proc. Natl. Acad. Sci. USA* **37**(1951), 760–766.
- [8] Z. Füredi and J. Komlós, The eigenvalues of random symmetric matrices, *Combinatorica* **1**(3) (1981) 233-241.
- [9] I. Gutman, The energy of a graph, *Ber. Math. Statist. Sect. Forschungsz. Graz* **103**(1978), 1–22.
- [10] I. Gutman, N.M.M. de Abreu, C.T.M. Vinagre, A.S. Bonifácio, S. Radenković, Relation between energy and Laplacian energy, *MATCH Commun. Math. Comput. Chem.* **59**(2008), 343–354.
- [11] I. Gutman, X. Li, J. Zhang, Graph Energy, in: M. Dehmer, F. Emmert-Streib (Eds.), *Analysis of Complex Networks: From Biology to Linguistics*, Wiley-VCH Verlag, Weinheim, 2009, 145-174.
- [12] I. Gutman and B. Zhou, Laplacian energy of a graph, *Linear Algebra Appl.* **414**(2006), 29–37.
- [13] S. Janson, T. Luczak, A. Ruciński, *Random Graphs*, Wiley, Hoboken, NJ. 2000.
- [14] J. Liu, B. Liu, On the relation between energy and Laplacian energy, *MATCH Commun. Math. Comput. Chem.* **61**(2009), 403–406.
- [15] M.L. Mehta, *Random Matrices. 2nd ed.* Academic Press, 1991.
- [16] V. Nikiforov, The energy of graphs and matrices, *J. Math. Anal. Appl.* **326**(2007), 1472-1475.
- [17] W. So, M. Robbiano, N.M.M. de Abreu, I. Gutman, Applications of a theorem by Ky Fan in the theory of graph energy, *Linear Algebra Appl.* (2009), doi:10.1016/j.laa.2009.01.006.
- [18] R. Speicher, Free probability theory and non-crossing partitions, *Sém. Lothar. Combin.* **39** (1997), Art. B39c, (electronic).
- [19] D. Stevanović, I. Stanković, M. Milošević, More on the relation between energy and Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **61**(2009), 395–401.
- [20] D.V. Voiculescu, Symmetries of some reduced free product C^* -algebras, *Let. Notes Math.* **1132**(1985), 556–588.

- [21] D.V. Voiculescu, Limit laws for random matrices and free products, *Invent. Math.* **104**(1991), 201–220.
- [22] E.P. Wigner, Characteristic vectors of bordered matrices with infinite dimensions, *Ann. Math.* **62**(1955), 548–564.
- [23] E.P. Wigner, On the distribution of the roots of certain symmetric matrices, *Ann. Math.* **67**(1958), 325–327.
- [24] J. Wishart, The generalized product moment distribution in samples from a normal multivariate population. *Biometrika* **20A**(1928), 32–52.