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The Laplacian energy of random graphs ☆

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ABSTRACT

Gutman et al. introduced the concepts of energy $\mathscr{E}(G)$ and Laplacian energy $\mathscr{E}_L(G)$ for a simple graph G, and furthermore, they proposed a conjecture that for every graph G, $\mathscr{E}(G)$ is not more than $\mathscr{E}_L(G)$. 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.

1. Introduction

Throughout this paper, G denotes a simple graph of order n. The eigenvalues $\lambda_1, \ldots, \lambda_n$ of the adjacency matrix $\mathbf{A}(G) = (a_{ij})_{n\times n}$ of G 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 Hüchkel molecular orbital approximation, the total π-electron energy $\mathscr{E}$ in a conjugated hydrocarbon 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 [8] extended the concept of energy to all simple graphs G, and defined that

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

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. It is rather hard, however, to compute the eigenvalues for a large matrix, even for a large symmetric $(0,1)$-matrix like $\mathbf{A}(G)$. 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 the readers to the comprehensive survey [10]. 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 $\mathscr{E}(G)$ 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.

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In spectral graph theory, the matrix $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$ is called the *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, $i = 1, \ldots, n$. Gutman et al. [11] 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* $\mathscr{E}_L(G)$ *of* G, *i.e.*,

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

where $\zeta_1, \ldots, \zeta_n$ are the eigenvalues of $\bar{\mathbf{L}}(G)$. Obviously, we can easily evaluate the Laplacian energy $\mathscr{E}_L(G)$ 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 Erdös–Rényi model [3].

In a recent paper [9], 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 $\mathscr{E}(G) \leqslant \mathscr{E}_L(G)$.*

Unfortunately, the conjecture turns out to be incorrect. In fact, Liu et al. [13] and Stevanović et al. [18] constructed two classes of graphs violating the assertion. However, So et al. [16] proved that the conjecture is true for bipartite graphs. In Section 3 we shall show that the conjecture is true for almost all graphs by comparing the energy with the Laplacian energy of a random graph.

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 Erdös–Rényi model $\mathcal{G}_n(p)$ [3], which consists of all graphs with vertex set $[n] = \{1, 2, \ldots, n\}$ 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 [23]. We refer readers to [1,6,14] 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*,

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

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;
- $\mathbb{V}\mathrm{ar}(x_{ij}) = \sigma_2^2 < \infty$ for all $1 \leqslant i < j \leqslant n$.

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

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

Wigner [21,22] considered the limiting spectral distribution (LSD) of $\mathbf{X}_n(x)$, and obtained the semi-circle law.

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

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

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*

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

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. Moreover, there exists only one eigenvalue which is of $O(n)$, while the others are not more than $2\sigma_2\sqrt{n}+O(n^{1/3}\log n)$ with probability 1 as n tends to infinity (see [7], 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 $x\geqslant 0$ 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. By means of Theorem 1, we have

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

According to the remark above, for any given $\epsilon>0$, there exists an integer N such that for all $n>N$, except only one eigenvalue, the eigenvalues of $n^{-1/2}\mathbf{X}_n$ are not more than $2\sigma_2+\epsilon$. Invoking Egoroff's theorem yields

$$\begin{aligned}\lim_{n\to\infty}\int|x|\,d\Phi_{n^{-1/2}\mathbf{A}(G_n(p))}(x)&=\lim_{n\to\infty}\left(\int_{-2\sigma_2-\epsilon}^{2\sigma_2+\epsilon}|x|\,d\Phi_{n^{-1/2}\mathbf{A}(G_n(p))}(x)+O(\sqrt{n})\cdot\frac{1}{n}\right)\quad\text{a.s.}\\&=\int_{-2\sigma_2-\epsilon}^{2\sigma_2+\epsilon}|x|\,d\Phi(x)\quad\text{a.s.}\\&=\int|x|\,d\Phi(x).\end{aligned}$$

Suppose $\lambda_1,\dots,\lambda_n$ and $\lambda'_1,\dots,\lambda'_n$ are the eigenvalues of $\mathbf{A}(G_n(p))$ and $n^{-1/2}\mathbf{A}(G_n(p))$, respectively. Clearly, $\sum_{i=1}^n|\lambda_i|=n^{1/2}\sum_{i=1}^n|\lambda'_i|$. Therefore, by the definition of the energy we can deduce that for a.e. random graph $G_n(p)$,

$$\begin{aligned}\mathscr{E}\big(G_n(p)\big)/n^{3/2}&=\frac{1}{n^{3/2}}\sum_{i=1}^n|\lambda_i|\\&=\frac{1}{n}\sum_{i=1}^n|\lambda'_i|\\&=\int|x|\,d\Phi_{n^{-1/2}\mathbf{A}(G_n(p))}(x)\\&\to\int|x|\,d\Phi(x)\quad\text{almost surely as } n\to\infty\\&=\frac{1}{2\pi\sigma_2^2}\int_{-2\sigma_2}^{2\sigma_2}|x|\sqrt{4\sigma_2^2-x^2}\,dx\\&=\frac{8}{3\pi}\sigma_2=\frac{8}{3\pi}\sqrt{p(1-p)}.\end{aligned}$$

Note that for $p=\frac{1}{2}$, Nikiforov in [15] got the above result. 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 exploring the LSD of $\bar{\mathbf{L}}=\bar{\mathbf{L}}(G_n(p))$. 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 of $\bar{\mathbf{L}}$

We begin with another random matrix. 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 a 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 $\phi_{0,1}(x) = \frac{1}{2\pi}\sqrt{4-x^2}\mathbf{1}_{|x|\leqslant 2}$.

Theorem 2. *(See 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 with probability 1, $\Phi_{n^{-1/2}\mathbf{M}_n}(x)$ converges weakly to a distribution $\Psi(x)$ as n tends to infinity, where $\Psi(x)$ is the free convolution of the standard semi-circle law $\Phi_{0,1}(x)$ 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. employed the moment approach. In fact, they showed that for each positive integer k,

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

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 was introduced by Voiculescu [19] via C^*-algebraic, which 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 $\mathbf{A}(G_n(p))$. The main result of this part is concerned with the LSD of $\bar{\mathbf{L}}$.

Theorem 3. *Let $G_n(p)$ be a random graph of $\mathcal{G}_n(p)$. Then with probability 1, $\Phi_{(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}}(x)$ converges weakly to the distribution $\Psi(x)$ as n tends to infinity.*

To prove the theorem above, we introduce two auxiliary matrices as follows:

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

and

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

where $\mathbf{J}_n$ is the matrix in which all elements equal 1.

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 $-\mathbf{D}(G_n(p)) + (n-1)p\mathbf{I}_n$. Thus $\sigma^{-1}\mathbf{L}_2$ is a Markov matrix such that the off-diagonal entries have mean 0 and variance 1. Since the LSD $\Psi(x)$ does not depend on the random variables x_{ij}, Theorem 2 yields

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

In what follows, we shall show that $(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}$, $(\sigma\sqrt{n})^{-1}\mathbf{L}_1$ and $(\sigma\sqrt{n})^{-1}\mathbf{L}_2$ have the same LSD $\Psi(x)$, by which Theorem 3 follows.

To this end, we first estimate the difference $(\sigma\sqrt{n})^{-1}(\mathbf{L}_1 - \mathbf{L}_2)$ by Chernoff's inequality (see [12, p. 26] for instance) and show that $(\sigma\sqrt{n})^{-1}\mathbf{L}_1$ has the same LSD as $(\sigma\sqrt{n})^{-1}\mathbf{L}_2$.

Lemma 4 *(Chernoff's inequality). Let X be a random variable with binomial distribution $Bi(n, p)$. Then, for any $\epsilon > 0$,*

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

Apparently,

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

Denote $(\sigma\sqrt{n})^{-1}(2\sum_{i=1}^{n}\sum_{j>i} a_{ij}/n - np)$ by Δ_n for convenience. Note that in the brackets the multiplied times of variable p is n. By Lemma 4, for any given $\epsilon > 0$, we have

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

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

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

and thus

$$\Delta_n\to 0\quad\text{a.s. } (n\to\infty).$$

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 ESD, it follows that

$$\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x)=\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x+\Delta_n). \tag{2}$$

Clearly, for any $\epsilon>0$, there exists an 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

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

Consequently,

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

Moreover, since the density of $\Psi(x)$ is smooth, $\Psi(x)$ is continuous. Together with the fact that $\epsilon>0$ is arbitrary, we conclude

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

We now turn to the LSD's of $(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}$ and $(\sigma\sqrt{n})^{-1}\mathbf{L}_1$. For a function f, set $\|f\|=\sup_x|f(x)|$.

Lemma 5 *(Rank inequality). (See [1].) Let $\mathbf{U}_n$ and $\mathbf{V}_n$ be two real symmetric matrices. Then*

$$\left\|\Phi_{\mathbf{U}_n}(x)-\Phi_{\mathbf{V}_n}(x)\right\|\leqslant\frac{1}{n}\operatorname{rank}(\mathbf{U}_n-\mathbf{V}_n).$$

Evidently,

$$(\sigma\sqrt{n})^{-1}\mathbf{L}_1-(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}=(\sigma\sqrt{n})^{-1}p\mathbf{J}_n.$$

Note that the rank of $\mathbf{J}_n$ is 1, and then we conclude, by Lemma 5, that the LSD's of $(\sigma\sqrt{n})^{-1}\mathbf{L}_1$ and $(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}$ are the same.

Therefore, $(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}$, $(\sigma\sqrt{n})^{-1}\mathbf{L}_1$ and $(\sigma\sqrt{n})^{-1}\mathbf{L}_2$ have the same LSD $\Psi(x)$, as we set out to show.

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

In this part, we shall establish the lower and upper bounds of $\mathscr{E}_L(G_n(p))$ by employing Theorem 3 and the trace method, and then show that Conjecture 1 is true for almost all graphs.

Let ξ_n be a random variable with the distribution $\Phi_{(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}}(x)$. Then, by the definition of the Laplacian energy, we have

$$\mathscr{E}_L\big(G_n(p)\big)=\sigma n^{3/2}\mathbb{E}|\xi_n|.$$

Evidently, to estimate $\mathscr{E}_L(G_n(p))$, it suffices to evaluate $\mathbb{E}|\xi_n|$. Let X be a random variable with distribution $\Psi(x)$. We shall apply $\mathbb{E}|X|$ to evaluate $\mathbb{E}|\xi_n|$ by employing Theorem 3 and the trace method.

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 law $\Phi_{0,1}(x)$ and the standard normal measure, let us further investigate the free convolution. Here, we follow the notation given by Voiculescu [20]. 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 [4,17]) 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

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

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

$$T_{\mu\boxplus\nu}(z) = T_\mu(z) + T_\nu(z). \tag{3}$$

It is not difficult to see that this definition is coincident with the analytical one (see [17]).

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

$$M_{\mu,n}(z) \equiv 1 + zM_{\mu,n-1}(z)T_{\mu,n-1}\big(zM_{\mu,n-1}(z)\big) \mod z^{n+1},\ n \geqslant 1,$$

and

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

Therefore, combining with the formula (3), 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

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

we have

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

and

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

Therefore,

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

We shall establish the lower bound of $\mathbb{E}|\xi_n|$ at first. Since $\mathbb{E}|X| = \int |x|\,d\Psi(x) \leqslant \sqrt{2}$, for any given $\epsilon > 0$, there exists an integer K such that

$$\left| \int |x|\,d\Psi(x) - \int_{-K}^{K} |x|\,d\Psi(x) \right| < \epsilon,$$

and thus Egoroff's theorem implies

$$\begin{aligned} \mathbb{E}|\xi_n| &= \int |x|\,d\Phi_{(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}}(x) \\ &\geqslant \int_{-K}^{K} |x|\,d\Phi_{(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}}(x) \\ &\to \int_{-K}^{K} |x|\,d\Psi(x) \quad \text{a.s.} \\ &\geqslant \int |x|\,d\Psi(x) - \epsilon \geqslant \frac{2\sqrt{2}}{3} - \epsilon. \end{aligned}$$

Consequently,

$$\lim_{n\to\infty} \mathbb{E}|\xi_n| \geqslant \frac{2\sqrt{2}}{3},$$

because ϵ is arbitrary.

We proceed to evaluate the upper bound of $\mathbb{E}|\xi_n|$. 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 the assertion (1), that for each positive integer k,

$$\lim_{n\to\infty} \int x^k\,d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x) = \int x^k\,d\Psi(x) \quad \text{a.s.} \tag{4}$$

According to the equality (2), we have

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

Since $\lim_{n\to\infty} \Delta_n \to 0$ a.s., the equality (4) implies that

$$\lim_{n\to\infty} \int x^2\,d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) = \lim_{n\to\infty} \int x^2\,d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_2}(x) = \int x^2\,d\Psi(x) \quad \text{a.s.} \tag{5}$$

We shall employ the trace method to estimate $\mathbb{E}(\xi_n^2) = \int x^2\,d\Phi_{(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}}(x)$ in what follows. It is not difficult to see that

$$\int x^2\,d\Phi_{(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}}(x) = n^{-1}\,\mathrm{trace}\left(\left(\frac{1}{\sigma\sqrt{n}}\bar{\mathbf{L}}\right)^2\right) = (\sigma n)^{-2}\,\mathrm{trace}\big(\bar{\mathbf{L}}^2\big).$$

Since $\mathbf{L}_1 = \bar{\mathbf{L}} + p\mathbf{J}_n$, we have

$$\begin{aligned} \int x^2\,d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) - \int x^2\,d\Phi_{(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}}(x) &= (\sigma n)^{-2}\big(\mathrm{trace}\big(\mathbf{L}_1^2\big) - \mathrm{trace}\big(\bar{\mathbf{L}}^2\big)\big) \\ &= (\sigma n)^{-2}\,\mathrm{trace}\big(p\bar{\mathbf{L}}\mathbf{J}_n + p\mathbf{J}_n\bar{\mathbf{L}} + p^2\mathbf{J}_n^2\big) \\ &= (\sigma n)^{-2}\big(2p\,\mathrm{trace}(\mathbf{J}_n\bar{\mathbf{L}}) + p^2\,\mathrm{trace}\big(\mathbf{J}_n^2\big)\big). \end{aligned} \tag{6}$$

For convenience, we shall use **A** and **D** to denote the matrices $\mathbf{A}(G_n(p))$ and $\mathbf{D}(G_n(p))$, respectively. Set $\varepsilon = \sum_{i=1}^{n}\sum_{j>i} a_{ij}/n$. In accordance with the definition of $\bar{\mathbf{L}}$, we have $\bar{\mathbf{L}} = \mathbf{D} - \mathbf{A} - \frac{2\varepsilon}{n}\mathbf{I}_n$, and thus

$$\operatorname{trace}(\mathbf{J}_n\bar{\mathbf{L}}) = \operatorname{trace}\left(\mathbf{J}_n\left(\mathbf{D} - \mathbf{A} - \frac{2\varepsilon}{n}\mathbf{I}_n\right)\right) = \operatorname{trace}(\mathbf{J}_n\mathbf{D}) - \operatorname{trace}(\mathbf{J}_n\mathbf{A}) - \frac{2\varepsilon}{n}\operatorname{trace}(\mathbf{J}_n).$$

It is easily seen that $\operatorname{trace}(\mathbf{J}_n\mathbf{D}) = \operatorname{trace}(\mathbf{J}_n\mathbf{A}) = \frac{2\varepsilon}{n}\operatorname{trace}(\mathbf{J}_n) = 2\varepsilon$. Recall that $\sigma = \sqrt{p(1-p)}$. Invoking the strong law of large number, we can deduce that

$$\begin{aligned}\lim_{n\to\infty}(\sigma n)^{-2}\big(2p\operatorname{trace}(\mathbf{J}_n\bar{\mathbf{L}}) + p^2\operatorname{trace}(\mathbf{J}_n^2)\big) &= \lim_{n\to\infty}(\sigma n)^{-2}\big(p^2n^2 - 4p\varepsilon\big)\\ &= \lim_{n\to\infty}\frac{p}{p(1-p)}\left(p - 2\frac{2\varepsilon}{n^2}\right)\\ &= -\frac{p}{(1-p)} \quad \text{a.s.}\end{aligned}$$

By means of the relations of (5) and (6), we have

$$\begin{aligned}\lim_{n\to\infty}\mathbb{E}\big(\xi_n^2\big) &= \lim_{n\to\infty}\int x^2\,d\Phi_{(\sigma\sqrt{n})^{-1}\bar{\mathbf{L}}}(x)\\ &= \lim_{n\to\infty}\int x^2\,d\Phi_{(\sigma\sqrt{n})^{-1}\mathbf{L}_1}(x) - \lim_{n\to\infty}(\sigma n)^{-2}\big(2p\operatorname{trace}(\mathbf{J}_n\bar{\mathbf{L}}) + p^2\operatorname{trace}(\mathbf{J}_n^2)\big)\\ &= \mathbb{E}X^2 + \frac{p}{(1-p)} \quad \text{a.s.}\\ &= 2 + \frac{p}{(1-p)}.\end{aligned}$$

Since $\mathbb{E}|\xi_n| \leqslant \sqrt{\mathbb{E}\xi_n^2}$, it follows that

$$\lim_{n\to\infty}\mathbb{E}|\xi_n| \leqslant \sqrt{2 + \frac{p}{(1-p)}} \quad \text{a.s.}$$

Therefore, the following inequality holds a.s.

$$\frac{2\sqrt{2}}{3} + o(1) \leqslant \mathbb{E}|\xi_n| \leqslant \sqrt{2 + \frac{p}{(1-p)}} + o(1).$$

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

Theorem 7. *Almost every random graph $G_n(p)$ satisfies*

$$\left(\frac{2\sqrt{2}}{3}\sqrt{p(1-p)} + o(1)\right)\cdot n^{3/2} \leqslant \mathscr{E}_L\big(G_n(p)\big) \leqslant \big(\sqrt{2p - p^2} + o(1)\big)\cdot n^{3/2}.$$

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

$$\lim_{n\to\infty}\frac{\mathscr{E}(G_n(p))}{n^{3/2}} = \frac{8}{3\pi}\sqrt{p(1-p)} < \frac{2\sqrt{2}}{3}\sqrt{p(1-p)} \leqslant \lim_{n\to\infty}\frac{\mathscr{E}_L(G_n(p))}{n^{3/2}},$$

we thus establish the result below.

Theorem 8. *For almost every random graph $G_n(p)$, $\mathscr{E}(G_n(p)) < \mathscr{E}_L(G_n(p))$.*

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

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