Asymptotic behavior of Laplacian-energy-like invariant of some graphs *

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Abstract

Let G be a connected graph of order n with Laplacian eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$. The Laplacian-energy-like invariant (LEL for short) of G is defined as $LEL = \sum_{i=1}^{n-1} \sqrt{\mu_i}$. In this paper, we consider the asymptotic behavior of the LEL of iterated line graphs of regular graphs. In addition, the formula and asymptotic formula of the LEL of the square (resp. hexagonal, triangular) lattices with toroidal boundary condition are obtained.

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1 Introduction

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Denote by $A(G)$ and $D(G)$ the adjacency matrix and the diagonal matrix with the vertex degrees of G on the diagonal, respectively. The matrix $L(G) = D(G) - A(G)$ is called the Laplacian matrix of G, for details on Laplacian matrix see [9]. Since $A(G)$ and $L(G)$ are real symmetric matrices, their eigenvalues are real numbers. So we can assume that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ (resp., $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$) are the adjacency (resp., Laplacian) eigenvalues of G. We write $\lambda_i(G)$ and $\mu_i(G)$ instead of λ_i and μ_i, respectively, when

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more than one graph are under discussion. It is well-known that $\mu_n = 0$ and the multiplicity of zero is equal to the number of connected components of G, see [1].

The Laplacian-energy-like invariant of a graph G (LEL for short) defined by

$$LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i} \tag{1}$$

was first introduced by J. Liu and B. Liu [8]. The motivation for introducing LEL was in its analogy to the earlier studied graph energy [2, 4] and Laplacian energy [5]. In [14], it was shown that LEL describes well the properties which are accounted by the majority of molecular descriptors: motor octane number, entropy, molar volume, molar refraction, particularly the acentric factor AF parameter, but also more difficult properties like boiling point, melting point and partition coefficient $LogP$. In a set of polycyclic aromatic hydrocarbons, LEL was proved [14] to be as good as the Randić index and better than the Wiener index. For further results on the LEL, the readers refer to the comprehensive survey [7].

The rest of this paper is organized as follows. In Section 2, we determine the growth rate of the LEL of iterated line graphs of an r-regular graph G. We prove that their growth rates are independent of the structure of G and only dependent on r and the number of vertices of G. In Section 3, we explore the asymptotic behavior of the LEL of a square lattice (resp., hexagonal lattice, triangular lattice) with toroidal boundary condition. We show that the growth rate of the LEL of these toroidal lattices is only dependent on the number of vertices of them.

2 The LEL of iterated line graphs of regular graphs

In this section, we will explore the asymptotic behavior of LEL of iterated line graphs of regular graphs.

The line graph $\mathcal{L}(G)$ of a graph G is the graph whose vertex set is in one-to-one correspondence with the set of edges of G where two vertices of $\mathcal{L}(G)$ are adjacent if and only if the corresponding edges in G have a vertex in common. If G is a graph and $\mathcal{L}(G) = \mathcal{L}^1(G)$ is its line graph, then $\mathcal{L}^k(G), k = 2, 3, \ldots$, defined recursively via $\mathcal{L}^k(G) = \mathcal{L}(\mathcal{L}^{k-1}(G))$, are the iterated line graphs of G. It is both consistent and convenient to set $G = \mathcal{L}^0(G)$. Recently, several papers on iterated line graph have been published [3, 8, 12, 15]. For example, Yan et al. [15] considered the asymptotic behavior of the number of spanning trees and the Kirchhoff index of iterated line graphs of a regular graph G. An upper bound for incidence energy of the iterated line graph of a regular graph G is obtained in [3].

Let G be a regular graph of order n_0 and of degree r_0. Then $\mathcal{L}^s(G)$ is regular for $s = 1, 2, \ldots, k$. Denote by n_s and r_s the order and degree of $\mathcal{L}^s(G)$, respectively. Then

$$n_k = \frac{1}{2} r_{k-1} n_{k-1} \quad \text{and} \quad r_k = 2r_{k-1} - 2, \quad k = 1, 2, 3, \ldots$$

and so

$$n_k = \frac{n_0}{2^k} \prod_{j=0}^{k-1} r_j = \frac{n_0}{2^k} \prod_{j=0}^{k-1} (2^j r_0 - 2^{j+1} + 2), \quad r_k = 2^k r_0 - 2^{k+1} + 2 \qquad (2)$$

for $k = 1, 2, \ldots$

Lemma 2.1 *[8] Let G be an r_0-regular graph of order n_0. Then*

$$LEL(\mathcal{L}^k(G)) = LEL(\mathcal{L}^{k-1}(G)) + \sqrt{2r_{k-1}}(n_k - n_{k-1}), \ k = 1, 2, \ldots$$

Lemma 2.2 *[15] Let $\{y_k\}_{k \geq 0}$, $\{f_k\}_{k \geq 0}$, $\{g_k\}_{k \geq 0}$ be three sequences satisfying the following recurrence relation:*

$$y_{k+1} = f_k y_k + g_k, \ k \geq 0.$$

Then

$$y_{k+1} = \left(y_0 + \sum_{i=0}^{k} h_i \right) \prod_{j=0}^{k} f_j,$$

where $h_k = s_{k+1} g_k$, $s_{k+1} = (\prod_{i=0}^{k} f_i)^{-1}$, $s_0 = 1$.

Theorem 2.3 *Let G be an r-regular graph of order n. Then*

$$LEL(\mathcal{L}^k(G)) \sim \frac{n}{2^k \sqrt{2^k r - 2^{k+1} + 2}} \prod_{j=0}^{k} (2^j r - 2^{j+1} + 2), \ (k \to \infty). \qquad (3)$$

Hence the asymptotic value of the LEL of iterated line graphs of a regular graph is independent of the structure of G.

Proof. Let r_k and n_k be defined as (2). Then $\mathcal{L}^k(G)$ is an r_k-regular graph of order n_k. By Lemma 2.1,

$$LEL(\mathcal{L}^k(G)) = LEL(\mathcal{L}^{k-1}(G)) + \sqrt{2r_{k-1}}(n_k - n_{k-1}), k \geq 1.$$

Set $y_k = LEL(\mathcal{L}^k(G))$, $f_k = 1$, $g_k = \sqrt{2r_{k-1}}(n_k - n_{k-1})$, $k = 1, 2, \ldots$. Then

$$y_{k+1} = f_k y_k + g_k,\ y_0 = LEL(G), k \geq 0.$$

By Lemma 2.2, we obtain

$$LEL(\mathcal{L}^{k+1}(G)) = LEL(G) + \sum_{i=0}^{k} \sqrt{2r_i}(n_{i+1} - n_i). \tag{4}$$

Let $t_i = \sqrt{2r_i}(n_{i+1} - n_i), i = 1, 2, \ldots, k-1$. Note that $r_i = 2^i r - 2^{i+1} + 2$, $n_i = \frac{n}{2^i}\prod_{j=0}^{i-1} r_j$. Obviously, if $r > 2$, then $r_k \to \infty$, $(k \to \infty)$. Hence, for all $i = 0, 1, 2, \ldots, k-1$, we have

$$\begin{aligned}
k\frac{t_i}{\sqrt{r_k}n_{k+1}} &= k\left[\frac{\sqrt{2r_i}n_{i+1}}{\sqrt{r_k}n_{k+1}} - \frac{\sqrt{2r_i}n_i}{\sqrt{r_k}n_{k+1}}\right] \\
&= \frac{k\sqrt{2r_i}\frac{n}{2^{i+1}}\prod_{j=0}^{i} r_j}{\sqrt{r_k}\frac{n}{2^{k+1}}\prod_{j=0}^{k} r_j} - \frac{k\sqrt{2r_i}\frac{n}{2^i}\prod_{j=0}^{i-1} r_j}{\sqrt{r_k}\frac{n}{2^{k+1}}\prod_{j=0}^{k} r_j} \\
&= \frac{k2^{k-i}\sqrt{\frac{2r_i}{r_k}}}{\prod_{j=i+1}^{k} r_j} - \frac{k2^{k-i+1}\sqrt{\frac{2r_i}{r_k}}}{\prod_{j=i}^{k} r_j} \\
&\to 0 \quad (k \to \infty).
\end{aligned}$$

Let $t = \max_{0 \leq i \leq k-1} t_i$. It is clear that

$$\begin{aligned}
&\lim_{k\to\infty} \frac{kt}{n_{k+1}\sqrt{r_k}} = 0, \\
&\lim_{k\to\infty} \frac{LEL(G)}{n_{k+1}\sqrt{r_k}} = 0, \\
&\lim_{k\to\infty} \frac{\sqrt{2r_k}(n_{k+1} - n_k)}{n_{k+1}\sqrt{r_k}} = \sqrt{2}.
\end{aligned} \tag{5}$$

By (4), we deduce that

$$\frac{\sqrt{2r_k}(n_{k+1} - n_k)}{n_{k+1}\sqrt{r_k}} \leq \frac{LEL(\mathcal{L}^{k+1}(G))}{n_{k+1}\sqrt{r_k}}, \tag{6}$$

$$\begin{aligned}
\frac{LEL(\mathcal{L}^{k+1}(G))}{n_{k+1}\sqrt{r_k}} \leq \frac{LEL(G)}{n_{k+1}\sqrt{r_k}} &+ \frac{\sum_{i=0}^{k-1}\sqrt{2r_i}(n_{i+1} - n_i)}{n_{k+1}\sqrt{r_k}} \\
&+ \frac{\sqrt{2r_k}(n_{k+1} - n_k)}{n_{k+1}\sqrt{r_k}}.
\end{aligned} \tag{7}$$

It follows from (5), (6) and (7) that

$$\lim_{k\to\infty} \frac{LEL(\mathcal{L}^{k+1}(G))}{n_{k+1}\sqrt{r_k}} = \sqrt{2},$$

which implies the result in the theorem. □

Corollary 2.4 *Let G be an r-regular graph of order n. Then*

$$\lim_{k\to\infty} \frac{LEL(\mathcal{L}^{k+1}(G))}{n_{k+1}\sqrt{r_k}} = \sqrt{2}.$$

Remark 1 *It should be pointed out that, in [11], the authors showed that the energy (the energy of a graph G is defined as the sum absolute values of eigenvalues of G) of iterated line graphs of a regular graph is independent of graph structure. Here, Theorem 2.3, in a sense, supports the point of view in [6] that the Laplacian-energy like invariant is an energy like invariant.*

3 The LEL of some toroidal lattices

In this section, we consider the asymptotic behavior of the LEL of a square lattice (resp., hexagonal lattice, triangular lattice) with toroidal boundary condition.

The following lemma is well known.

Lemma 3.1 *[1] The Laplacian eigenvalues of the Cartesian product $G_1 \times G_2$ of graphs G_1 and G_2 are equal to all the possible sums of eigenvalues of the two factors:*

$$\mu_i(G_1) + \mu_j(G_2), \quad i = 1, 2, \ldots, |V(G_1)|, \quad j = 1, 2, \ldots, |V(G_2)|. \tag{8}$$

Let P_m and C_n be the path with m vertices and the cycle with n vertices, respectively.

Theorem 3.2 *Let $P_m \times P_n$ be the square lattice with free boundary condition. Then*

$$LEL(P_m \times P_n) = \sum_{i=0}^{m-1}\sum_{j=0}^{n-1} \sqrt{4 - 2\cos\frac{i\pi}{m} - 2\cos\frac{j\pi}{n}};$$

$$LEL(P_m \times P_n) \approx 1.91618mn. \tag{9}$$

Proof. Recall that [10] the Laplacian spectrum of P_m is

$$2 - \cos\frac{i\pi}{2}, i = 0, 1, \ldots, m - 1.$$

By applying Lemma 3.1 we can easily determine the Laplacian spectrum of $P_m \times P_n$ is

$$\mu_{ij}(P_m \times P_n) = 4 - 2\cos\frac{i\pi}{m} - 2\cos\frac{j\pi}{n}, 0 \leq i \leq m-1, 0 \leq j \leq n-1.$$

It follows from (1) that

$$LEL(P_m \times P_n) = \sum_{i=0}^{m-1}\sum_{j=0}^{n-1}\sqrt{4 - 2\cos\frac{i\pi}{m} - 2\cos\frac{j\pi}{n}}.$$

Hence,

$$\lim_{m,n\to\infty}\frac{LEL(P_m \times P_n)}{mn} = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi\sqrt{4 - 2\cos x - 2\cos y}d_x d_y.$$

Using the computer software Mathematica, we have

$$\lim_{m,n\to\infty}\frac{LEL(P_m \times P_n)}{mn} \approx 1.91618.$$

Thus

$$LEL(P_m \times P_n) \approx 1.91618mn.$$

□

Recall that the Laplacian spectrum of C_n is

$$2 - \cos\frac{2j\pi}{2},\ j = 0, 1, \ldots, n - 1.$$

By Lemma 3.1, the Laplacian eigenvalues of the Cartesian product $P_m \times C_n$ and $C_m \times C_n$ are $\mu_{ij}(P_m \times C_n) = 4 - 2\cos\frac{i\pi}{m} - 2\cos\frac{2j\pi}{n}$ and $\mu_{ij}(C_m \times C_n) = 4 - 2\cos\frac{2i\pi}{m} - 2\cos\frac{2j\pi}{n}$, $0 \leq i \leq m-1$, $0 \leq j \leq n-1$, respectively. An argument analogous to the proof of Theorem 3.2 establishes that

$$LEL(P_m \times C_n) = LEL(C_m \times C_n) \approx 1.91618mn. \tag{10}$$

Remark 2 *It follows from* (9) *and* (10) *that* $P_m \times P_n, P_m \times C_n$ *and* $C_m \times C_n$ *have the same asymptotic* $LEL(\approx 1.91618mn)$, *that is, the asymptotic LEL of square lattices is independent on the three boundary conditions (i.e., the free, cylindrical and toroidal boundary conditions).*

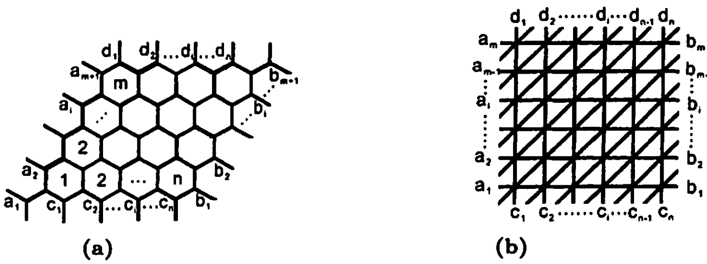

Figure 1: (a) The hexagonal lattice $H(m,n)$. (b) The triangular lattice graph $T(m,n)$.

The hexagonal lattice with toroidal boundary condition, denoted by $H(m,n)$, is illustrated in Figure 1(a), where (a_1,b_1), (a_2,b_2), $\cdots$, (a_{m+1}, b_{m+1}), (a_1,d_1), (c_1,d_2), (c_2,d_3), (c_{n-1},d_n), (c_n,b_{m+1}) are edges in $H(m,n)$.

Theorem 3.3 *Let $H(m,n)$ be the hexagonal lattice with toroidal boundary condition. Then*

$$\begin{aligned} LEL(H(m,n)) &= \sum_{i=0}^{m}\sum_{j=0}^{n}\left(\sqrt{3+\sqrt{3+2\cos\alpha+2\cos\beta+2\cos(\alpha+\beta)}}\right. \\ &\quad \left. +\sqrt{3-\sqrt{3+2\cos\alpha+2\cos\beta+2\cos(\alpha+\beta)}}\right), \end{aligned}$$

where $\alpha=\frac{2i\pi}{n+1}, \beta=\frac{2j\pi}{m+1}$;

$$LEL(H(m,n)) \approx 3.28747(m+1)(n+1).$$

Proof. Denote by $L(H(m,n))$ the Laplacian matrix of $H(m,n)$. It follows from Eq. (6.2.2) [13] that $L(H(m,n))$ is similar to the block diagonal matrix whose diagonal blocks are $H(i,j), 0\le i\le m, 0\le j\le n$, where

$$H(i,j)=\begin{pmatrix} 3 & -1-\xi_{n+1}^{-i}-\xi_{m+1}^{j} \\ -1-\xi_{n+1}^{i}-\xi_{m+1}^{-j} & 3 \end{pmatrix},$$

$\xi_t=\cos\frac{2\pi}{t}+i\sin\frac{2\pi}{t}, i^2=-1$. Thus the Laplacian eigenvalues of $H(m,n)$ are

$$3\pm\sqrt{3+2\cos\frac{2i\pi}{n+1}+2\cos\frac{2j\pi}{m+1}+2\cos\left(\frac{2i\pi}{n+1}+\frac{2j\pi}{m+1}\right)}, \qquad (11)$$

$0\le i\le m, 0\le j\le n$.

It follows from (1) and (11) that

$$LEL(H(m,n)) = \sum_{i=0}^{m}\sum_{j=0}^{n}\left(\sqrt{3+\sqrt{3+2\cos\alpha+2\cos\beta+2\cos(\alpha+\beta)}}\right.$$
$$\left.+\sqrt{3-\sqrt{3+2\cos\alpha+2\cos\beta+2\cos(\alpha+\beta)}}\right),$$

where $\alpha=\frac{2i\pi}{n+1}, \beta=\frac{2j\pi}{m+1}$. Hence

$$\lim_{m,n\to\infty}\frac{LEL(H(m,n))}{(m+1)(n+1)}$$
$$= \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi}\left(\sqrt{3+\sqrt{3+2\cos x+2\cos y+2\cos(x+y)}}\right.$$
$$\left.+\sqrt{3-\sqrt{3+2\cos x+2\cos y+2\cos(x+y)}}\right)d_xd_y.$$

Similarly, using the computer software Mathematica, we easily get

$$\lim_{m,n\to\infty}\frac{LEL(H(m,n))}{(m+1)(n+1)}\approx 3.28747.$$

Therefore

$$LEL(H(m,n))\approx 3.28747(m+1)(n+1).$$

□

Denote by $Tr(m,n)$ the triangular lattice with toroidal boundary condition. $Tr(m,n)$ can be regarded as an $m\times n$ square lattice with toroidal boundary condition with an additional diagonal edge added, in the same way, to every square, see Figure 1(b) for an illustration, where (a_1,b_1), $(a_2,b_2),\cdots,(a_m,b_m)$; (c_1,d_1), $(c_2,d_2),\cdots,(c_n,d_n)$; (d_1,c_2), $(d_2,c_3),\cdots$, (d_{n-1},c_n), $(d_n,c_1)=(b_m,a_1)$; $(b_1,a_2),(b_2,a_3),\cdots,(b_{m-1},a_m)$ are edges in $Tr(m,n)$.

Theorem 3.4 *Let $Tr(m,n)$ be the triangular lattice with toroidal boundary condition. Then*

$$LEL(Tr(m,n))=\sum_{i=0}^{n-1}\sum_{j=0}^{m-1}\left(\sqrt{6-2\cos\alpha-2\cos\beta-2\cos(\alpha+\beta)}\right),$$

where $\alpha=\frac{2i\pi}{n},\beta=\frac{2j\pi}{m}$;

$$LEL(Tr(m,n))\approx 2.37047mn.$$

Proof. Let $L(Tr(m,n))$ be the Laplacian matrix of $Tr(m,n)$. By Eq. (6.1.1) [13], the eigenvalues of $L(Tr(m,n))$ are

$$6 - 2\cos\frac{2i\pi}{n} - 2\cos\frac{2j\pi}{m} - 2\cos\left(\frac{2i\pi}{n} + \frac{2j\pi}{m}\right),$$

$0 \leq i \leq n-1, 0 \leq j \leq m-1$. Hence by the definition of LEL, we immediately get

$$LEL(Tr(m,n)) = \sum_{i=0}^{n-1}\sum_{j=0}^{m-1}\left(\sqrt{6 - 2\cos\alpha - 2\cos\beta - 2\cos(\alpha+\beta)}\right),$$

where $\alpha = \frac{2i\pi}{n}, \beta = \frac{2j\pi}{m}$. The rest of the proof is then fully analogous to the proof of Theorem 3.3. □

Remark 3 *It follows from Remark 2, Theorem 3.3 and Theorem 3.4 that the growth rate of the LEL of a square lattice (resp., hexagonal lattice, triangular lattice) with toroidal boundary condition is only dependent on the number of vertices of it.*

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