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The Eigen-chromatic Ratio of Classes of Graphs:Asymptotes, Areas and Molecular Stability

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Abstract

In this paper, we present a new ratio associated with classes of graphs, called the *eigen-chromatic ratio*, by combining the two graph theoretical concepts of *energy* and *chromatic number*.

The energy of a graph, the sum of the absolute values of the eigenvalues of the adjacency matrix of a graph, arose historically as a result of the energy of the benzene ring being identical to that of the sum of the absolute values of the eigenvalues of the adjacency matrix of the cycle graph on *n* vertices (see [18]).

The chromatic number of a graph is the smallest number of colour classes that we can partition the vertices of a graph such that each edge of the graph has ends that do not belong to the same colour class, and applications to the real world abound (see [30]). Applying this idea to molecular graph theory, for example, the water molecule would have its two hydrogen atoms coloured with the same colour different to that of the oxygen molecule.

Ratios involving graph theoretical concepts form a large subset of graph theoretical research(see [3], [16], [48]). The eigen-chromatic ratio of a class of graph provides a form of energy distribution among the colour classes determined by the chromatic number of such a class of graphs. The asymptote associated with this eigen-chromatic ratio allows for the behavioral analysis in terms of stability of molecules in molecular graph theory where a large number of atoms are involved.

This asymptote can be associated with the concept of graphs being hyper-or hypo- energetic (see [48]).

Keywords: Eigenvalue; Energy of graph; Chromatic number; Ratio; Asymptote; Area.

1.INTRODUCTION

We provided some basic notions of Graph theory which will be required later in this paper. We have used the graph theoretical notation of Harris, Hirst, and Mossimgho (see [27]). All graphs are simple, loopless and on *n* vertices and *m* edges.

1.1 Eigenvalue and Energy of Graphs

For a graphG = (V,E) with *n* vertices and *m* edges, we define its *eigenvalues* as the eigenvalues of its adjacency matrix

$$A(G)=(a_{ij})_{i,j=1}^{n} \quad \text{where} \quad a_{ij}=\begin{cases}1 & if\ v_iv_j\in E\ and\ v_1,v_2,\ldots,v_n\in V\\ 0 & otherwise\end{cases}$$

The energy of graph G is the sum of the absolute values of the eigenvalues of the adjacency matrix of G, i.e., for an *n*-vertex graph G, with adjacency matrix A, having eigen values $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$, the energy of G, denoted by E(G), is defined as:

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

Much research has been done involving the energy of graph (see Coulson, Leary and Mallion[18], Gustmam [26], Brualdi [15], Indual and Vijayakumar [28], and Stevanovic [35]).

1.2 Chromatic Number

Given a graph G, what is the least number of colours required to colour its vertices in such away no two adjacent vertices receive the same colour? The required number of colours is called the *chromatic number* of G and is denoted by χ(G). No formula exits for the chromatic number of an arbitrary graph. Thus, for the most part, one must be content with supplying bounds for the chromatic number of graphs.

The chromatic idea can be translated to a molecular construction. So, the chromatic number associated with the molecular graph (the atoms are vertices and edges are bonds between the atoms) would involve the partitioning of the atoms into the smallest number of sets of like atoms so that like atoms are not bonded. For example, the water molecule H_2O has two hydrogen atoms bonded to an oxygen atom, the hydrogen atoms are not bonded, so that, the molecular graphic version would involve the chromatic number of 2, where the oxygen atom has a different colour to the hydrogen atoms which are assigned the same colour. On the other hand, the benzene ring molecule C_6H_6 has same atoms (carbon atoms) bonded. There are other examples: the hydrogen sulfide molecule H_2S, the ammonia molecule H_3N, the methane moleculeCH_4 have respectively two, three, four hydrogen atoms bonded to another atom, such that same atoms are not bonded. The atoms bond to form molecules, and different atoms are forced to bond in order to get *stability*; different atoms come together to achieve the noble gas configuration. This coming together and sharing of electron pairs leads to the formation of a chemical bond know as a covalent bond.
A *covalent bond* is a shared pair of electrons between two different nonmetal atoms. These electrons can originate from one atom, or one electron can originate from each of the two atoms. The two electrons in the bond are attracted to both atomic nuclei and are shared between the two atoms. Two different atoms share the electrons because atoms (other than hydrogen and helium) are most stable when surrounded by eight electrons (an octet), which means that an atom with a full octet of electrons has lower energy (is more stable) than one without a full octet (See Coulson, Lary and Mallion [18], Wiswesser [51], Agida, Bayad, Gustman and Srinivas [2], Ballhausen and Gray [7], Gray [24]).

Remarks:(see Winter [37],[38])

(i) The chromatic number of a *k*-partite graph is *k*;
(ii) The chromatic number of the complete graph K_n on *n* vertices is $\chi(K_n) = n$.

1.3 Ratios

Ratios have always been an important aspect of graph theoretical definitions. The following are examples of various ratios which have been studied which provide motivation for the new ratios which we discuss here: Expanders (see Alon and Spencer [4]), The central ratio of graph (see Buckley [16]), Eigen-pair ratio of classes of graphs (see Winter and Jessop [42]), Independence and Hall ratios (see Gabor [21]), Tree-cover ratio of graphs (see Winter and Adewusi [41]), The eigen-energy formation ratio of graphs (see Winter and Sarvate [50]), The chromatic-cover ratio of graphs (see Winter [38]), The eigen-complete difference ratio (see Winter and Ojako [49]), The eigen-cover ratios (see Winter and Jessop [43], [46], [47]), The t-complete eigen ratio of graphs (see Winter, Jessop and Adewusi [44]) and Ratios of classes of graphs (see Winter [39]).

2. EIGEN-CHROMATIC RATIO AND ASYMPTOTE

In this paper, we combine the two concepts of energy and chromatic number of graphs to forma ratio, the eigen-chromatic ratio. If the eigen-chromatic ratio is a function of *n*, the order of graphs belonging to a particular class of graphs, then we investigated its asymptotic behavior (see Winter [37],[39],[40], Winter and Adewusi [41], Winter and Ojako [49], Winter and Sarvate [50], Adewusi [1], Gabor [21], Ojako [33], Winter and Jessop [42], [43], [46], [47]).

Definition 2.1

The *eigen-chromatic ratio* of a graph G, of order *n,* is denoted by eig_χ(G) and defined as

$$eig_{\chi}(G) = \frac{\chi(G)}{E(G)}$$

where $\chi(G)$ is the chromatic number of G and $E(G)$ the energy of G.

Definition 2.2

If $eig_{\chi}(G) = f(n)$ for every graph $G \in \mathfrak{I}$, where $\mathfrak{I}$ is a class of graphs, then the asymptotic behaviour of *f(n)* is called the *eigen-chromatic asymptote* of G and denoted by $Asyeig_{\chi}(G)$, and then

$$Asyeig_{\chi}(G) = \lim_{n \to \infty} f(n).$$

This asymptote gives a measure of the *asymptote* effect of the chromatic number on the energy of the original graph, for large values of *n,* and is referred to as the *eigen-chromatic asymptote* effect. This idea translates to the effect in the molecular graph theory.

Eigen-Chromatic stability: The Hyper/Hypo Chromatic Stability Effect.

The eigen-chromatic ratio of a graph G is a form of energy distribution among the colour classes determined by $\chi(G)$. The eigen-chromatic asymptote gives an indication of this distribution when a large number of vertices are involved as in molecular graph theory. We show that the eigen-chromatic asymptote for the complete graph on *n* vertices is $\frac{1}{2}$, while most graphs have 0 such asymptote, which motivates for the following two definitions (see [26]):

- A graph G is said to be *eigen-chromatically stable* if the eigen-chromatic asymptote is not zero i.e. if

$$Asyeig_{\chi}(G) \neq 0;$$

  otherwise it is *eigen-chromatically unstable.*

- A graph G is said to *be hyper eigen-chromatically stable* if its eigen-chromatic asymptote is bigger or equal to $\frac{1}{2}$, i.e. if

$$Asyeig_{\chi}(G) \geq \frac{1}{2}$$

  and *hypoeigen-chromatically stable* if its eigen-chromatic asymptote is less than $\frac{1}{2}$ and positive, i.e. if

$$0 < Asyeig_{\chi}(G) < \frac{1}{2}.$$

3. EXEMPLES OF EIGEN-CHROMATIC RATIOS AND ASYMPTOTES

In this section, we use energies of graphs already found, based on the articles by Winter and Jessop [43], [45], [48]. For the chromatic number of graphs, see Winter [37],[38].

3.1 The Complete Graphs

Let K_n be a complete graph on *n* vertices. Then, we have its chromatic number $\chi(K_n) = n$ and its energy

$$E(K_n) = \sum_{i=1}^{n} |\lambda_i| = 2(n-1)$$

(see Winter and Jessop [43], [46]).

So that, the *eigen-chromatic ratio* of the complete graph K_n, of order *n* is

$$eig_{\chi}(K_n) = \frac{\chi(K_n)}{E(K_n)} = \frac{n}{2(n-1)} = \frac{n}{2n-2};$$

The *eigen-chromatic asymptote* of K_n is $Asyeig_{\chi}(K_n) = \lim_{n\to\infty} \frac{n}{2n-2} = \frac{1}{2}$.

3.2 The Path Graph

Let P_n be a path on *n* vertices, with *n* even. The chromatic number of P_n is $\chi(P_n) = 2$ and its energy is

$$E(P_n) = 2\left[\cos ec \frac{\pi}{2(n+1)} - 1\right]$$ (see Winter and Jessop [43], [45], [48]).

We have:

$$eig_{\chi}(P_n) = \frac{\chi(P_n)}{E(P_n)} = \frac{2}{2\left[\cos ec \frac{\pi}{2(n+1)} - 1\right]} = \frac{1}{\left[\cos ec \frac{\pi}{2(n+1)} - 1\right]};$$

and

$$Asyeig_{\chi}(P_n) = \lim_{n\to\infty} \frac{1}{\cos ec \frac{\pi}{2(n+1)} - 1} = \lim_{n\to\infty} \frac{1}{\frac{2n}{\pi}} = \lim_{n\to\infty} \frac{\pi}{2n} = 0.$$

3.3 The Cycle Graph

Let C_n be a cycle graph on *n* vertices, with *n* even. The chromatic number of C_n is $\chi(C_n) = 2,$ and its energy is

$$E(C_n) = \sum_{j=0}^{n-1} \left| 2\cos\left(\frac{2\pi j}{n}\right) \right| = 4\cot\left(\frac{\pi}{n}\right)$$ (see Winter and Jessop [43], [45], [48]).

The eigen-chromatic ratio of C_n is

$$eig_{\chi}(C_n) = \frac{\chi(C_n)}{E(C_n)} = \frac{2}{4\cot\left(\frac{\pi}{n}\right)} = \frac{1}{2\cot\left(\frac{\pi}{n}\right)};$$

And its eigen-chromatic asymptote is

$$Asyeig_{\chi}(C_n) = \lim_{n\to\infty} \frac{1}{2\cot\left(\frac{\pi}{n}\right)} = 0.$$

3.4 The Wheel Graph

Let W_n be the wheel graph, on *n* vertices, with *n* even, *n* – 1 spokes, and *n* ≥4. The wheel graph W_n have the chromatic number $\chi(W_n) = 4$ and the energy

$$E(W_n) = 2\sqrt{n} - 2 + 2\cos ec\left(\frac{\pi}{2(n-1)}\right)$$ (see Winter and Jessop [43], [45], [48]).

So that, the eigen-chromatic ratio of W_n is

$$eig_\chi(W_n) = \frac{\chi(W_n)}{E(W_n)} = \frac{4}{2\sqrt{n} - 2 + 2\cos ec\left(\frac{\pi}{2(n-1)}\right)} = \frac{2}{\sqrt{n} - 1 + \cos ec\left(\frac{\pi}{2(n-1)}\right)}$$

and the eigen-chromatic asymptote of W_n is

$$Asyeig_\chi(W_n) = \lim_{n\to\infty} \frac{2}{\sqrt{n} - 1 + \cos ec\left(\frac{\pi}{2(n-1)}\right)} = 0.$$

3.5 Star Graphs of length 1

Let $S_{n-1,1}$ be the star graph on n vertices, and with $n-1$ rays of length 1, $n \geq 2$. The star graphs $S_{n-1,1}$ have the chromatic number

$$\chi(S_{n-1,1}) = 2,$$

and the energy

$$E(S_{n-1,1}) = 2\sqrt{n-1}$$ (see Winter and Jessop [43], [45], [48]).

Then, the eigen-chromatic ratio of $S_{n-1,1}$ is

$$eig_\chi(S_{n-1,1}) = \frac{\chi(S_{n-1,1})}{E(S_{n-1,1})} = \frac{2}{2\sqrt{n-1}} = \frac{1}{\sqrt{n-1}}$$

and its eigen-chromatic asymptote is

$$Asyeig_\chi(S_{n-1,1}) = \lim_{n\to\infty} \frac{1}{\sqrt{n-1}} = \lim_{n\to\infty} \frac{1}{\sqrt{n}} = 0.$$

3.6 Star Graphs of length 2

Let $S_{\frac{n-1}{2},2}$ be the star graph on n vertices, and with $\frac{n-1}{2}$ rays of length 2, $n \geq 7$. Then the chromatic number of $S_{\frac{n-1}{2},2}$ is

$$\chi(S_{\frac{n-1}{2},2}) = 2,$$

and its energy is

$$E(S_{\frac{n-1}{2},2}) = n - 3 + \sqrt{2(n+1)}$$ (see Winter and Jessop [43], [45], [48]).

So that the eigen-chromatic ratio of $S_{\frac{n-1}{2},2}$ is

$$eig_\chi(S_{\frac{n-1}{2},2}) = \frac{\chi(S_{\frac{n-1}{2},2})}{E(S_{\frac{n-1}{2},2})} = \frac{2}{n - 3 + \sqrt{2(n+1)}}$$

and its eigen-chromatic asymptote is

$$Asyeig_{\chi}(S_{\frac{n-1}{2},2}) = \lim_{n\to\infty} \frac{2}{n-3+\sqrt{2(n+1)}} = 0.$$

3.7 The Lollipop Graphs

Let LP_n be the lollipop graph comprising of the complete graph K_{n-1} on $(n - 1)$ vertices, joined to a single end vertex x_2 by an edge x_1x_2, with $n \geq 3$. The chromatic number and the energy of LP_n are respectively: $\chi(LP_n) = n-1$, and

$$E(LP_n) = (n-3) + \sqrt{n^2 - 4n + 8}$$ (see Winter and Jessop [43], [45], [48]).

Then, the eigen-chromatic ratio of LP_n is

$$eig_{\chi}(LP_n) = \frac{\chi(LP_n)}{E(LP_n)} = \frac{n-1}{(n-3)+\sqrt{n^2-4n+8}}$$

and its eigen-chromatic asymptote is

$$Asyeig_{\chi}(LP_n) = \lim_{n\to\infty} \frac{n-1}{(n-3)+\sqrt{n^2-4n+8}} = \lim_{n\to\infty} \frac{n-1}{2n} = \frac{1}{2}.$$

3.8 The Complete Split-bipartite Graph

Let $K_{\frac{n}{2},\frac{n}{2}}$ be the complete split-bipartite graph on n vertices, and with $\frac{n^2}{4}$ edges. Then the chromatic number of the complete split-bipartite graphs is $\chi(K_{\frac{n}{2},\frac{n}{2}}) = 2$; and its energy is:

$$E(K_{\frac{n}{2},\frac{n}{2}}) = n$$ (see Winter and Jessop [43], [45], [48]).

So that, the eigen-chromatic ratio of $K_{\frac{n}{2},\frac{n}{2}}$ is

$$eig_{\chi}(K_{\frac{n}{2},\frac{n}{2}}) = \frac{\chi(K_{\frac{n}{2},\frac{n}{2}})}{E(K_{\frac{n}{2},\frac{n}{2}})} = \frac{2}{n}$$

and its eigen-chromatic asymptote is

$$Asyeig_{\chi}(K_{\frac{n}{2},\frac{n}{2}}) = \lim_{n\to\infty} \frac{2}{n} = 0.$$

3.9 The Friendship Graph

Let F_n be a friendship graph on $2n + 1$ vertices and $3n$ edges, constructed by joining n copies of the cycle graph C_3, with a common vertex. Then, the chromatic number and energy of F_n are respectively:

$$\chi(F_n) = 3,$$

and

$$E(F_n) = (2n-1) + \sqrt{1+8n}$$ (see Rajesh Kanna and all [34]).

We have the eigen-chromatic ratio of F_n :

$$eig_{\chi}(F_n) = \frac{\chi(F_n)}{E(F_n)} = \frac{3}{(2n-1)+\sqrt{1+8n}}$$

and its eigen-chromatic asymptote:

$$Asyeig_{\chi}(F_n) = \lim_{n\to\infty} \frac{3}{(2n-1)+\sqrt{1+8n}} = 0.$$

3.10 The Complete Sun Graph

Let $CompSun(h, p)$ be the complete sun graph which consists of the complete graph K_p , with h end vertices appended to each of the p vertices in K_p . Then $CompSun(h, p)$ has $n = (h+1)p$ vertices and $p(\frac{p-1}{2}+h)$ edges.

The chromatic number and energy of the complete sun graph $CompSun(h, p)$ are respectively:

$$\chi(CompSun(h, p)) = p$$

and

$$E(CompSun(h, p)) = (p-1)\sqrt{1+4h} + \sqrt{(p-1)^2+4h}$$ (see Winter and Jessop [45], [48]).

So that, the eigen-chromatic ratio of $CompSun(h, p)$ is

$$eig_{\chi}(CompSun(h, p)) = \frac{\chi(CompSun(h, p))}{E(CompSun(h, p))} = \frac{p}{(p-1)\sqrt{1+4n} + \sqrt{(p-1)^2+4h}}$$

and its eigen-chromatic asymptote:

$$Asyeig_{\chi}(CompSun(h, p)) = \lim_{n\to\infty} \frac{p}{(p-1)\sqrt{1+4n} + \sqrt{(p-1)^2+4h}}$$

$$= \lim_{(h+1)p\to\infty} \frac{p}{(p-1)\sqrt{1+4n} + \sqrt{(p-1)^2+4h}}$$

$$= \lim_{p\to\infty} \frac{p}{(p-1)\sqrt{1+4n} + \sqrt{(p-1)^2+4h}} = \frac{1}{\sqrt{1+4h}+1}.$$

So, for

$$h = 1,\ Asyeig_{\chi}(CompSun(1, p)) = \frac{1}{\sqrt{5}+1} \cong 0.309$$

$$h = 2,\ Asyeig_{\chi}(CompSun(2, p)) = \frac{1}{\sqrt{9}+1} \cong 0.25$$

$$h = 3,\ Asyeig_{\chi}(CompSun(3, p)) = \frac{1}{\sqrt{13}+1} \cong 0.217$$

.
.
.

$$h = 100,\ Asyeig_{\chi}(CompSun(100, p)) = \frac{1}{\sqrt{401}+1} \cong 0.047$$

$$\vdots$$

This implies that $0 < Asyeig_{\chi}(CompSun(h, p)) < \frac{1}{2}$.

Remark: The asymptote of the complete sun graph with h=1 is 0.309 which is $\frac{1}{2}$ golden ratio (see Winter and Jessop [48], Buckley [16]) of 0.618.

We get the golden ratio for $h = 1$, then $p = \frac{n}{2}$, so

$$eig_{\chi}(CompSun(1, \frac{n}{2})) = \frac{n}{\frac{\sqrt{5}}{2}(n-2) + \frac{1}{2}\sqrt{(n-2)^2+16}} = \frac{2n}{(n-2)\sqrt{5} + \sqrt{(n-2)^2+16}}$$

and

$$Asyeig_{\chi}(CompSun(1, \frac{n}{2})) = \lim_{n\to\infty} \frac{2n}{(n-2)\sqrt{5} + \sqrt{(n-2)^2+16}} = \frac{2}{2\sqrt{5}+1} \cong 0.35.$$

3.11 The Complete Split-bipartite Sun Graph

Let $BipSun(h, p)$ be the complete split-bipartite sun graph which consists of the complete split-bipartite graph $K_{\frac{p}{2},\frac{p}{2}}$, with h end vertices appended to each of the p vertices in $K_{\frac{p}{2},\frac{p}{2}}$. Then $BipSun(h, p)$ has $n = (h+1)p$ vertices and $\frac{p^2}{4} + ph$ edges.

The chromatic number and energy of the complete split-bipartite sun graph are respectively:

$$\chi(BipSun(h, p)) = 2$$

and

$$E(BipSun(h, p)) = \sqrt{p^2+16h} + 2(p-2)\sqrt{h}$$ (see Winter and Jessop [45], [48]).

So that, the eigen-chromatic ratio of $BipSun(h, p)$ is

$$eig_{\chi}(BipSun(h, p)) = \frac{\chi(BipSun(h, p))}{E(BipSun(h, p))} = \frac{2}{\sqrt{p^2+16h} + 2(p-2)\sqrt{h}}$$

and its eigen-chromatic asymptote:

$$Asyeig_{\chi}(BipSun(h, p)) = \lim_{n\to\infty} \frac{2}{\sqrt{p^2+16h} + 2(p-2)\sqrt{h}}$$

$$= \lim_{(h+1)p\to\infty} \frac{2}{\sqrt{p^2+16h} + 2(p-2)\sqrt{h}}$$

$$= \lim_{p\to\infty} \frac{2}{\sqrt{p^2+16h} + 2(p-2)\sqrt{h}} = 0.$$

3.12 The Star Sun Graph

Let $StarSun(h, p)$ be the star sun graph which consists of the star graph $S_{n-1,1}$, with *h* end vertices appended to each of the *p* vertices in $S_{n-1,1}$. Then $StarSun(h, p)$ has $n=(h+1)p$ vertices and $(h+1)(p-1)+h$ edges.
The energy of the star sun graph is

$$E(StarSun(h,p)) = 2\sqrt{p-1+4h} + 2(p-2)\sqrt{h} \text{ (see Winter and Jessop [45], [48])}$$

and its chromatic number

$$\chi(StarSun(h,p)) = 2.$$

Then, the eigen-chromatic ratio of $StarSun(h, p)$ is

$$eig_{\chi}(StarSun(h,p)) = \frac{\chi(StarSun(h,p))}{E(StarSun(h,p))} = \frac{2}{2\sqrt{p-1+4h}+2(p-2)\sqrt{h}} = \frac{1}{\sqrt{p-1+4h}+(p-2)\sqrt{h}}$$

and its eigen-chromatic asymptote:

$$Asyeig_{\chi}(StarSun(h,p)) = \lim_{(h+1)p\to\infty} \frac{1}{\sqrt{p-1+4h}+(p-2)\sqrt{h}}$$

$$= \lim_{p\to\infty} \frac{1}{\sqrt{p-1+4h}+(p-2)\sqrt{h}} = 0.$$

Conjecture 1. The eigen-chromatic asymptote of all the classes of graphs lies on the interval $[0, \frac{1}{2}]$.

Theorem 3.1 The eigen-chromatic ratio and asymptotes for all the classes $\Im$ of graphs studied in this paper are summarized in the following table.

$\Im$	$eig_{\chi}(\Im)$	$Asyeig_{\chi}(\Im)$
K_n	$\frac{n}{2n-2}$	$\frac{1}{2}$
P_n	$\frac{1}{\operatorname{cosec}\frac{\pi}{2(n+1)}-1}$	0
C_n	$\frac{1}{2\cot\left(\frac{\pi}{n}\right)}$	0
W_n	$\frac{2}{\sqrt{n}-1+\operatorname{cosec}\left(\frac{\pi}{2(n-1)}\right)}$	0
$S_{n-1,1}$	$\frac{1}{\sqrt{n-1}}$	0

$S_{\frac{n-1}{2},2}$	$\frac{2}{n-3+\sqrt{2(n+1)}}$	0
LP_n	$\frac{n-1}{(n-3)+\sqrt{n^2-4n+8}}$	$\frac{1}{2}$
$K_{\frac{n}{2},\frac{n}{2}}$	$\frac{2}{n}$	0
F_n	$\frac{3}{(2n-1)+\sqrt{1+8n}}$	0
$CompSun(h,p)$	$\frac{p}{(p-1)\sqrt{1+4n}+\sqrt{(p-1)^2+4h}}$	$(0,\frac{1}{2})$
$BipSun(h,p)$	$\frac{2}{\sqrt{p^2+16h}+2(p-2)\sqrt{h}}$	0
$StarSun(h,p)$	$\frac{1}{\sqrt{p-1+4h}+(p-2)\sqrt{h}}$	0

Corollary 3.1 The complete, the lollipop and the complete sun graph are the only eigen-chromatically stable classes of graphs in the collection of classes discussed above.

4. SECOND ORDER DIFFERENTIAL EQUATION ASSOCIATED WITH THE EIGEN-CHROMATIC RATIO OF THE COMPLETE GRAPH: PAIRED SOLUTIONS

An important step is to notice that if f and g are two solutions of an ordinary differential equation, then so is the sum; in fact, so is any linear combination $\alpha f+\beta g$ where α and β are constants. And such two solutions f and g satisfying the same differential equation are called *paired solutions*. For example, cosine and sine functions are paired solutions for the ordinary differential equation $y''+y=0$; cosh and sinh funcions are paired sloutions, for the ordinary differential equation $y''-y=0$ (See Zill[53], Zill and Wright [54]).

Now, the eigen-chromatic ratio of the complete graph on *n* vertices in $\frac{n}{2n-2}$.

Setting

$$y=\frac{n}{2n-2},$$

now

$$y'=\frac{dy}{dn}=\frac{d}{dn}\left[\frac{n}{2n-2}\right]=\frac{-2}{(2n-2)^2}=\frac{d}{dn}\left[\frac{1}{2n-2}\right].$$

Also:

$$y''=\frac{dy'}{dn}=-2\frac{d}{dn}\left[\frac{1}{(2n-2)^2}\right]=\frac{8}{(2n-2)^3}.$$

Thus:

$$2y'+(n-1)y''=\frac{-4}{(2n-2)^2}+(n-1)\frac{8}{(2n-2)^3}=0.$$

So that:

$$y''+\frac{2}{n-1}y'=0.$$

Put $P=y'\Rightarrow P'=y''$, so

$$P'+\frac{2}{n-1}P=0.$$

Integrating factor is $e^{2\int\frac{dn}{n-1}}=(n-1)^2$, so that $(n-1)^2P=C$, Hence $P=\frac{C}{(n-1)^2}$. So that

$$y'=\frac{C}{(n-1)^2}.$$

We thus have:

$$y=\frac{-C}{n-1}+C'\Rightarrow y=\frac{K}{n-1}+K'(\text{with } K,K'\in\mathbb{R}).$$

Thus the two distinct functions

$$y=\frac{n}{2n-2} \quad \text{and} \quad y=\frac{K}{n-1}+K'$$

satisfy the same differential equation:

$$2y'+(n-1)y''=0$$

and are hence paired solutions.

5. EIGEN-CHROMATIC AREA OF CLASSES OF GRAPHS

By introducing the average degree of a graph together with the Riemann integral of each new ratio defined, the eigen-chromatic ratio, we associate *eigen-chromatic area* with classes of graphs(see Adewusi [1], Ojako [33], Winter [37], [38], Winter and Adewusi [41], Winter and Jessop[42],[43], Winter and Sarvate [50], Winter, Jessop and Adewusi [44], Winter and Ojako [49]).The idea of eigen-chromatic area provides a further comparative analysis between the different classes of graphs analysed. This analysis confirms previous research that the area (defined in terms of different ratios) of the complete graph dominates the appropriate area of all other classes of graphs. The eigen-chromatic area of the complete graph is of order $\frac{n^2}{2}$ for large values of n.

Definition 5.1

If $\Im$ is a class of graphs and $eig_{\chi}(G)=\frac{\chi(G)}{E(G)}=f(n)$ for every graph $G\in\Im$ with n vertices and m edges, then the *eigen-chromatic area* is defined as (see Winter [37], [38], Winter and Jessop [41] etc):

$$A^{\chi}_{\Im(n)}=\frac{2m}{n}\int f(n)dn$$

with $A^{\chi}_{\Im(k)}=0$ where k is the smallest number of vertices for which $eig_{\chi}(G)=f(n)$ is defined, and $\frac{2m}{n}$ is the average degree of $G\in\Im$, referred to as the *length* of G. The integral part is referred to as its *height*, which we always make positive.

5.1 Examples of Eigen-chromatic Area of Classes of Graphs

5.1.1 The Complete Graph

A complete graph has $m=\frac{2(n-1)}{2}$ edges. Then, the eigen-chromatic area of the complete graph K_n is

$$A_{K_n}^{\chi}=\frac{2m}{n}\int\frac{n}{2n-2}dn=n-1\int\frac{n}{2n-2}dn=\frac{n-1}{2}\int\frac{n}{n-1}dn=\frac{n-1}{2}(n+\ln|n-1|+C).$$

The function $f(n)=\frac{n}{2n-2}$ is defined if $2n-2\neq 0$ i.e. if $n\neq 1,$ so that with smallest order 2 we have:

$$A_{K_2}^{\chi}=\frac{2-1}{2}(2+\ln|2-1|+C)=0\Rightarrow C=-2,$$

So that,

$$A_{K_n}^{\chi}=\frac{n-1}{2}(n+\ln|n-1|-2).$$

5.1.2 The Path Graph

A path graph has $m=n-2$ edges. Then, the eigen-chromatic area of the path graph P_n is

$$A_{P_n}^{\chi}=\frac{2m}{n}\int\frac{1}{\cos ec\frac{\pi}{2(n+1)}-1}dn$$

$$=\frac{2(n-2)}{n}\int\frac{1}{\cos ec\frac{\pi}{2(n+1)}-1}dn.$$

5.1.3 The Cycle Graph

A cycle graph has $m=n$ edges. Then, the eigen-chromatic area of the cycle graph C_n is

$$A_{C_n}^{\chi}=\frac{2m}{n}\int\frac{1}{2\cot\left(\frac{\pi}{n}\right)}dn=2\int\frac{1}{2\cot\left(\frac{\pi}{n}\right)}dn$$

$$=\int\frac{1}{\cot\frac{\pi}{n}}dn.$$

5.1.4 The Wheel Graph

The wheel graph has $m=(2n-2)$ edges. Then, the eigen-chromatic area of the wheel graph W_n is

$$A_{W_n}^{\chi}=\frac{2m}{n}\int\frac{2}{\sqrt{n}-1+\cos ec\left(\frac{\pi}{2(n-1)}\right)}dn=2.\frac{2n-2}{n}\int\frac{2}{\sqrt{n}-1+\cos ec\left(\frac{\pi}{2(n-1)}\right)}dn$$

$$= 8.\frac{n-1}{n}\int \frac{1}{\sqrt{n}-1+\cos ec\left(\frac{\pi}{2(n-1)}\right)}dn.$$

5.1.5 The Star graph of length 1

The star graph has $m = n-1$ edges. Then, the eigen-chromatic area of the star graph $S_{n-1,1}$ is

$$A^{\chi}_{S_{n-1,1}} = \frac{2m}{n}\int \frac{1}{\sqrt{n-1}}dn = \frac{2(n-1)}{n}\int \frac{1}{\sqrt{n-1}}dn$$

$$= \frac{2(n-1)}{n}(2\sqrt{n-1}+C).$$

The function $f(n) = \frac{1}{\sqrt{n-1}}$ is defined if $n-1>0$ i.e. if $n>1$, so that with smallest order 2 we have:

$$A^{\chi}_{S_{1,1}} = \frac{2(2-1)}{2}(2\sqrt{2-1}+C) = 0 \Rightarrow C = -2,$$

So that

$$A^{\chi}_{S_{n-1,1}} = \frac{2(n-1)}{n}(2\sqrt{n-1}-2) = \frac{4(n-1)}{n}(\sqrt{n-1}-1).$$

5.1.6 The Star graph of length 2

The star graph $S_{\frac{n-1}{2},2}$ of length 2 has $m = n-1$ edges, so its eigen-chromatic area is

$$A^{\chi}_{S_{\frac{n-1}{2},2}} = \frac{2m}{n}\int \frac{2}{n-3+\sqrt{2(n+1)}}dn = \frac{2(n-1)}{n}\int \frac{2}{n-3+\sqrt{2(n+1)}}dn$$
$$= \frac{4(n-1)}{n}\int \frac{1}{n-3+\sqrt{2(n+1)}}dn$$

Let us compute $I = \int \frac{1}{n-3+\sqrt{2(n+1)}}dn,$ setting $\sqrt{2(n+1)} = t \Rightarrow n = \frac{1}{2}(t^2-2) \Rightarrow dn = tdt$

$$\Rightarrow I = 2\int \frac{1}{t^2+2t-8}tdt,$$

So, $I = \frac{2}{3}(\ln[(t-2)(t+4)^2]) + C = \frac{2}{3}(\ln[\sqrt{2(n+1)}-2)(\sqrt{2(n+1)}+4)^2]) + C,$ and

$$A^{\chi}_{S_{\frac{n-1}{2},2}} = \frac{4(n-1)}{n}(\frac{2}{3}(\ln[\sqrt{2(n+1)}-2)(\sqrt{2(n+1)}+4)^2]) + C).$$

With smallest order 2 we have:

$$\frac{4(2-1)}{2}(\frac{2}{3}(\ln[\sqrt{2(2+1)}-2)(\sqrt{2(2+1)}+4)^2]) + C) = 0 \Rightarrow C = -\frac{2}{3}\ln(4+\sqrt{6});$$

So

$$A^{\chi}_{S_{\frac{n-1}{2},2}} = \frac{4(n-1)}{n}(\frac{2}{3}(\ln[\sqrt{2(n+1)}-2)(\sqrt{2(n+1)}+4)^2]) - \frac{2}{3}\ln(4+\sqrt{6})).$$

And finally we have:

$$A^{\chi}_{S_{\frac{n-1}{2},2}}=\frac{8(n-1)}{3n}\ln\left(\frac{(\sqrt{2(n+1)}-2)(\sqrt{2(n+1)}+4)^2}{4+\sqrt{6}}\right).$$

5.1.7 The Lollipop Graph

The lollipop graph has $m=(n-1)(n-2)+1$ edges. Then, the eigen-chromatic area of the lollipop graph LP_n is

$$A^{\chi}_{LP_n}=\frac{2m}{n}\int\frac{n-1}{(n-3)+\sqrt{n^2-4n+8}}dn=\frac{2((n-1)(n-2)+1)}{n}\int\frac{n-1}{(n-3)+\sqrt{n^2-4n+8}}dn.$$

So

$$A^{\chi}_{LP_n}=\frac{2((n-1)(n-2)+1)}{n}\int\frac{n-1}{(n-3)+\sqrt{(n-2)^2+4}}dn.$$

5.1.8 The Complete Split-bipartite Graph

The Complete Split-bipartite graph has $m=\frac{n^2}{4}$ edges. Then, the eigen-chromatic area of the Complete Split-bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ is

$$A^{\chi}_{K_{\frac{n}{2},\frac{n}{2}}}=\frac{2m}{n}\int\frac{2}{n}dn=\frac{\frac{2n^2}{4}}{n}\int\frac{2}{n}dn=\frac{n}{2}\int\frac{2}{n}dn=n(\ln(n)+C)$$

With smallest order 2 we have: $C=-\ln 2,$ so

$$A^{\chi}_{K_{\frac{n}{2},\frac{n}{2}}}=n(\ln(n)-\ln 2)$$

$$=n(\ln\left(\frac{n}{2}\right)).$$

5.1.9 The Friendship Graph

The friendship graph has $m=3n$ edges. Then, the eigen-chromatic area of the friendship graph F_n is

$$A^{\chi}_{F_n}=\frac{2m}{n}\int\frac{3}{(2n-1)+\sqrt{1+8n}}dn=6\int\frac{3}{(2n-1)+\sqrt{1+8n}}dn.$$

$$=18\int\frac{1}{(2n-1)+\sqrt{1+8n}}dn=\frac{9}{2}\int\frac{(2n-1)-\sqrt{1+8n}}{n^2-3n}dn,$$

So

$$A^{\chi}_{F_n}=\frac{3}{2}(\ln(n)+\ln(n-3)^5)-\frac{9}{2}\int\frac{\sqrt{1+8n}}{n^2-3n}dn,$$

$$=\frac{3}{2}(\ln(n(n-3)^5)-\frac{9}{2}\int\frac{\sqrt{1+8n}}{n^2-3n}dn.$$

5.1.10 The Complete Sun Graph

The complete sun graph has $n=(h+1)p$ vertices and $m=p(\frac{p-1}{2}+h)$ edges. Then, the eigen-chromatic area of the complete sun graph $CompSun(h,p),$ for $h=1,$ is

$$A^{\chi}_{CompSun(1,\frac{n}{2})}=\frac{n+2}{4}\int\frac{n}{\frac{\sqrt{5}}{2}(n-2)+\frac{1}{2}\sqrt{(n-2)^2+16}}dn$$

$$=\frac{n+2}{2}\int\frac{n}{(n-2)\sqrt{5}+\sqrt{(n-2)^2+16}}dn.$$

5.1.11 The Complete Split-bipartite Sun Graph

The complete split-bipartite sun graph has $n=(h+1)p$ vertices and $m=\frac{p^2}{4}+ph$ edges. If $h=1$ then $p=\frac{n}{2}$ and the eigen-chromatic area of the complete split-bipartite sun graph $BipSun(h,p)$ is

$$A^{\chi}_{BipSun(1,\frac{n}{2})}=\frac{2.\frac{n}{16}(n+8)}{n}\int\frac{2}{\sqrt{(\frac{n}{2})^2+16+2(\frac{n}{2}-2)}}dn$$

$$=\frac{n+8}{4}\int\frac{1}{\sqrt{(\frac{n}{2})^2+16+2(\frac{n}{2}-2)}}dn$$

$$=\frac{n+8}{4}\int\frac{1}{\sqrt{n^2+64+2n-8}}dn.$$

5.1.12 The star Sun Graph

The star sun graph has $n=(h+1)p$ vertices and $m=(h+1)(p-1)+h$ edges. If $h=1$ then $p=\frac{n}{2}$ and the eigen-chromatic area of the star sun graph $StarSun(h,p)$ is

$$A^{\chi}_{StarSun(1,\frac{n}{2})}=\frac{2(n-1)}{n}\int\frac{1}{\sqrt{\frac{n}{2}-1+4+(\frac{n}{2}-2)\sqrt{1}}}dn$$

$$=\frac{2(n-1)}{n}\int\frac{1}{\sqrt{\frac{n}{2}+3+(\frac{n}{2}-2)}}dn.$$

Theorem 5.1 The eigen-chromatic areas for all the classes $\Im$ of graphs studied in this paper are summarized in the following table.

$\mathfrak{I}$	$A^{\chi}_{\mathfrak{I}(n)}$
K_n	$\frac{n-1}{2}(n+\ln\|n-1\|-2)$
P_n	$\frac{2(n-2)}{n}\int \frac{1}{\cos ec\frac{\pi}{2(n+1)}-1}dn$
C_n	$\int \frac{1}{\cot\frac{\pi}{n}}dn$
W_n	$8.\frac{n-1}{n}\int \frac{1}{\sqrt{n}-1+\cos ec\left(\frac{\pi}{2(n-1)}\right)}dn$
$S_{n-1,1}$	$\frac{4(n-1)}{n}(\sqrt{n-1}-1)$
$S_{\frac{n-1}{2},2}$	$\frac{8(n-1)}{3n}\ln(\frac{(\sqrt{2(n+1)}-2)(\sqrt{2(n+1)}+4)^2}{4+\sqrt{6}})$
LP_n	$\frac{2((n-1)(n-2)+1)}{n}\int \frac{n-1}{(n-3)+\sqrt{(n-2)^2+4}}dn$
$K_{\frac{n}{2},\frac{n}{2}}$	$n(\ln\left(\frac{n}{2}\right))$
F_n	$\frac{3}{2}(\ln(n(n-3)^5)-\frac{9}{2}\int \frac{\sqrt{1+8n}}{n^2-3n}dn$
$CompSun(h,p)$	$\frac{n+2}{2}\int \frac{n}{(n-2)\sqrt{5}+\sqrt{(n-2)^2+16}}dn$
$BipSun(h,p)$	$\frac{n+8}{4}\int \frac{1}{\sqrt{n^2+64}+2n-8}dn$
$StarSun(h,p)$	$\frac{2(n-1)}{n}\int \frac{1}{\sqrt{\frac{n}{2}+3+(\frac{n}{2}-2)}}dn$

Hypothesis 5.1 The eigen-chromatic area of the complete graph is the largest off classes of graphs for large *n*.

6. CONCLUSION

The motivation for combining the energy, and chromatic number of a graph, into a ratio, arose from the need to understand, in molecular graph theory, the energy distribution among the atoms of a molecule, where only different atoms are bonded (for example, covalent bonding). In molecules where a large number of atoms are involved, classes of graphs involving the complete graph appears to give the most stable of such an energy distribution. We propose that the eigen-chromatic area of the complete graph is the largest of all such areas of all classes of graphs. We found the eigen-chromatic ratio of the complete graph on n vertices, as a function of n, to be paired with another function, as solutions of a second order ordinary differential equation.

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