ADV MATH SCI JOURNAL
Advances in Mathematics: Scientific Journal **3** (2014), no.2, 133–147
ISSN 1857-8365

THE H-EIGEN ENERGY FORMATION NUMBER OF H-DECOMPOSABLE CLASSES OF GRAPHS- FORMATION RATIOS, ASYMPTOTES AND POWER

PAUL AUGUST WINTER[1] AND DINISH SARVATE

ABSTRACT. The study of graph decomposition is well known, so is the energy of graphs in terms of its eigenvalues. The union of these two ideas has been presented recently where the idea of the energy used in forming a "graphical molecule" from its decomposed parts was muted. In this paper, we inherit the idea of the *Hückel de-localization or deformation energy*, which correlates with the experimental heat of combustion associated with a molecule, to introduce the idea of the *formation energy* of a H-decomposable class of graphs. We consider the *average formation energy* (as a ratio) and discuss classes of graphs which have *asymptotic* convergence. The idea of the *formation power* of a class of graphs is developed using the Riemann integral of the formation energy, which allowed for the investigation of classes of graphs on a large number of vertices whose formation powers converge in a constant "reciprocal" manner.

1. INTRODUCTION

All graphs G are simple, connected, loopless and without multiple edges and on n vertices and m edges. We shall adopt the graph-theoretical notation of [7].

The idea of H-decomposition (see [8]) and the energy of a graph (see [5]) are combined in this paper to consider the idea of the energy involved in the formation of a molecule, where a graph theoretical representation is provided for the molecule, assigning vertices as atoms and the edges as bonds between the atoms. The formation energy of a graph representation G, of a molecule, is the difference between the energy of the graph, and the sum of energy of each of its H-decomposable parts. Dividing this formation energy, by the number of edges of G, we obtain the formation energy ratio associated with G and consider its asymptotic properties. If this ratio is a function $f(n)$, of the order of G, we combine the average degree of G, with the Riemann integral of $f(n)$, to introduce the idea of the formation power of G. We provide the basic definitions involved below.

Definition 1.1. *Consider a decomposition of G into t subgraphs belonging to the set, $P = \{G_1, G_2, \dots, G_t\}$, such that any edge of G is an edge of exactly one of the*

[1] *corresponding author*
2010 *Mathematics Subject Classification.* 05C99.
Key words and phrases. eigenvalues, graph decomposition, energy, ratios, asymptotes.

G_i's, and the G_i's are isomorphic to the graph H - such a decomposition is called a ***H-decomposition of G*** *. The G_i are called the base graphs of the decomposition. If $H = K_2$, then the decomposition is called the* ***trivial decomposition****.*

Definition 1.2. *Define*

$$\alpha_f(G, H) = \min_P \sum_i f(G_i)$$

where $P = \{G_1, G_2, \ldots, G_t\}$ ranges over all H-decompositions of G, and $f(G_i)$ is some non-negative value (such as weight or energy, see below) assigned to G_i, or its **cost function.**

Definition 1.3. *The Huckel Molecular Orbital theory provided the motivation for the idea of the energy of a graph - the sum of the absolute values of the eigenvalues associated with the graph (see* [5], [1]*):*

$$\sum_{i=1}^{n} |\lambda_i|,$$

$|\lambda_i|$ is the eigenvalues of the adjacency matrix of the graph G.

The Hückel method or Hückel molecular orbital method (HMO), proposed by Erich Hückel in 1930, is a very simple linear combination of atomic orbitals molecular orbitals (LCAO MO) method for the determination of energies of molecular orbitals of pi electrons in conjugated hydrocarbon systems, such as benzene.

The eigenvalues of a cycle on n vertices are:

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

These eigenvalues are inherited by cyclic molecules such as benzene. For benzene, a hexagon is placed in a circle with radius 2β and center α, and the general solution of the energy system is:

$$E_j = \alpha + 2\beta\cos\frac{2\pi j}{6},\ j = 0, 1, \ldots, 5$$

The Hückel delocalization or deformation energy of a molecule correlates with the experimental heat of combustion associated with the molecule. This energy is defined as the difference between the total predicted pi energy of the molecule (in benzene 8β) and a hypothetical pi energy in which all ethylene molecular units are assumed isolated, each contributing 2β (making benzene $3 \times 2\beta = 6\beta$). The reverse of this process may be regarded as the formation energy of the benzene molecule (see [5]).

A molecular structure can be regarded as a collection of atoms bonded together which can be mapped onto a graph where the vertices are the atoms and the edges the bonds.

Thus, in terms of definition 1.2, we can compare the sum cost functions of each of the decomposed graphs to the total energy of the original graph (see [8]).

In terms of molecular formation energy we therefore have a motivation for the following definitions:

Definition 1.4. *Let the set $P = \{G_1, G_2, \ldots, G_t\}$, be associated with the H-decomposition of the graph G. Let the* ***H-decomposition-energy*** *of G with respect to the H-decomposition of G be defined as (since the energy of each $G \approx H$ is the same):*

$$E^H(G) = \alpha_E(G, H) = \min_P \sum_i E(G_i) = tE(H)$$

Then the ***H-formation energy*** *of the graph G is defined as:*

$$form_H E(G) = E(G) - E^H(G)$$

If $form_H E(G) > 0$, then the formation energy is exothermic, otherwise ($form_H E(G) < 0$), endothermic. If $form_H E(G)$ is a constant α, (or a function $f(n)$ of order n of $G \in \Omega$) for all graphs G belonging to a class Ω of graphs, then α (or $f(n)$) is called the **H-eigen energy formation number** of Ω and denoted by $form_E E(\Omega)$.

Ratios and Energy. Ratios have been an important aspect of graph theoretical definitions. Examples of ratios are: expanders, (see [2]), the central ratio of a graph (see [4]), eigen-pair ratio of classes of graphs (see [10]), Independence and Hall ratios (see [6]) and tree-cover ratio of graphs (see [9]).

The edges of a graph contribute to the non-zero entries of the adjacency matrix of a graph, and hence they affect the eigenvalues associated with the graph, which motivates the following definition:

Definition 1.5. *The ratio, consisting of $form_H E(\Omega)/m$, where m (as a function of n) is the number of edges of the graph G belonging to Ω can be regarded as the average H-eigen formation energy of Ω and is called the* ***H-eigen energy formation ratio*** *of Ω, denoted by: $ratio_H E(\Omega)$.*

Asymptotes of ratios have been investigated in [3], [9] and [10].

Definition 1.6. *If $ratio_H E(\Omega) = g(n)$, where n is the size of $G \in \Omega$, then the horizontal asymptote of $g(n)$ is called the* ***H-eigen energy formation asymptote*** *of and denoted by: $asymp_H E(\Omega)$. If $asymp_H E(\Omega) = asymp_H E(\Omega')$ for different classes Ω and Ω', then the classes Ω and Ω' are said to* **converge** *to the same H-eigen formation asymptote.*

2. Examples of K_2-Eigen Energy Formation Numbers, ratios, and Asymptotes of Classes of Graphs

2.1. **Complete graphs and its trivial decomposition.** The complete graph K_n on $n \geq 2$ has a K_2-decomposition involving $\frac{n(n-2)}{2}$ copies of subgraphs. Each K_2 has energy 2 and K_n has energy $(n-1) + 1(n-1) = 2n - 2$ so that:

$$form_H E(K_n) = E(K_n) - E^{K_2}(G) = 2n - 2 - n(n-1) = -n^2 + 3n - 2 \leq 0\,,$$

so that the formation energy member of $K_n = form_H E(K_n)$ is $-n^2 + 3n - 2$. This is zero when $n = 2$.

$$ratio_{k_2}(K_n) = 2\Big[\frac{-n^2 + 3n - 2}{n(n-1)}\Big] \Longrightarrow asympt_{k_2}(K_n) = -2\,.$$

2.2. **Complete split-bipartite graphs and its trivial decomposition.** Let $K_{n/2,n/2}$, n even be a complete split bipartite graph on n vertices. The non-zero eigenvalues are $\pm\frac{n}{2}$ so that $E(K_{n/2,n/2}) = n$ and the graph has $\frac{n^2}{4}$ copies of K_2 each having energy 2 so that:

$$form_{k_2}E(K_{n/2,n/2}) = E(K_{n/2,n/2}) - E^{K_2}(K_{n/2,n/2}) = n - \frac{n^2}{2} = \frac{2n-n^2}{2} \leq 0\,.$$

Also,

$$ratio_{k_2}E(K_{n/2,n/2}) = \frac{4(2n-n^2)}{2n^2} \Longrightarrow asymp_{k_2}E(K_{n/2,n/2}) = -2\,.$$

Thus, K_n and $K_{n/2,n/2}$, n even, converge to the same eigen-formation asymptote.

2.3. **Wheels and its trivial decomposition.** The Wheel, $W_{n'+1}$ with n' spokes and has $n'+1$ vertices and $2n'$ edges. The eigenvalues of $W_{n'+1}$ are:

$$\alpha_1, \alpha_2 = \frac{2 \pm \sqrt{4+4n'}}{2}, \quad \beta = 2\cos\frac{2\pi k}{n'}\ \ k = 1, 2, \ldots, n'-1\,,$$

so that its energy is:

$$\begin{aligned} E(W_{n'+1}) &= 1 + \frac{\sqrt{4+4n'}}{2} - 1 + \frac{\sqrt{4+4n'}}{2} + \sum_{k=1}^{n'-1} 2\left|\cos\frac{2\pi k}{n'}\right| \\ &= \sqrt{4+4n'} + \sum_{k=1}^{n'-1} 2\left|\cos\frac{2\pi k}{n'}\right|. \end{aligned}$$

Letting $n'+1 = n$ vertices, we have that:

$$\begin{aligned} E(W_n) &= 1 + \sqrt{n} - 1 + \sqrt{n} + \sum_{k=1}^{n-2} 2\left|\cos\frac{2\pi k}{n-1}\right| \\ &= 2\sqrt{n} + \sum_{k=1}^{n-2} 2\left|\cos\frac{2\pi k}{n-1}\right|. \end{aligned}$$

The number of edges are $2n' = 2(n-1)$, so that:

$$\begin{aligned} form_{K_2}E(W_n) &= E(W_n) - E^{K_2}(W_n) \\ &= \left(2\sqrt{n} + \sum_{k=1}^{n-2} 2\left|\cos\frac{2\pi k}{n-1}\right|\right) - 4n - 4\,. \end{aligned}$$

For n even, the sigma part must be less that or equal to $2(n-2)$, so:

$$form_{K_2}E(W_n) \leq (2\sqrt{n} + 2n - 4) - 4n + 4 = 2\sqrt{n} - 2n\,,$$

so that:

$$ratio_{K_2}E(W_n) \leq \frac{2\sqrt{n}-2n}{2n-2} = \frac{\sqrt{n}-n}{n-1} \Longrightarrow asymp_{K_2}E(W_n) \leq -1\,.$$

2.4. **Stars and their trivial decomposition.**

2.4.1. *Star graphs with rays of length 1.* The star graph on n vertices and $n-1$ edges with rays of length one is the same as the complete bipartite graph and denoted by $K_{1,n-1}$.

$$\begin{aligned} form_{K_2}E(K_{1,n-1}) &= E(K_{1,n-1}) - E^{K_2}(K_{1,n-1}) \\ &= 2\sqrt{n-1} - 2(n-1) \leq 0\,, \end{aligned}$$

so that:

$$ratio_{K_2}E(K_{1,n-1}) = \frac{2\sqrt{n-1} - 2n + 2}{n-1} \Longrightarrow asymp_{K_2}E(K_{1,n-1}) = -2\,.$$

2.4.2. *Star graphs with rays of length 2 and its trivial decomposition.* Star graphs on n vertices with q rays of length 2 (paths on 3 vertices) has $(n-1)$ edges and is denoted by S_{1,qP_3}. This graph has $2q+1$ vertices so that $q = \dfrac{n-1}{2}$ and $n-1$ must be even. The eigenvalues of S_{1,qP_3} are 1 and -1, each of multiplicity $q-1 = \dfrac{n-3}{2}$, one eigenvalue 0, and two eigenvalues $\lambda = \pm\sqrt{q+1} = \pm\sqrt{\dfrac{n+1}{2}}$.

$$\begin{aligned} form_{K_2}E(S_{1,qP_3}) &= E(S_{1,qP_3}) - E^{K_2}(S_{1,qP_3}) \\ &= n - 3 + \sqrt{2}\sqrt{n+1} - 2n + 2 < 0\,. \end{aligned}$$

Thus,

$$ratio_{K_2}E(S_{1,qP_3}) = \frac{-n-1+\sqrt{2}\sqrt{n+1}}{n-1} \Longrightarrow asymp_{K_2}E(S_{1,qP_3}) = -1\,.$$

Theorem 2.1. *$form_{K_2}E(\Omega)$, $ratio_{K_2}E(\Omega)$, and $asymp_{K_2}E(\Omega)$ are respectively:*

$$\Omega = K_n : \quad -n^2+3n-2, \quad \frac{2(-n^2+3n-2)}{n(n-1)}, \quad \textit{and} \quad -2\,;$$

$$\Omega = K_{n/2,n/2} : \quad \frac{2n-n^2}{2}, \quad \frac{2(2n-n^2)}{n^2}, \quad \textit{and} \quad -2\,;$$

$$\Omega = W_n : \quad \leq 2\sqrt{n} - 2n, \quad \leq \frac{\sqrt{n}-n}{n-1}, \quad \textit{and} \quad \leq -1\,;$$

$$\Omega = K_{1,n-1} : \quad 2\sqrt{n-1} - 2(n-1), \quad \frac{2\sqrt{n-1}-2n+2}{n-1}, \quad \textit{and} \quad -2\,;$$

$$\Omega = S_{1,qP_3} : \quad -n-1+\sqrt{2}\sqrt{n+1}, \quad \frac{-n-1+\sqrt{2}\sqrt{n+1}}{n-1}, \quad \textit{and} \quad -1\,.$$

3. P_3-EIGEN ENERGY FORMATION NUMBERS OF CLASSES OF GRAPHS

3.1. A P_3 -decomposition of the complete graph and the associated P_3-eigen energy formation number. For the P_3-decomposition of K_n, we need the necessary condition that: $n(n-1) \equiv 0 \mod 4$. If this condition holds, then K_n can be decomposed into $\frac{n(n-1)}{4}$ copies of P_3. Thus,

$$\begin{aligned} form_{P_3}E(K_n) &= E(K_n) - E^{P_3}(K_n) \\ &= 2n-2-\frac{n(n-1)}{4}2\sqrt{2} = \frac{8n-8-n(n-1)2\sqrt{2}}{4}, \end{aligned}$$

so that:

$$ratio_{P_3}E(K_n) = \frac{8n-8-n(n-1)2\sqrt{2}}{2n(n-1)} \Longrightarrow asymp_{P_3}E(K_n) = -\sqrt{2}.$$

We show that the $asymp_{P_3}E(K_n)$ is the same as $asymp_{P_3}E(K_{n/2,n/2})$ so that these classes of graphs converge to the same P_3-eigen formation asymptote.

3.2. A P_3-decomposition of the complete split-bipartite graph, $K_{n/2,n/2}; n$ even and the associated P_3-eigen energy formation number. The necessary condition for a P_3-decomposition of $K_{n/2,n/2}; n$ even is that $\frac{n^2}{4}$ must be even. Thus, when $\frac{n^2}{4} \equiv 0 \mod 2$, the number of copies of P_3 in the decomposition of the complete graph is $\frac{n^2}{8}$. Then,

$$\begin{aligned} form_{P_3}E(K_{n/2,n/2}) &= E(K_{n/2,n/2}) - E^{P_3}(K_{n/2,n/2}) \\ &= n-\frac{n^2}{8}2\sqrt{2} = n-\frac{n^2}{4}\sqrt{2} = \frac{4n-n^2\sqrt{2}}{4}, \end{aligned}$$

so that:

$$ratio_{P_3}E(K_{n/2,n/2}) = \frac{4n-n^2\sqrt{2}}{n^2} \Longrightarrow asymp_{P_3}E(K_{n/2,n/2}) = -\sqrt{2}.$$

Thus K_n and $K_{n/2,n/2}; n$ even converge to the same P_3-eigen formation asymptote.

3.3. A P_3-decomposition of the wheel on n vertices and $n-1$ spokes and the associated P_3-eigen energy formation number. The wheel on n vertices has $2n-2$ edges - this is even so it will have $n-1$ copies of P_3, each having energy $2\sqrt{2}$. Thus,

$$\begin{aligned} form_{P_3}E(W_n) &= E(W_n) - E^{P_3}(W_n) \\ &\leq (2\sqrt{n}-2n) - 2n\sqrt{2} + 2\sqrt{2} \\ &= n(-2-2\sqrt{2}) + 2\sqrt{n} + 2\sqrt{2}. \end{aligned}$$

Thus,

$$\begin{aligned} ratio_{P_3}E(W_n) &\leq \frac{n(-2-2\sqrt{2})+2\sqrt{n}+2\sqrt{2}}{2n-2} \\ &\Longrightarrow asymp_{P_3}E(W_n) \leq \frac{-2-2\sqrt{2}}{2} = -1-\sqrt{2}. \end{aligned}$$

3.4. **A P_3-decomposition of the star graph, $K_{1,n-1}$ on n vertices and the associated P_3-eigen energy formation number.** The necessary condition for a P_3-decomposition of $K_{1,n-1}$ is that $n-1$ be divisible by 2. If this is so, then, $K_{1,n-1}$ will have $\frac{n-1}{2}$ copies of P_3 each of energy $2\sqrt{2}$. Thus:

$$\begin{aligned} form_{P_3}E(K_{1,n-1}) &= E(K_{1,n-1}) - E^{P_3}(K_{1,n-1}) \\ &\leq (2\sqrt{n-1}) - \sqrt{2}(n-1) \leq 0, \text{ for } n \geq 3\,. \end{aligned}$$

Also,

$$\begin{aligned} ratio_{P_3}E(K_{1,n-1}) &\leq \frac{(2\sqrt{n-1}) - \sqrt{2}(n-1)}{n-1} \\ &\implies asymp_{P_3}E(K_{1,n-1}) = -\sqrt{2}\,. \end{aligned}$$

3.5. **A P_3-decomposition of the star graph, S_{1,qP_3} with q rays of length 2 and the associated P_3-eigen energy formation number.** The star graph on n vertices and $n-1$ edges with q rays of length 2 has a P_3-decomposition with $\frac{n-1}{2}$ copies of P_3 each of energy $2\sqrt{2}$. Hence,

$$\begin{aligned} form_{P_3}E(S_{1,qP_3}) &= E(S_{1,qP_3}) - E^{P_3}(S_{1,qP_3}) \\ &= n - 3 + (\sqrt{2}\sqrt{n+1}) - \sqrt{2}(n-1) \\ &= n(1-\sqrt{2}) + \sqrt{2} - 3 + \sqrt{2}\sqrt{n+1}\,. \end{aligned}$$

Thus:

$$\begin{aligned} ratio_{P_3}E(S_{1,qP_3}) &= \frac{n(1-\sqrt{2}) + \sqrt{2} - 3 + \sqrt{2}\sqrt{n+1}}{n-1} \\ &\implies asymp_{P_3}E(S_{1,qP_3}) = 1 - \sqrt{2}\,. \end{aligned}$$

Theorem 3.1. *$form_{P_3}E(\Omega)$, $ratio_{P_3}E(\Omega)$, and $asymp_{P_3}E(\Omega)$ are respectively:*

$$\Omega = K_n : \quad \frac{8n - 8 - n(n-1)2\sqrt{2}}{4}, \quad \frac{8n - 8 - n(n-1)2\sqrt{2}}{2n(n-1)}, \quad and \quad -\sqrt{2}\,;$$

$$\Omega = K_{n/2,n/2} : \quad \frac{4n - n^2\sqrt{2}}{4}, \quad \frac{(4n - n^2\sqrt{2})}{n^2}, \quad and \quad -\sqrt{2}\,;$$

$$\Omega = W_n : \quad \leq n(-2-2\sqrt{2}) + 2\sqrt{n} + 2\sqrt{2} \quad \leq \frac{n(-2-2\sqrt{2}) + 2\sqrt{n} + 2\sqrt{2}}{2n-2} \leq -1-\sqrt{2}\,;$$

$$\Omega = K_{1,n-1} : \quad 2\sqrt{n-1} - \sqrt{2}(n-1), \quad \frac{2\sqrt{n-1} - \sqrt{2}(n-1)}{n-1}, \quad and \quad -\sqrt{2}\,;\ n \geq 3\,;$$

$$\Omega = S_{1,qP_3} : \quad \frac{n(1-\sqrt{2}) + \sqrt{2} - 3 + \sqrt{2}\sqrt{n+1}}{n-1}, \frac{n(1-\sqrt{2}) + \sqrt{2} - 3 + \sqrt{2}\sqrt{n+1}}{n-1}$$
$$and \quad -1-\sqrt{2}\,.$$

Theorem 3.2. *K_n, $K_{1,n-1}$, and $K_{\frac{n}{2},\frac{n}{2}}$ (n even) converge to the same H-eigen formation asymptote for $H = K_2; P_3$.*

Proposition 3.1. *If a class Ω of graphs has an H-eigen energy formation asymptote, then this lies on the closed interval $[-2, 0)$, with equality at the end point -2 if Ω is the class of H-decomposable complete bipartite graphs, or K_n, where H is K_2.*

4. The H-eigen power formation number of classes of H-decomposable graphs

Integrating ratios and multiplying this integral by the average degree has been considered in [9] and [10]. In this section, we combine the H-eigen energy formation ratio and integration to develop the idea of power.

Definition 4.1. *If the class Ω of graphs of has an H-eigen energy formation ratio $f(n) = ratio_H E(\Omega)$, then the* ***H-eigen power formation number*** *of Ω is defined as:*

$$power_H E(\Omega) = av(deg) \Big| \int_a^n f(t)dt \Big| ,$$

where a is the number of vertices of the smallest graph $G \in \Omega$, for which an H-decomposition exists, and $av(deg)$ is the average degree of $G \in \Omega$; i.e. $\frac{1}{n}\sum_1^n deg(v_i)$.

The value of $power_H E(\Omega)$, for extremely large values of n for each $G \in \Omega$ is the *H-eigen formation extreme-power* of Ω and denoted by $extreme - power_H E(\Omega)$.

If $extreme - power_H E(\Omega) = kg(n)$, and $extreme - power_H E(\Omega) = \frac{g(n)}{k}$ for 2 different classes Ω,Ω', where k is a non-zero constant , then the classes Ω,Ω' are said to be k-*reciprocally H-eigen formation power convergent.*

4.1. The K_2-eigen power formation number of the class of complete graphs.

The K_2 -eigen energy formation ratio of K_n is:

$$ratio_{K_2} E(K_n) = \frac{2(-n^2 + 3n - 2)}{n(n-1)} ,$$

so that (ignoring the limits):

$$\begin{aligned}
(n-1)\int \frac{2(-t^2+3t-2)}{t(t-1)}dt &= (n-1)\int \frac{-2t^2+6t-4}{t^2-t}dt \\
&= (n-1)\int \frac{-2(t^2-t)}{t^2-t}dt + \int \frac{4t-4}{t^2-t}dt \\
&= (n-1)\Big(-2t + 2\int \frac{2t-1}{t^2-t}dt - 2\int \frac{dt}{t^2-t}\Big) \\
&= (n-1)\Big(-2t + 2\ln|t^2-t| - 2\ln|t-1| + 2\ln|t|\Big) + c \\
&= (n-1)(-2t + 4\ln|t| + c) ,
\end{aligned}$$

so that, since the smallest $G \in K_n$ which has a K_2- decomposition is K_2, we have:

$$\begin{aligned} power_{K_2}E(K_n) &= (n-1)\,\Big|\int_2^n f(t)dt\Big| \\ &= (n-1)|-2n+4\ln(n)+4-4\ln 2| \\ &= (n-1)|-2n+4\ln\frac{n}{2}+4|\,. \end{aligned}$$

Note that $power_{K_2}E(K_n) \approx 2n^2$ for n large, so that:

$$extreme - power_{K_2}E(K_n) = 2n^2\,.$$

4.2. The K_2 -eigen power formation number of the class of complete split bipartite graphs, $K_{\frac{n}{2},\frac{n}{2}}$, n even.

The K_2-eigen formation ratio of $K_{\frac{n}{2},\frac{n}{2}}$ n even, is:

$$ratio_{K_2}(K_{\frac{n}{2},\frac{n}{2}}) = \frac{2(-2n-n^2)}{n^2}\,,$$

so that the K_2-eigen power formation number is (the smallest $G \in K_{\frac{n}{2},\frac{n}{2}}$ which has a K_2-decomposition is K_2):

$$\begin{aligned} power_{K_2}E(K_{\frac{n}{2},\frac{n}{2}}) &= \frac{n}{2}\,\Big|\int_2^n \frac{2(2t-t^2)}{t^2}dt\Big| \\ &= \frac{n}{2}|4\ln(n)-2n-4\ln 2+4| \\ &= \frac{n}{2}|4\ln\frac{n}{2}-2n+4|\,. \end{aligned}$$

Thus, $power_{K_2}E(K_{\frac{n}{2},\frac{n}{2}})$ for n large:

$$extreme - power_{K_2}E(K_{\frac{n}{2},\frac{n}{2}}) = n^2\,.$$

4.3. The K_2-eigen power formation number of the class of wheels with $n-1$ spokes.

The wheel W_n with $n-1$ spokes has n vertices and $2n-2$ edges so that from section 3.3, we have that:

$$ratio_{K_2}E(W_n) \leq \frac{\sqrt{n}-n}{n-1}\,.$$

To find an upper bound on the K_2 eigen power formation number, we need the following:

$$\int \frac{\sqrt{t}-t}{t-1}dt = \int \frac{\sqrt{t}}{t-1}dt - \int \frac{t-1}{t+1}dt + \int \frac{dt}{t-1}dt = A - t + \ln|t-1|\,.$$

A; substitute $t = \sec^2 u \Longrightarrow \int \frac{\sqrt{t}}{t-1}dt = 2\int \frac{du}{\cos^2 u \sin u} = 2\int \sec^2 u\, cosec\, u\, du\,;$

parts $\longrightarrow 2(\tan u \mathrm{cosec}\, u + \int \mathrm{cosec}\, u du) = 2(\tan u \mathrm{cosec}\, u + \ln|\mathrm{cosec}\, u + \cot u|)\,. = 2(\sqrt{t} + \ln(\sqrt{t}-1) - \ln\sqrt{t-1})\,.$

Thus, since the smallest wheel graph that has a K_2 decomposition is on 4 vertices:

$$\int_4^n \frac{\sqrt{t}-t}{t-1}dt = 2\Big(\sqrt{n}+\ln(\sqrt{n}-1)-\ln(\sqrt{n}-1)\Big) - n + \ln(n-1) - 2(2-\ln 3) + 4 - \ln 3\,.$$

Since the average degree of the wheel graph is $\dfrac{4n-4}{n}$, then:

$$power_{K_2}E(W_n) \le \frac{4n-4}{n}\Big(2(\sqrt{n}+\ln(\sqrt{n}-1)-\ln(\sqrt{n}-1)\Big)-n+\ln(n-1)-2(2-\ln 3)+4-\ln 3\Big).$$

For n very large this becomes

$$extreme-power_{K_2}E(W_{n+1}) \le 4n\,.$$

4.4. **The K_2-eigen power formation number of the class of star graphs $K_{1,n-1}$.** From previous section, we have:

$$ratio_{K_2}E(K_{1,n-1}) = \frac{2\sqrt{n-1}-2n+2}{n-1}\,.$$

To find the K_2-eigen power formation number we compute:

$$\int \frac{2\sqrt{t-1}-2t+2}{t-1}dt = \int \frac{2\sqrt{t-1}}{t-1}dt - 2\frac{t-1}{t-1} = \int \frac{2}{\sqrt{t-1}}dt - 2t = 4\sqrt{t-1}-2t\,.$$

Hence,

$$\frac{2n-2}{n}\Big|\int_2^n \frac{2\sqrt{t-1}-2t+2}{t-1}dt\Big| = \frac{2n-2}{n}|4\sqrt{n-1}-2n|\,,$$

which behaves like $4n$ for extremely large n so that:

$$extreme-power_{K_2}E(K_{1,n-1}) = 4n\,.$$

4.5. **The K_2-eigen power formation number of the class of star graphs S_{1,qP_3} with q rays length 2.** From previous section, we have:

$$ratio_{K_2}E(K_{1,n-1}) = \frac{-n-1\sqrt{2}\sqrt{n+1}}{n-1}\,.$$

Thus, to evaluate the K_2-eigen power formation number we need to compute:

$$\int \frac{-t-1+\sqrt{2}\sqrt{t+1}}{t-1}dt = -\int \frac{t-1}{t-1}dt - 2\ln(t-1) + \int \frac{\sqrt{2}\sqrt{t+1}}{t-1}dt = -t-2\ln(t-1)+A\,,$$

and

$$A = \sqrt{2}\int \frac{\sqrt{t+1}}{t-1}dt\ :$$

substitute $t+1=u^2 \Longrightarrow$

$$\begin{aligned} A &= 2\sqrt{2}\int \frac{u^2}{u^2-2}du = 2\sqrt{2}\int \frac{u^2-2}{u^2-2}du + 4\sqrt{2}\int \frac{du}{u^2-2} \\ &= 2\sqrt{2}u + 2\ln(u-\sqrt{2}) - 2\ln(u+\sqrt{2}) = 2\sqrt{2}\sqrt{t+1} + 2\ln\Big[\frac{\sqrt{t+1}-\sqrt{2}}{\sqrt{t-1}+\sqrt{2}}\,. \end{aligned}$$

Thus, we consider:

$$\int \frac{-t-1+\sqrt{2}\sqrt{t+1}}{t-1}dt = -t-2\ln(t-1)+2\sqrt{2}\sqrt{t+1}+2\ln\frac{\sqrt{t+1}-\sqrt{2}}{\sqrt{t-1}+\sqrt{2}}\,.$$

Thus, the K_2-eigen power formation number of S_{1,qP_3} is : $\dfrac{2(n-1)}{n}$ multiplied by:

$$\left| -n - 2\ln(n-1) + 2\sqrt{2}\sqrt{n+1} + 2\ln\frac{\sqrt{n+1}-\sqrt{2}}{\sqrt{n-1}+\sqrt{2}} + 2 - 2\sqrt{6} - 2\ln\frac{\sqrt{3}-\sqrt{2}}{\sqrt{1}+\sqrt{2}} \right|,$$

which behaves like $2n$ for extremly large n so that:

$$extreme - power_{K_2} E(S_{1,qP_3}) = 2n\,.$$

4.6. **The P_3-eigen power formation number of the class of complete graphs.**

$$ratio_{P_3} E(K_n) = \frac{8n - 8 - n(n-1)2\sqrt{2}}{2n(n-1)}\,.$$

To evaluate the P_3-eigen-power formation number of K_n, we need to determine:

$$\begin{aligned}\int \frac{8t-8-t(t-1)2\sqrt{2}}{2t(t-1)}dt &= 4\ln|t-1| - \int \frac{4}{t(t-1)}dt - \sqrt{2}t\\ &= 4\ln(t-1) - \sqrt{2}t - 4\ln(t-1) + 4\ln t + c\\ &= 4\ln t - \sqrt{2}t + c\,.\end{aligned}$$

The P_3-eigen power formation number is then (the smallest complete graph with a P_3-decomposition is on a 4 vertices): $(n-1)|4\ln n - n\sqrt{2} - 4\ln 4 + 4\sqrt{2}|$, which imples that:

$$extreme - power_{P_3} E(K_n) = \sqrt{2}n^2\,.$$

4.7. **The P_3-eigen power formation number of the class of complete split-bipartite graph, $K_{\frac{n}{2},\frac{n}{2}}$.** From previous section:

$$ratio_{P_3} E(K_{\frac{n}{2},\frac{n}{2}}) = \frac{4n - n^2\sqrt{2}}{n^2}\,,$$

so that to evaluate the P_3-eigen power formation number, we need to compute

$$\int \frac{4t - t^2\sqrt{2}}{t^2}dt = 4\ln t - \sqrt{2}t + c\,.$$

Since the average degree of $K_{\frac{n}{2},\frac{n}{2}}$ is $\dfrac{n}{2}$, we need (the smallest n for which a P_3-decomposition of $K_{\frac{n}{2},\frac{n}{2}}$ exists is $n = 4$):

$$\frac{n}{2}\left|\int_4^n \frac{4t - t^2\sqrt{2}}{t^2}dt\right| = \frac{n}{2}\left|4\ln n - n\sqrt{2} - 4\ln 4 + 4\sqrt{2}\right|,$$

so that:

$$extreme - power_{P_3} E(K_{\frac{n}{2},\frac{n}{2}}) = \frac{n^2}{\sqrt{2}}\,,$$

which is the same as the class of complete graphs.

4.8. **The P_3-eigen power formation number of the class of the wheel graph on n vertices and $n-1$ spokes.** From previous sections:

$$\begin{aligned}\Omega &= W_n :\leq n(-2-2\sqrt{2})+2\sqrt{n}+2\sqrt{2} \\ &\Longrightarrow \; ratio_{P_3}E(W_n) \leq \frac{n(-2-2\sqrt{2})+2\sqrt{n}+2\sqrt{2}}{2n-2}\,.\end{aligned}$$

To compute the P_3-eigen power formation number, we need to evaluate:

$$\begin{aligned}\int \frac{t(-2-2\sqrt{2})+2\sqrt{t}+2\sqrt{2}}{2t-2}dt &= \frac{(-2-2\sqrt{2})}{2}\int\frac{2t-2}{2t-2}dt+\int\frac{(-2-2\sqrt{2})+2+4\sqrt{2}}{2t-2}dt \\ &+ \int\frac{\sqrt{t}}{t-1}dt \\ &= \frac{(-2-2\sqrt{2})}{2}t+2\sqrt{2}\int\frac{dt}{2t-2}+\int\frac{\sqrt{t}}{t-1}dt \\ &= \frac{(-2-2\sqrt{2})}{2}t+\sqrt{2}\ln(t-1)+\int\frac{\sqrt{t}}{t-1}dt\,.\end{aligned}$$

Now,

$$\frac{\sqrt{t}}{t-1}(t=\sec^2 u) \Longrightarrow 2\int \sec^2 u \operatorname{cosec} u du :$$

Parts $\Longrightarrow 2(\tan u \operatorname{cosec} u + \int \tan u \operatorname{cosec} u \cot u du) = 2(\tan u \operatorname{cosec} u + \ln|\operatorname{cosec} u - \cot u|)$

$$= 2\sqrt{t-1}\frac{\sqrt{t}}{\sqrt{t-1}}+\ln\left|\frac{\sqrt{t}}{\sqrt{t-1}}-\frac{1}{\sqrt{t-1}}\right| = 2\sqrt{t}+2\ln|\sqrt{t}-1|-\ln(t-1)\,.$$

Thus, we consider $\frac{(-2-2\sqrt{2})}{2}t+(\sqrt{2}-1)\ln(t-1)+2\sqrt{t}+2\ln|\sqrt{t}-1|+c$, so that the P_3-eigen power formation number is (the smallest n for which a P_3-decomposition of W_n exists is $n=4$):

$$\leq \frac{(4n-4)}{n}\Big|\frac{(-2-2\sqrt{2})}{2}n\ln(n-1)+2\sqrt{n}+2\ln|\sqrt{n}-1|-\frac{(-2-2\sqrt{2})}{2}4-(\sqrt{2}-1)\ln 3-4\,.$$

So that:

$$extreme-power_{P_3}E(W_n) \leq (4+4\sqrt{2})n\,.$$

4.9. **The P_3-eigen power formation number of the classes of star graphs with rays of length 1.** The necessary condition for a P_3-decomposition of $K_{1,n-1}$ is that $n-1$ be divisible by 2. If this is so, then $K_{1,n-1}$ will have $\frac{n-1}{2}$ copies of P_3 each of energy $2\sqrt{2}$. So that from previous section:

$$ratio_{P_3}E(K_{1,n-1}) = \frac{2\sqrt{n-1}-\sqrt{2}(n-1)}{n-1}\,.$$

To evaluate the P_3-eigen formation power number of $K_{1,n-1}$, we need to compute:

$$\int\frac{2\sqrt{t-1}-\sqrt{2}(t-1)}{t-1}dt = 2\int\frac{dt}{\sqrt{t-1}}-\sqrt{2t} = 4\sqrt{t-1}-\sqrt{2t}+c\,.$$

Since the smallest n for which $K_{1,n-1}$ has a P_3-decomposition is $n = 3$. Thus the number we seek is:

$$\frac{2(n-1)}{n}|4\sqrt{n-1} - n\sqrt{2} - 4\sqrt{2} + 3\sqrt{2}|\,,$$

so that:

$$extreme - power_{P_3}E(K_{1,n}) = 2\sqrt{2}n\,.$$

4.10. **The P_3-eigen power formation number of the class of star graphs, S_{1,qP_3} with rays of length 2.** The smallest graph for which S_{1,qP_3} has a P_3-decomposition has $n = 5(q = 2)$. From previous section:

$$ratio_{P_3}E(S_{1,qP_3}) = \frac{n(1-\sqrt{2}) + \sqrt{2} - 3 + \sqrt{2}\sqrt{n+1}}{n-1}\,.$$

Thus to evaluate the P_3-eigen power formation number of S_{1,qP_3}, we need to compute:

$$\begin{aligned}\int \frac{t(1-\sqrt{2}) + \sqrt{2} - 3 + \sqrt{2}\sqrt{t+1}}{t-1}dt &= (1-\sqrt{2})\int \frac{t-1}{t-1}dt + (1-\sqrt{2})\ln(t-1)\\ &+ (\sqrt{2}-3)\ln(t-1) + \sqrt{2}\int \frac{\sqrt{t+1}}{t-1}dt\\ &= (1-\sqrt{2})t - 2\ln(t-1) + A\,,\end{aligned}$$

where:

$$A = \sqrt{2}\int \frac{\sqrt{t+1}}{t-1}dt\,.$$

Substituting $t + 1 = u^2$ implies that:

$$\begin{aligned}2\sqrt{2}\int \frac{u^2}{u^2-2}du &= 2\sqrt{2}\int \frac{u^2-2}{u^2-2}du + 4\sqrt{2}\int \frac{du}{u^2-2}\\ &= 2\sqrt{2}u + 2\ln(u-\sqrt{2}) - 2\ln(u+\sqrt{2}) = 2\sqrt{2}\sqrt{t+1} + 2\ln\frac{\sqrt{t+1}-\sqrt{2}}{\sqrt{t+1}+\sqrt{2}}\,.\end{aligned}$$

Thus, integrating between 5 and n, we get:

$$\left|(1-\sqrt{2})n - 2\ln(n-1) + 2\sqrt{2}\sqrt{n+1} + 2\ln\frac{\sqrt{n+1}-\sqrt{2}}{\sqrt{n+1}+\sqrt{2}} - (1-\sqrt{2})5 - 2\ln 4 - 2\sqrt{12} - 2\ln\frac{\sqrt{6}-\sqrt{2}}{\sqrt{6}+\sqrt{2}}\right|.$$

The average degree of S_{1,qP_3} is $\dfrac{2(n-1)}{n}$ so that the P_3-eigen power formation number becomes:

$$\frac{2(n-1)}{n} \times \Bigg|((\sqrt{2}-1)n - 2\ln n) + 2\sqrt{2}\sqrt{n+1} +$$

$$2\ln\frac{\sqrt{n+1}-\sqrt{2}}{\sqrt{n+1}+\sqrt{2}} - (\sqrt{2}-1)5 - 2\ln 4 - 2\sqrt{12} - 2\ln\frac{\sqrt{6}-\sqrt{2}}{\sqrt{6}+\sqrt{2}}\Bigg|\,,$$

so that:

$$extreme - power_{P_3}E(S_{1,qP_3}) = 2(1-\sqrt{2})n\,.$$

Theorem 4.1. *The power*$_{K_2}E(\Omega)$ *and extreme−power*$_{K_2}E(\Omega)$; $\Omega = K_n, K_{\frac{n}{2},\frac{n}{2}}, W_n, K_{1,n}, S_{1,qP_3}$ *respectively are:*

$$\Omega = K_n : \quad (n-1)|-2n + 4\ln\frac{n}{2} + 4| \quad and \quad 2n^2\,;$$

$$\Omega = K_{\frac{n}{2},\frac{n}{2}} : \frac{n}{2}|4\ln\frac{n}{2} - n + 2| \quad and \quad \frac{n^2}{2}\,;$$

$$\Omega = W_n : \quad \leq \frac{4n-4}{n}\Big|[2(n+\ln(\sqrt{n}-1)) - \ln(\sqrt{n}-1)] - n - \ln(n+1) - 2(2-\ln 3) + 4 - \ln 3$$

and $\leq 4n$;

$$\Omega = K_{1,n-1} : \frac{2n-2}{n}|4\sqrt{n-1} - 2n| \quad and \quad 4n\,;$$

$$\Omega = S_{1,qP_3} : \frac{2(n-1)}{n}\ multiplied\ by$$

$$\Big|-n - 2\ln(n-1) + 2\sqrt{2}\sqrt{n+1} + 2\ln\frac{\sqrt{n+1}-\sqrt{2}}{\sqrt{n-1}+\sqrt{2}} + 2 - 2\sqrt{6} - 2\ln\frac{\sqrt{3}-\sqrt{2}}{\sqrt{1}+\sqrt{2}}\Big| \quad and \quad 2n\,.$$

Theorem 4.2. *The power*$_{P_3}(\Omega)$ *and extreme−power*$_{P_3}(\Omega)$; $\Omega = K_n, K_{\frac{n}{2},\frac{n}{2}}, W_n, K_{1,n}, S_{1,qP_3}$ *respectively are:*

$$\Omega = K_n : \quad (n-1)|4\ln n - n\sqrt{2} - 4\ln 4 + 4\sqrt{2}| \quad and \quad \sqrt{2}n^2\,;$$

$$\Omega = K_{\frac{n}{2},\frac{n}{2}} : \frac{n}{2}|4\ln n - n\sqrt{2} - 4\ln 4 + 4\sqrt{2}| \quad and \quad \frac{n^2}{\sqrt{2}}\,;$$

$$\begin{aligned} \Omega \quad &= \quad W_n :\leq \frac{(4n-4)}{n}\Big|\frac{(-2-2\sqrt{2})}{2}n + (\sqrt{2}-1)\ln(n-1) + 2\sqrt{n} + 2\ln|\sqrt{n}-1| \\ &- \quad \frac{(-2-2\sqrt{2})}{2}4 - (\sqrt{2}-1)\ln 3 - 4\Big| \end{aligned}$$

and $\leq 2(2\sqrt{2}+2)n$;

$$\Omega = K_{1,n-1} : \frac{2(n-1)}{n}|4\sqrt{n-1} - n\sqrt{2} - 4\sqrt{2} + 3\sqrt{2}| \quad and \quad 2\sqrt{2}n\,;$$

$$\begin{aligned} \Omega \quad &= \quad S_{1,qP_3} : \frac{2(n-1)}{n}\Big|(1-\sqrt{2})n - 2\ln(n-1) + 2\sqrt{2}\sqrt{n+1} + 2\ln\Big[\frac{\sqrt{n+1}-\sqrt{2}}{\sqrt{n+1}+\sqrt{2}}\Big] \\ & (1-\sqrt{2})5 + 2\ln(4) - 2\sqrt{12} - 2\ln\Big[\frac{\sqrt{6}-\sqrt{2}}{\sqrt{6}+\sqrt{2}}\Big]\Big| \quad and \end{aligned}$$

$2(1-\sqrt{2})n$; $n \geq 5$.

Theorem 4.3. K_n *and* $K_{\frac{n}{2},\frac{n}{2}}$ *are 2-reciprocal* K_2*-eigen formation power and* $\sqrt{2}$*-reciprocal* P_3*-eigen formation power convergent.*

Proposition 4.1. *The H-eigen power formation number of any class of graphs is bounded above by power*$_{K_2}(K_n)$.

5. Conclusion

The idea of H-decomposition and the energy of a graph are combined in this chapter to consider the idea of the energy involved in the *formation* of a molecule, where a graph theoretical representation is provided for the molecule, assigning vertices as atoms and the edges as bonds between the atoms. We used the difference between the energy of a graph and the sum of the energy of its H-decomposable elements to define the H-eigen energy formation number of a graph. If this number as a function $f(n)$, of the order of graphs, belongs to a class of graphs, then we considered the ratio $f(n)/m$ and its convergent properties. We combined the average degree with the Riemann integral of this ratio to consider the idea of H-eigen energy formation power of classes of graphs. We believe that the H-eigen energy formation asymptote lies on the interval $[-2, 0)$ for all classes of graphs and that the complete graph has the maximum H-eigen energy formation power over all classes of graphs.

References

[1] C. Adiga, A. Bayad, I. Gutman, S. A. Srinivas: *The minimum Covering Energy of a Graph*, Kragujevac J. Sci. **34**, (2012), 39–56.
[2] N. Alon, J.H. Spencer: *Eigenvalues and Expanders, The Probabilistic Method (3rd ed.)*, John Wiley & Sons, 1991.
[3] M. Bousquet-M' elouy, K. Weller: *Asymptotic properties of some minor-closed classes of graphs*, DMTCS proc. AS: (2013) 629 - 640.
[4] F. Buckley: *The central ratio of a graph*, Discrete Mathematics, **38**(1), (1982), 17–21.
[5] C.A Coulson, B. O'Leary, R.B Mallion: *Hückel Theory for organic Chemists*, Academic Press, 1978.
[6] S. Gabor: *Asymptotic values of the Hall-ratio for graph powers*, Discrete Mathematics, **306**(19-20), (2006), 2593–2601.
[7] J.M Harris, J.L Hirst, M. Mossinghoff: *Combinatorial and Graph Theory*, Springer, New York, 2008.
[8] D. Sarvate, P. A Winter, Z. Li: *A Fundamental Theorem of Multigraph Decomposition of* $\lambda K_{m,n}$, Journal of Combinatorial Mathematics and Combinatorial Computing (to appear).
[9] P.A Winter, F.J Adewusi: *Tree-cover ratio of graphs with asymptotic convergence identical to the secretary problem*, Advances in Mathematic: Scientific Journal; **3**(1), (2014), 47–61.
[10] P.A Winter, C.L Jessop: *Integral eigen-pair balanced classes of graphs: ratios, asymptotes, areas and involution complementary*, International Journal of Graph Theory, Volume 2014, Article ID 148690, 16 pages http://dx.doi.org/10.1155/2014/148690

Department of Mathematics
University of Kwazulu-Natal
Howard College, Durban
E-mail address: winter@ukzn.ac.za

Department of Mathematics
College of Charleston
South Carolina, United States
E-mail address: winter@ukzn.ac.za