# On Maximum Independent χ - Energy of Graphs

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**Abstract**

Maximum independent χ - energy (Color Energy) $E_{I\chi}$ of a simple graph Ω is obtained by calculating the absolute sum of its independent χ - eigen/latent values. Few standard results regarding Maximum independent χ - energy $E_{I\chi}$ and the Maximum independent χ - energy value for certain standard graphs has also been shown here. As an application of this energy, drug Cisplatin has been taken into consideration and its $E_{I\chi}$ value has been computed here.

**Key words**: Color energy, Color latent values, Color matrix, Maximum independent colored set.

## 1. PRELUDE

Let Ω = (V, E) be a connected but undirected graph. A Subset I ⊆ V becomes independent if its vertices doesn't form any edges. The highest cardinality of such a set is called independence number which is usually denoted as β (Ω).

The ideologies pertaining to the concepts namely The Energy of a Graph [3], Coloring a Graph [2], Color Energy of a Graph [2] and the Maximum independent vertex energy [6] are the main motivation to conceptualize Maximum independent χ - energy 'EIχ' of a graph Ω and to determine the χ – energy EIχ of certain standard graphs. Mathematical aspects concerning Energy of a Graph can be seen in [1], [4] and [5].

It has been discovered that Energy of a Graph has exceptional applications in the study of chemical molecules and in other fields.

Similar studies are also found in [7] and [8].

The standard results regarding EIχ of any graph Ω are obtained by studying characteristic polynomial of its maximum independent colored matrix.

Inorder to connect with chemical applications, We have computed the mathematical value of EIχ for the chemical cancer drug Cisplatin.

## 2. MAXIMUM INDEPENDENT χ - ENERGY – EIχ

Let Ω be a graph with r edges and s vertices. Let Iχ be its maximum independent colored set of vertices.

The maximum independent colored matrix of Ω is a s × s adjacency square matrix AIχ (Ω) = (bij ), where

$$
b_{ij} = \begin{cases} 1 & \text{if } i = j \text{ if } v_i \in I\chi \text{ or the vertices } v_i \text{ and } v_j \text{ constitutes an edge and } c(v_i) \neq c(v_j) \\ -1 & \text{if vertices } v_i \text{ and } v_j \text{ doesn't constitute an edge but } c(v_i) = c(v_j) \\ 0 & \text{elsewhere} \end{cases}
$$

Then the characteristic polynomial obtained from its adjacency matrix AIχ (Ω) denoted by $h_s(\Omega, \lambda_c)$ is elucidated as $h_s(\Omega, \lambda_c) = \det(\lambda_c I - AI\chi(\Omega))$.

As it is evident that the adjacency matrix AIχ (Ω) consists of real symmetric numbers, its independent χ - eigenvalues are also real and we specify them as $\lambda_{c1}, \lambda_{c2}, \lambda_{c3}, \ldots, \lambda_{cs}$. The maximum independent χ - energy of Ω is defined as : $EI\chi(\Omega) = \sum_{i=1}^{s} |\lambda ci|$

In the later section of this paper, we have computed the numerical values of EIχ for certain standard graphs namely Star $K_{1,s-1}$, Complete Bipartite $K_{s,s}$ and Friendship $F_s$ Graphs after studying the basic properties of EIχ.

## 3. BASIC THEOREMS ON EIχ

**Theorem 1**. Let Ω be a simple connected graph with independence number β (Ω). If the order and size of Ω is s and r respectively with $h_s(\Omega, \lambda_c) = b_0\lambda^s c + b_1\lambda^{s-1}_c + \ldots + b_s$ being the characteristic polynomial obtained from Iχ of Ω, then

1) $b_0=1$
2) $b_1 = -\beta(\Omega)$
3) $b_2 = \binom{\beta(\Omega)}{2} - [r'\chi + r]$, $r'\chi$ being $\frac{\text{number of vertices that doesn't form edges but identical in color}}{2}$

**Proof.** (1) It is obvious that $h_S(\Omega, \lambda c) := \det(\lambda_c I - AI\chi(\Omega))$ which yields $b_0=1$.

(2)As the total of the diagonal elements in AIχ (Ω) is evidently equal to independence number β(Ω) of its corresponding graph Ω, thus we get $b_1 = -\beta(\Omega)$.

(3) Since $(-1)^2 b_2$ equals total of determinants of all principal submatrices of AIχ (Ω) of order 2 × 2, it leads to

$$b_2 = \sum_{1 \le i < j \le s} \begin{vmatrix} b_{ii} & b_{ij} \\ b_{ji} & b_{jj} \end{vmatrix}$$

$$= \sum_{1\le i<j\le s} \left(b_{ii}b_{jj} - b_{ij}b_{ji}\right)$$

$$= \sum_{1\le i<j\le s}\left(b_{ii}b_{jj}\right) - \sum_{1\le i<j\le s}\left({b_{ij}}^2\right)$$

$$= \binom{\beta(\Omega)}{2} - [r'\chi + r],$$

where r'χ being $\frac{\text{number of vertices that doesn't form edges but identical in color}}{2}$

**Theorem 2**. Let Ω be a graph. Let $\lambda_c 1, \lambda_c 2, \lambda_c 3, \ldots, \lambda_c s$ be the latent values of maximum independent colored adjacency matrix AIχ (Ω). Then

(1). $\sum_{i=1}^{s} \lambda ci = \beta(\Omega)$,

(2). $\sum_{i=1}^{s} \lambda^2 ci = 2[r'\chi + r] + \beta(\Omega)$ where r'χ being $\frac{\text{number of vertices that doesn't form edges but identical in color}}{2}$

**Proof**. (1) Since the total of the latent values of AIχ (Ω) equals the trace of AIχ (Ω), we get $\sum_{i=1}^{s} \lambda ci = \sum_{i=1}^{s} b_{ii} = |I\chi| = \beta(\Omega)$ where β (Ω) denotes the cardinality of maximum independent colored vertex set.

(2) Also likewise the Sum of the squares of latent values of the AIχ (Ω) matches the trace of the ($A^2$ Iχ (Ω)).

Thus

$$\sum_{i=1}^{s} \lambda^2 ci = \sum_{i=1}^{s}\sum_{j=1}^{s} b_{ij}b_{ji}$$

$$= 2\sum_{i\ne j}^{s} b_{ij}b_{ji} + \sum_{i=1}^{s}\left({b_{ii}}^2\right)$$

$$= 2\sum_{i<j}^{s}\left({b_{ij}}^2\right) + \sum_{i=1}^{s}\left({b_{ii}}^2\right)$$

$$\text{So } \sum_{i=1}^{s} \lambda^2 ci = 2[r'\chi + r] + \beta(\Omega)$$

**Theorem 3**. Consider Ω to be a simple connected graph containing a maximum independent colored set Iχ. If the EIχ is a rational number, Then EIχ (Ω) ≡ |Iχ|(mod2).

**Proof**. Let $\lambda_{c1}, \lambda_{c2}, \lambda_{c3}, \ldots, \lambda_{cs}$ be the maximum independent χ - latent values of a graph Ω. Let $\lambda_{c1}, \lambda_{c2}, \lambda_{c3}, \ldots, \lambda_{cs}$ (for t < s) be the non negative latent values and the balance being negative values, we get

$\sum_{i=1}^{s} |\lambda ci| = (\lambda_{c1} + \lambda_{c2} + \lambda_{c3} + \ldots + \lambda_{ct}) - (\lambda_{ct+1} + \lambda_{ct+2} + \lambda_{ct+3} + .. + \lambda_{cs})$

$= 2(\lambda_{c1} + \lambda_{c2} + \lambda_{c3} + \ldots + \lambda_{ct}) - (\lambda_{c1} + \lambda_{c2} + \lambda_{c3} + \ldots + \lambda_{cs})$ ................ (3.1)

$= 2(\lambda_{c1} + \lambda_{c2} + \lambda_{c3} + \ldots + \lambda_{ct}) - \beta(\Omega)$

Therefore, EI$\chi$ ($\Omega$) = 2k − $\beta$ ($\Omega$) where k = ($\lambda_{c1} + \lambda_{c2} + \lambda_{c3} + .... + \lambda_{ct}$)

Here the latent values $\lambda_{c1}$, $\lambda_{c2}$, $\lambda_{c3}$, ...., $\lambda$cs are integers,so their total will also be an integer value. Then, the value of 'k' is also integer as the value of EI$\chi$ ($\Omega$) is a rational.

## 4. EI$\chi$ OF CERTAIN COMMON FAMILIES OF GRAPHS

**Theorem 4.** For s ≥ 2, EI$\chi$ ($K_{1,s-1}$) = $(2s - 4) + \sqrt{s^2 - 2s + 5}$

**Proof.** For a Star graph $K_{1,s-1}$ with s vertices V = {$v_1, v_2, ..., v_s$}, its highest independent set I$\chi$ = {$v_s$}

Since its chromatic number $\chi$ = 2 and $\beta$ ($K_{1,s-1}$) = s − 1, we obtain

$$AI\chi(K_{1,s-1}) = \begin{bmatrix} 0 & 1 & \cdots & 1 & 1 \\ 1 & 1 & & -1 & -1 \\ \vdots & & \ddots & & \vdots \\ 1 & -1 & & 1 & -1 \\ 1 & -1 & \cdots & -1 & 1 \end{bmatrix}_{(s \times s)}$$

Characteristic polynomial is obtained as $(-1)^s (\lambda_c - 2)^{s-2} (\lambda^2_c + (s - 3)\lambda_c - (s - 1))$

$$\text{Spectrum, SpecI}\chi(K_{1,s-1}) = \begin{pmatrix} 2 & \frac{-(s-3)\pm\sqrt{s^2-2s+5}}{2} \\ s-2 & 1 \end{pmatrix}$$

Therefore, EI$\chi$ ($K_{1,s-1}$) = $\sum_{i=1}^{s} |\lambda ci|$

$$= |2|(s - 2) + \left|\frac{-(s-3)\pm\sqrt{s^2-2s+5}}{2}\right| 1$$

$$= (2s - 4) + \sqrt{s^2 - 2s + 5}$$

Thus EI$\chi$ ($K_{1,s-1}$) is $(2s - 4) + \sqrt{s^2 - 2s + 5}$.

**Theorem 5.** For s ≥ 2 , EI$\chi$ ($K_{s,s}$) = (3s − 3) + $\sqrt{4s^2 + 1}$.

**Proof.** Let $K_{s,s}$ be a Complete Bipartite graph with vertices V = {$u_1, u_2, ..., u_s, v_1, v_2, ..., v_s$}, then its I$\chi$ = {$u_1, v_1$}.

Since its chromatic number $\chi$ = 2 and the independence number $\beta(K_{s,s})$ = s, we obtain

$$AI\chi(K_{s,s}) = \begin{bmatrix} 0 & 1 & \cdots & 1 & 1 \\ 1 & 1 & & -1 & -1 \\ \vdots & & \ddots & & \vdots \\ 1 & -1 & & 1 & -1 \\ 1 & -1 & \cdots & -1 & 1 \end{bmatrix}_{(2s \times 2s)}$$

Characteristic polynomial of $K_{s,s}$ is found to be $(\lambda_c - 1)^{s-1} (\lambda_c - 2)^{s-1} (\lambda^2_c + (2s - 3)\lambda_c + (2-3s))$

$$\text{Its Spectrum, SpecI}\chi(K_{s,s}) = \begin{pmatrix} 1 & 2 & \frac{-(2s-3)\pm\sqrt{4s^2+1}}{2} \\ s-1 & s-1 & 1 \end{pmatrix}$$

Then EIχ ($K_{s,s}$) = $\sum_{i=1}^{s} |\lambda ci|$

$= |1|(s-1) + |2|(s-1) + \left|\frac{-(2s-3)\pm\sqrt{4s^2+1}}{2}\right| 1$

$= (s-1) + (2s-2) + \sqrt{4s^2+1}$

$= (3s-3) + \sqrt{4s^2+1}$

Thus EIχ ($K_{s,s}$) is $(3s-3) + \sqrt{4s^2+1}$.

**Theorem 6.** For s ≥ 2, EIχ (Fs) is $(s-1)\sqrt{5} + s + \sqrt{s^2+2s+5}$

**Proof.** For a Friendship graph $F_s$ of order (2s + 1), it assumes the maximum independent set as Iχ = {$v_0$}.

Since its chromatic number χ=3 and the independence number β($F_s$) = s, we obtain

$$AI\chi\,(Fs) = \begin{bmatrix} 1 & 1 & \cdots & 1 & 1 \\ 1 & 1 & & -1 & 0 \\ \vdots & & \ddots & \vdots & \\ 1 & -1 & \cdots & 1 & 1 \\ 1 & 0 & & 1 & 0 \end{bmatrix}_{(2s+1 \times 2s+1)}$$

Characteristic polynomial of $F_s$ is given by $(-1)(\lambda_c+s)\,(\lambda^2_c - 3\lambda_c + 1)^{s-1}\,(\lambda^2_c + (s-3)\,\lambda_c + (1-2s))$

Spectrum, Spec Iχ ($F_s$) = $\begin{pmatrix} \frac{3\pm\sqrt{5}}{2} & -s & \frac{-(s-3)\pm\sqrt{s^2+2s+5}}{2} \\ s-1 & 1 & 1 \end{pmatrix}$

Then EIχ ($F_s$) = $\sum_{i=1}^{s} |\lambda ci|$

$= \left|\frac{3\pm\sqrt{5}}{2}\right|(s-1) + |-s|1 + \left|\frac{-(s-3)\pm\sqrt{s^2+2s+5}}{2}\right| 1$

$= (s-1)\sqrt{5} + s + \sqrt{s^2+2s+5}$

Thus EIχ (Fs) is $(s-1)\sqrt{5} + s + \sqrt{s^2+2s+5}$.

## 5. CHEMICAL APPLICATION OF EIχ

Cisplatin is a strong medicinal drug which is extensively used for chemotherapy purpose against Cancer disease. Maximum independent Color energy EIχ of Cisplatin has been computed below which might be useful for further development that involves Cancer treatment.

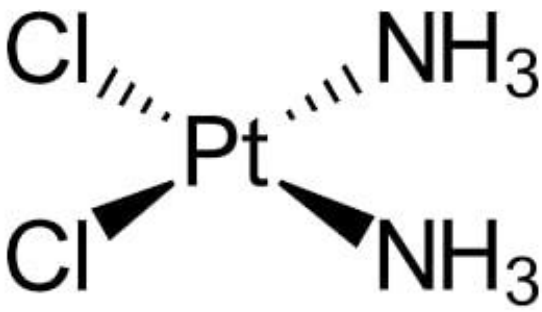


Fig 1. Cisplatin: Structural Formula

Here, the maximum independent colored set is I$\chi$ = {Cl, Cl, $NH_3$, $NH_3$}.

$$A\ I\chi = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 0 & 0 \\ 1 & -1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & -1 \\ 1 & 0 & 0 & 1 & 1 \end{bmatrix}$$

The Characteristic polynomial is found to $(\lambda_c)(\lambda_c - 2)^3 (\lambda_c + 2)$

Spectrum of Cisplatin, Spec I$\chi$ = $\begin{bmatrix} 0 & -2 & 2 \\ 1 & 1 & 3 \end{bmatrix}$

Thus, EI$\chi$ of Cisplatin = 8.

## 6. CONCLUSION

The numerical values of EI$\chi$ of certain well known standard graphs are established here. It is noticed that the selection of the maximum independent colored vertex set acts as an important criteria in calculating the $\chi$ – energy EI$\chi$ of a particular graph. It can be applied to any drug's structural formula transferred to a graph and can be analysed and compared with its corresponding Pharmaceutical properties.

## REFERENCES

1. Bapat R B, Graphs and Matrices, Hindustan Book Agency , (2011)
2. Chandrashekar Adiga, Sampathkumar E , Sriraj M.A, Shrikanth A. S, Color Energy of a Graph ,Proceedings of the Jangjeon Mathematical Society, 16 (2013), 335 - 351.
3. Gutman I, The energy of a graph, Ber. Math. Stat. Sekt. Forschungsz. Graz , 103 (1978), 1 – 22.
4. Gutman I, Li X, Zhang J, Graph Energy , Streib., Anal. Comp. Net., From Biology to Linguistics, Wiley-VCH, Weinheim, (2009), 145-174
5. Li X, Shi Y, Gutman I, Graph Energy, Springer, New York Heid. Dord., London (2012)
6. Murthy K.B, Puttaswamy, Naji A.M, The Maximum Independent Vertex Energy of a Graph , International Journal of Mathematics And its Applications, 3(4)(2016), 63-71
7. Rajesh Kanna M.R., Pradeep Kumar R, Jagadeesh R, Minimum Covering Color Energy of a Graph, International Journal of Mathematical Analysis, 9(8)(2015), 351-364

8. Sreeja S, Mary U, Minimum hub Color energy of a graph, Malaya Journal of Mathematik, 9(1)(2021), 494 - 497.