PREFACE

"Spectral graph theory" is a branch of graph theory in which linear algebra, particularly matrix theory, plays an important role. On one hand, various concepts from matrix theory have facilitated the construction of graphs and are explored as tools in computer science. On the other hand, graph theory has also contributed to characterizing certain properties of matrices. Over the last decade, there has been a growing interest in the extensive investigation of graphs with the aid of matrix theory.

In this thesis, we highlight the rich interplay between the two topics viz matrix theory and graph theory. In particular, we focus on the structural properties of graphs with the help of a signless Laplacian matrix. We begin by introducing the necessary concepts and definitions from both matrix theory and graph theory. Next, we discuss the importance of the signless Laplacian matrix among various other graph matrices, followed by a brief literature survey on Q-integral graphs that motivated this thesis. From Chapter 2 to Chapter 3, we study simple graphs. In Chapter 4, we explore the addition of self-loops to simple connected Q-integral graphs.

In 2019, Park and Sano [32] studied simple connected Q-integral graphs with maximum edge-degree at most 6. They provided a structural classification for such graphs G when Q-spectral radius of G is 6. Inspired by their work, in ***Chapter 2***, we study simple connected Q-integral graphs G whose maximum edge-degree is at most 8 and give a structural characterization when G has Q-spectral radius 7. We show that if $G \neq K_{1,4} \square K_2$, then G must be bipartite and contain one of the four special subgraphs $\mathcal{S}_4^2(m)(m = 0, 1, 2)$ (see Figure 1.2(c)) as an induced subgraph when Q-spectral radius of G is 7 and its maximum edge-degree is 8.

In addition, we give a bound for the maximum edge-degree in terms of the Q-spectral radius for connected graphs with integer-valued Q-spectral radius. Furthermore, as an application, we prove that the Q-spectral radius of a connected edge-non-regular graph G having integer-valued Q-spectral radius and maximum edge-degree 5 is always equal to 6 (which was unsolved earlier). Additionally, we show that there does not exist any connected edge-non-regular graph with integer-valued Q-spectral radius less than 5.

For the Q-spectral radius (q) of a simple connected Q-integral graph G, equal to 5 and 6, we surprisingly notice that the double star $\mathcal{S}^2_{q-3}$ (see Figure 1.2(a)) is always a subgraph of G when its maximum edge-degree is $2q-6$ (see [32, 35]). Eventually, a question about the existence of the double star $\mathcal{S}^2_{q-3}$ in a simple connected Q-integral graph with maximum edge-degree $2q-6$, also arises in our mind.

To answer this question, in ***Chapter 3***, we study simple connected graphs with integral Q-spectral radius (q) and maximum edge-degree equal to $2q-6$. We provide necessary and sufficient conditions for such a connected graph G to contain $\mathcal{S}^2_{q-3}$ and $\mathcal{S}^{2,1}_{q-3}$ (see Figures 1.2(a), 1.2(b)) as subgraphs. We also give a necessary and sufficient condition for connected graphs, whose least Q-eigenvalue is not in $(0,1)$, to contain only the double star $\mathcal{S}^2_{q-3}$ as a subgraph for $q \in \{7,8,9\}$. In 2008, Simić and Stanić [35] showed that the only connected edge-non-regular Q-integral graphs with maximum edge-degree 4 are $\mathcal{H}^*$ and $K_{1,2}\Box K_2$, see Figure 3.5. In this chapter, we extend their result by characterizing all such edge-non-regular connected graphs when G is not necessarily Q-integral, but instead has only the smallest Q-eigenvalue outside the interval $(0,1)$ and integer-valued Q-spectral radius.

Finally, we move our attention to graphs containing self-loops (representing heteroatoms) since they are of evident chemical significance. Moreover, graph energy and graph eigenvalues are interconnected, and graphs with integral Q-spectrum are of high interest now, which motivates us to observe the effect of adding self-loops on the Q-integrality of a Q-integral graph.

In ***Chapter 4***, we prove that the graph, obtained by adding self-loops to each vertex of a non-empty proper subset of vertices of $K_{p,p}$, is Q-integral if and only if $p = 4$ and self-loops are added to exactly two vertices of each partite set, or $p = 2$ and self-loops are added to all vertices of one partite set. Besides, we prove that the graph, obtained by adding self-loops to each vertex of a non-empty proper subset of vertices of the star graph $K_{1,p}$, is Q-integral if and only if $p = 4$ and self-loops are added to all the pendant vertices. Using this results, we also answer when $Spec(M + 3D') \subseteq \mathbb{Z}$, where M is permutation similar to either $\begin{pmatrix} \mathrm{O}_p & \mathrm{J} \\ \mathrm{J} & \mathrm{O}_p \end{pmatrix}$ or $\begin{pmatrix} p & \mathrm{J} \\ \mathrm{J} & I_p \end{pmatrix}$, and D' is any $(0, 1)$-diagonal matrix.

At the last, in ***Chapter 5***, we conclude the thesis by presenting a comprehensive summary and outlining the potential directions for future research.

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