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Regular graphs with maximal energy per vertex

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ABSTRACT

We study the energy per vertex in regular graphs. For every $k \geqslant 2$, we give an upper bound for the energy per vertex of a k-regular graph, and show that a graph attains the upper bound if and only if it is the disjoint union of incidence graphs of projective planes of order $k-1$ or, in case $k = 2$, the disjoint union of triangles and hexagons. For every k, we also construct k-regular subgraphs of incidence graphs of projective planes for which the energy per vertex is close to the upper bound. In this way, we show that this upper bound is asymptotically tight.

1. Introduction

The energy of a graph is the sum of the absolute values of the eigenvalues of its adjacency matrix. This concept was introduced by Gutman [10] as a way to model the total π-electron energy of a molecule. For details and an overview of the results on graph energy, we refer to the recent book by Li, Shi, and Gutman [12] (and the references therein).

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Several results on graphs with maximal energy have been obtained. In particular, Koolen and Moulton [11] showed that a graph on n vertices has energy at most $n(1+\sqrt{n})/2$, and characterized the case of equality. Nikiforov [14] showed that this upper bound is asymptotically tight by constructing graphs on n vertices that have energy close to the upper bound, for every n. Another result, which follows easily from a bound by McClelland [13], is that a graph with m edges has energy at most $2m$, with equality if and only if the graph is the disjoint union of isolated vertices and m edges (a matching) (see also [12, Thm. 5.2]).

In this paper, we consider the (average) energy *per vertex* of a graph Γ, that is,

$$\overline{\mathcal{E}}(\Gamma) = \frac{1}{n}\sum_{i=1}^{n} |\lambda_i|,$$

where n is the number of vertices and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of Γ. At an AIM workshop in 2006, the problem was posed to find upper bounds for the energy per vertex of regular graphs, and it was conjectured that the incidence graph of a projective plane has maximal energy per vertex; cf. [6, Conj. 3.11]. In this paper, we prove this conjecture – among other results.

In Section 2 we give an upper bound for the energy per vertex of a k-regular graph in terms of k, and show that a graph attains the upper bound if and only if it is the disjoint union of incidence graphs of projective planes of order $k-1$ or, in case $k=2$, the disjoint union of triangles and hexagons. In order to prove this result, we reduce the problem to a constrained optimization problem that we solve in Section 3 using the Karush–Kuhn–Tucker conditions. Projective planes of order $k-1$ are only known to exist when $k-1$ is a prime power. We therefore construct, in Section 4, k-regular subgraphs of incidence graphs of certain elliptic semiplanes (that are substructures of projective planes) for which the energy per vertex is close to the upper bound, for every k. In this way, we show that our upper bound is asymptotically tight.

2. Maximal energy per vertex

Theorem 1. *Let $k \geqslant 2$, and let Γ be a k-regular graph. Then the energy per vertex of Γ is at most*

$$\frac{k+(k^2-k)\sqrt{k-1}}{k^2-k+1}$$

with equality if and only if Γ is the disjoint union of incidence graphs of projective planes of order $k-1$ or, in case $k=2$, the disjoint union of triangles and hexagons.

Proof. First of all, we note that the incidence graph of a projective plane of order $k-1$ (for $k=2$ this is the hexagon) has spectrum