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Coxeter energy of graphs

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ABSTRACT

We study the concept of the Coxeter energy of graphs and digraphs (quivers) as an analogue of Gutman's adjacency energy, which has applications in theoretical chemistry and is a recently widely investigated graph invariant. Coxeter energy $\mathcal{CE}(G)$ of a (di)graph G is defined to be the sum of the absolute values of all complex eigenvalues of the Coxeter matrix associated with G. Our main inspiration for the study comes from the Coxeter formalism appearing in group theory, Lie theory, representation theory of algebras, mathematical physics and other contexts. We focus on the Coxeter energy of trees and we prove that the path (resp. the maximal star) has the smallest (resp. the greatest) Coxeter energy among all trees (resp. two large subclasses of trees) with fixed number of vertices. We provide several other related results, as the characterization of trees with second smallest and second greatest Coxeter energy, bounds for Coxeter energy, and general facts on Coxeter spectra of graphs extending known results e.g. for Salem trees and for certain special real Coxeter eigenvalues of trees. Additionally, we discuss few other energy-like quantities for the Coxeter spectra of (di)graphs, including Coxeter energy "normalized" by the trace of the Coxeter matrix and the quantities derived from variants of Coulson integral formula.

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1. Introduction

The energy of a (simple, undirected) graph G with $n \geq 1$ vertices was defined in 1978 by Gutman [23] to be the quantity

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\mu_i|, \tag{1}$$

where $\mu_1, \ldots, \mu_n$ denote the eigenvalues of the symmetric adjacency matrix $\mathrm{Ad}_G \in \mathbb{M}_n(\mathbb{Z})$, together with multiplicities (for all basic definitions of spectral graph theory we refer to [11] and [5,6]). We recall that the idea of the energy of a graph has its origin in computational chemistry. Briefly speaking, the total π-electron energy in a conjugated hydrocarbon can be approximated by the energy $\mathcal{E}(G)$ of the associated "molecular" graph G. For more details on the properties of graph energy and its chemical applications we refer to the survey [24] and the handbook [39].

On the other hand, graph energy is an interesting abstract graph invariant, recently intensively studied from purely mathematical point of view, see [39] and the rich literature quoted therein. We refer also to [52] (resp. [19,53]), where the authors generalize the definition of energy for digraphs (resp. signed graphs, signed digraphs). Moreover, one considers other variants of this concept, such as the Laplacian energy, defined in [25] by setting

$$\mathcal{LE}(G) = \sum_{i=1}^{n} |\nu_i - \overline{\nu}|, \tag{2}$$

for a graph G with $n \geq 1$ vertices, where $\nu_1, \ldots, \nu_n$ are the eigenvalues of the Laplacian matrix [21] $L_G = \Delta_G - \mathrm{Ad}_G$, where $\Delta_G \in \mathbb{M}_n(\mathbb{Z})$ is the diagonal matrix whose diagonal elements are the vertex degrees and $\overline{\nu} := \frac{\sum_{i=1}^{n} \nu_i}{n} = \frac{\mathrm{tr}(L_G)}{n}$ is the arithmetic mean of the eigenvalues of L_G (which clearly coincides with the average vertex degree). Note that all eigenvalues of the adjacency matrix Ad_G and the Laplacian matrix L_G are real, since these matrices are real-symmetric.

In the present paper we introduce an energy-like quantity for the spectrum of another matrix associated with a graph. Namely, let $\lambda_1, \ldots, \lambda_n$ be all (complex) eigenvalues of the Coxeter matrix $\mathrm{Cox}_G \in \mathbb{M}_n(\mathbb{Z})$ of a graph G with $n \geq 1$ vertices (see Section 2 for detailed definitions; note that we will consider, more generally, multigraphs and multidigraphs). We define the *Coxeter energy* of G to be the real number

$$\mathcal{CE}(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{3}$$

We note that analogous quantity was defined by de la Peña in [50] for the Coxeter matrix associated with a finite dimensional algebra over a field. Recall that the Coxeter spectral properties of graphs (including edge-bipartite graphs [57], a class of signed