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Topological Indices Based on Vertex Energy

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Abstract

The energy $\mathcal{E}(v) = |A|_{vv}$ of a vertex v of a graph G, introduced by Arizmendi, Fernández Hidalgo and Juárez-Romero, is the diagonal entry of the absolute value $|A| = (A^2)^{1/2}$ of the adjacency matrix, so that the graph energy $\mathcal{E}(G)$ splits as $\sum_v \mathcal{E}(v)$. Replacing vertex degrees by vertex energies in the classical bond-incident-degree scheme, we introduce a family of *vertex-energy topological indices* $\mathrm{VE}_f(G) = \sum_{uv\in E(G)} f\big(\mathcal{E}(u), \mathcal{E}(v)\big)$, together with its vertex-sum companions, and study in detail the first and second vertex-energy Zagreb indices $\mathrm{EM}_1, \mathrm{EM}_2$, the energy-degree index ED, the vertex-energy Randić index ER and the vertex-energy Sombor index ESO. We first prove two-sided pointwise bounds on vertex energy: a Hölder-type lower bound $\mathcal{E}(v) \geq d_v^{3/2}/\sqrt{W_4(v)}$, which simultaneously sharpens the known bounds d_v/Δ and $\sqrt{d_v/\Delta}$ and whose equality case forces a complete bipartite graph, and a new upper bound $\mathcal{E}(v)^2 \leq d_v - \big(W_4(v) - d_v^2\big)/(\sqrt{d_v} + \lambda_1)^2$ that refines $\mathcal{E}(v) \leq \sqrt{d_v}$. Here $W_4(v)$ is the number of closed 4-walks at v. Second, for adjacent vertices we strengthen the inequality $\mathcal{E}(u)\mathcal{E}(v) \geq 1$ of Arizmendi and Arizmendi to $\mathcal{E}(u)\mathcal{E}(v) \geq (1 + ||A|_{uv}|)^2$, characterize the edges with $\mathcal{E}(u)\mathcal{E}(v) = 1$, prove that $\mathcal{E}(u)\mathcal{E}(v) = 1$ on all edges of a connected graph exactly for complete bipartite graphs, and prove that equality $\mathcal{E}(u)\mathcal{E}(v) = (1 + |A|_{uv})^2$ with $|A|_{uv} \geq 0$ on all edges characterizes complete multipartite graphs. As a consequence we obtain a refinement of the inequality $\mathcal{E}(G) \geq 2R(G)$ that

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is sharp for all complete graphs. Third, we derive sharp bounds for EM_1, EM_2, ER and ESO in terms of n, m, λ_1, Δ, δ, the number of quadrangles, the Zagreb, Randić and Sombor indices and the energy; among the consequences are a strengthening of McClelland's bound and improvements of recent inequalities relating graph energy and the Sombor index. Fourth, removing the Perron atom from the spectral measure of a vertex, we obtain two-sided Perron-refined bounds whose sum over the vertices is a vertex decomposition of the Koolen–Moulton inequality; for regular graphs this yields explicit bounds for every monotone vertex-energy index and vertex-level Nordhaus–Gaddum inequalities $2(n-1)/n \le \mathcal{E}_G(v) + \mathcal{E}_{\overline{G}}(v)$, with equality exactly for K_n and $\overline{K_n}$. Finally, we prove that vertex energies are multiplicative under the tensor product, that $\max\{\mathcal{E}_G(g), \mathcal{E}_H(h)\} \le \mathcal{E}_{G\Box H}(g,h) \le \mathcal{E}_G(g) + \mathcal{E}_H(h)$ for the Cartesian product (with an exact formula for prisms and hypercubes), and that the join of two regular graphs raises every vertex energy by an explicit positive amount; we derive product and join formulas for the new indices, introduce a vertex-energy irregularity index, treat quadrangle-free graphs and trees, compute the indices for many families (wheels, friendship and complete split graphs, hypercubes, prisms), and report on exhaustive computations.

1 Introduction

Let G be a simple graph with vertex set $V(G)$, $|V(G)| = n$, edge set $E(G)$, $|E(G)| = m$, and adjacency matrix $A = A(G)$ with eigenvalues $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$. The *energy* of G,

$$\mathcal{E}(G) = \sum_{j=1}^{n} |\lambda_j|,$$

was introduced by Gutman [19] as a mathematical abstraction of the total π-electron energy of conjugated hydrocarbons in the Hückel molecular orbital theory [29]. Energy has become one of the most intensively investigated graph invariants; see the monograph [36], the surveys [23,27] and the references therein. Among its classical bounds are McClelland's inequality $\mathcal{E}(G) \le \sqrt{2mn}$ [40], the Koolen–Moulton bound [35] and the observation of Nikiforov [43] that $\mathcal{E}(G) = \operatorname{tr}|A|$ is the trace (nuclear) norm of A, where $|A| = (AA^{\mathsf{T}})^{1/2}$.

Nikiforov's observation suggests splitting $\mathcal{E}(G)$ into local contributions.

Following Arizmendi and Juárez-Romero [5] and Arizmendi, Fernández Hidalgo and Juárez-Romero [4], the *energy of the vertex* v is

$$\mathcal{E}_G(v) = |A|_{vv}, \qquad \text{so that} \qquad \mathcal{E}(G) = \sum_{v \in V(G)} \mathcal{E}_G(v).$$

Vertex energy turned out to be a powerful tool. In [4] it was shown that $d_v/\Delta \le \mathcal{E}(v) \le \sqrt{d_v}$ and several further local inequalities were derived. G. Arizmendi and O. Arizmendi [1] proved the striking fact that $\mathcal{E}(u)\mathcal{E}(v) \ge 1$ for every edge uv, and deduced the first relation between energy and a degree-based index, namely $\mathcal{E}(G) \ge 2R(G)$, where $R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-1/2}$ is the Randić index [44]. Yan et al. [53] complemented this by an upper bound involving the maximum degree. Motivated by these results, Ülker, Gürsoy and Gürsoy [50] and Ülker, Gürsoy, Gürsoy and Gutman [51] related the energy to the Sombor index

$$\mathrm{SO}(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}$$

introduced by Gutman [20]; for instance, they proved $\mathcal{E}(G) < \mathrm{SO}(G)$ for connected graphs with $n \ge 3$, and $\mathrm{SO}(G) \le \frac{\Delta^2}{\sqrt{2}} \mathcal{E}(G)$.

Since 2020 the theory of vertex energy has developed rapidly. Arizmendi, Luna-Olivera and Ramírez Ibáñez [6] established a Coulson integral formula for vertex energy; G. Arizmendi and O. Arizmendi extended vertex energies and the energy–Randić inequality to digraphs [2] and interpreted the vector of vertex energies as the payoff vector of a cooperative "graph energy game" [3]; Arizmendi and Sigarreta [7] discovered an alternating pattern in the change of vertex energies when a tree is coalesced with a bipartite graph; Guerrero [18] introduced Laplacian energies of vertices; Gutman and Furtula [24] wrote a tutorial on the computation of vertex energies; and vertex energies have been computed for integral graphs [47], double graphs and bipartite double covers [14], regular graph structures [42], and splitting and shadow graphs [31]. In parallel, the Sombor index has generated a large literature on extremal problems and bounds [12, 13, 15, 32, 37, 39, 41, 46] and on its chemical applicabil-

ity [10,45], and a spectral theory of Sombor-type matrices and their energies has emerged [16, 21, 28, 33, 38]. Relations between graph energy and degree-based indices, and between such indices and their own energies, were further studied in [26, 34]; see also [25] for a broad view of degree-based indices beyond the Zagreb indices.

All these results use vertex energy only as an intermediate device. The purpose of the present paper is to put vertex energy into the *definition* of topological indices. Bond-incident-degree (BID) indices have the form $\mathrm{BID}_f(G) = \sum_{uv\in E(G)} f(d_u, d_v)$ for a symmetric function f, and include the Zagreb, Randić, harmonic, sum-connectivity and Sombor indices [20, 22, 49, 54]. Since, by the results recalled above, $\mathcal{E}(v)$ is squeezed between d_v/λ_1 and $\sqrt{d_v}$, it behaves like a spectrally corrected (square root of the) degree. This leads naturally to the following family.

Definition 1. For a symmetric function $f : (0,\infty)^2 \to \mathbb{R}$ and a graph G, the *vertex-energy index* associated with f is

$$\mathrm{VE}_f(G) = \sum_{uv\in E(G)} f\big(\mathcal{E}_G(u), \mathcal{E}_G(v)\big).$$

Well-defined positivity of $\mathcal{E}(u)$ for non-isolated u is proved in Lemma 3. The particular members studied here are listed in Definition 2. Our main results can be summarized as follows.

(1) **Pointwise bounds** (Theorems 2 and 3). For every non-isolated vertex v,

$$\max\left\{\frac{d_v}{\lambda_1}, \sqrt{\frac{d_v}{\Delta}}\right\} \le \frac{d_v^{3/2}}{\sqrt{W_4(v)}} \le \mathcal{E}(v) \le \sqrt{d_v - \frac{W_4(v) - d_v^2}{(\sqrt{d_v} + \lambda_1)^2}} \le \sqrt{d_v},$$

where $W_4(v)$ is the number of closed walks of length four starting at v; the equality cases are completely determined. This yields a general *transfer principle* (Theorem 4) bounding every monotone vertex-energy index by two BID indices.

(2) **Adjacent vertices** (Theorems 5 and 6). For every edge uv, $\mathcal{E}(u)\mathcal{E}(v) \ge (1 + ||A|_{uv}|)^2$. Equality $\mathcal{E}(u)\mathcal{E}(v) = 1$ holds on every edge

of a connected graph if and only if the graph is complete bipartite, and equality $\mathcal{E}(u)\mathcal{E}(v) = (1 + |A|_{uv})^2$ with $|A|_{uv} \geq 0$ holds on every edge if and only if the graph is complete multipartite. A corollary (Corollary 4) sharpens $\mathcal{E}(G) \geq 2R(G)$ and is attained, e.g., by all complete graphs.

(3) **Zagreb-type indices** (Theorems 8 and 9). For instance,

$$\frac{\mathcal{E}(G)^2}{n} \leq \mathrm{EM}_1(G) \leq 2m - \frac{M_1(G) - 2m + 8q}{(\sqrt{\Delta} + \lambda_1)^2},$$

where M_1 is the first Zagreb index and q the number of quadrangles, which improves McClelland's inequality.

(4) **Sombor-type index** (Theorem 10). We prove $\sqrt{2}\,m \leq \mathrm{ESO}(G)$, $\mathrm{SO}(G)/\lambda_1 \leq \mathrm{ESO}(G) \leq \sum_{uv} \sqrt{d_u + d_v}$ and $\frac{\delta}{\sqrt{2}}\mathcal{E}(G) \leq \mathrm{ESO}(G) < \Delta\mathcal{E}(G)$, with all equality cases, and we improve the energy–Sombor inequalities of [50, 51].

(5) **Products, trees and computations** (Theorems 11 and 12). Vertex energy is multiplicative under the tensor (Kronecker) product, which yields product formulas for all multiplicative vertex-energy indices; explicit sharp bounds are given for quadrangle-free graphs and trees. Exhaustive computations on all connected graphs with at most seven vertices and all trees with at most 18 vertices confirm all results and suggest further extremal properties (Section 17).

(6) **Perron-refined bounds** (Theorem 13 and Corollary 9). Removing the Perron atom x_v^2 from the spectral measure of v gives

$$\frac{d_v^{3/2}}{\sqrt{W_4(v)}} \leq \lambda_1 x_v^2 + \frac{\sigma_v^{3/2}}{\sqrt{\tau_v}} \leq \mathcal{E}(v) \leq \lambda_1 x_v^2 + \sqrt{(1 - x_v^2)\sigma_v} \leq \sqrt{d_v},$$

with $\sigma_v = d_v - \lambda_1^2 x_v^2$, $\tau_v = W_4(v) - \lambda_1^4 x_v^2$; the upper bound is strictly below $\sqrt{d_v}$ except at star centres, and its sum over v is a vertex decomposition of the Koolen–Moulton inequality.

(7) **Regular graphs and complements** (Theorems 14 and 15). Explicit

two-sided bounds for r-regular graphs, and the vertex-level Nordhaus–Gaddum inequality $2(n-1)/n \le \mathcal{E}_G(v)+\mathcal{E}_{\overline{G}}(v)$, with equality at every vertex exactly for K_n and $\overline{K_n}$.

(8) **Cartesian products and joins** (Theorems 16 and 18).

$$\max\{\mathcal{E}_G(g), \mathcal{E}_H(h)\} \le \mathcal{E}_{G\Box H}(g,h) \le \mathcal{E}_G(g) + \mathcal{E}_H(h),$$

with an exact formula for prisms $G\Box K_2$ and hypercubes (Corollary 11 and Proposition 17); for regular G, H the join raises all vertex energies by explicit constants $\alpha, \beta > 0$, giving closed forms for wheels, friendship graphs and complete split graphs and exact join formulas for EM_1, EM_2 and ED (Corollaries 13 and 14).

(9) **Irregularity** (Propositions 19 and 20). A vertex-energy irregularity index and the sandwich $\mathrm{ED}/\sqrt{2} \le \mathrm{ESO} \le \mathrm{ED}/\sqrt{2} + (1 - 1/\sqrt{2})\,\mathrm{EIrr}$.

The paper is organized as follows. Section 2 collects the spectral tools. Section 3 introduces the indices and elementary examples. Sections 4 and 5 contain the local theory (pointwise and edge inequalities). Sections 6, 7 and 8 study the individual indices. Section 9 deals with tensor products and Section 10 with quadrangle-free graphs and trees. Sections 11 and 12 contain the Perron-refined bounds and the theory for regular graphs and their complements, Sections 13 and 14 treat Cartesian products and joins, Section 15 deals with irregularity, Section 16 collects further examples, and Section 17 contains explicit values and computational evidence. Section 18 contains concluding remarks.

2 Preliminaries

2.1 Notation

All graphs are finite, simple and undirected. For $v \in V(G)$ we write $N(v)$ for its neighbourhood, $d_v = |N(v)|$ for its degree, and δ, Δ for the minimum and maximum degree. For distinct v, w let $c_{vw} = |N(v) \cap N(w)|$ be the number of common neighbours. A *quadrangle* is a subgraph isomorphic

to C_4; $q = q(G)$ denotes the number of quadrangles and q_v the number of quadrangles containing v. We use the classical degree-based indices

$$M_1(G) = \sum_v d_v^2, \qquad M_2(G) = \sum_{uv \in E} d_u d_v,$$
$$R_\alpha(G) = \sum_{uv \in E} (d_u d_v)^\alpha, \qquad \chi_\alpha(G) = \sum_{uv \in E} (d_u + d_v)^\alpha,$$

so that $R = R_{-1/2}$ is the Randić index [44], R_α the general Randić index [8] and χ_α the general sum-connectivity index [54].

The spectral radius of A is $\lambda_1 = \lambda_1(G)$. Since A is nonnegative, $\lambda_1 \geq |\lambda_j|$ for all j, and the operator norm of A equals λ_1. The tensor (Kronecker) product $G \times H$ has vertex set $V(G) \times V(H)$, with $(g,h) \sim (g',h')$ if and only if $g \sim g'$ in G and $h \sim h'$ in H; its adjacency matrix is $A(G) \otimes A(H)$ [30,52].

2.2 Spectral decomposition and vertex energy

Write $A = U \Lambda U^{\mathsf{T}}$ where $U = (u_{vj})$ is orthogonal, its j-th column u_j is a unit eigenvector for λ_j, and $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. For a real function φ defined on the spectrum, $\varphi(A) = U \varphi(\Lambda) U^{\mathsf{T}}$; in particular $|A| = U|\Lambda|U^{\mathsf{T}}$ is the unique positive semidefinite square root of A^2 and does not depend on the choice of U. We put

$$p_{vj} = u_{vj}^2 \qquad (v \in V(G),\ 1 \leq j \leq n).$$

Lemma 1 ([4]). *The matrix $P = (p_{vj})$ is doubly stochastic, and for every function φ on the spectrum and every vertex v,*

$$\varphi(A)_{vv} = \sum_{j=1}^{n} p_{vj}\, \varphi(\lambda_j).$$

In particular $\mathcal{E}(v) = \sum_j p_{vj} |\lambda_j|$, and $W_k(v) := (A^k)_{vv} = \sum_j p_{vj} \lambda_j^k$ is the number of closed walks of length k starting at v.

Proof. Rows and columns of an orthogonal matrix have unit Euclidean length, hence $\sum_j p_{vj} = \sum_v p_{vj} = 1$. The formula follows from $\varphi(A)_{vv} = \sum_j u_{vj} \varphi(\lambda_j) u_{vj}$. The walk interpretation of $(A^k)_{vv}$ is standard [11]. ∎

Thus $\mu_v = \sum_j p_{vj}\delta_{\lambda_j}$ is a probability measure (the *spectral measure of* v) whose moments are the closed walk counts at v, and $\mathcal{E}(v)$ is its first absolute moment. We shall use the following walk counts.

Lemma 2. *Let v be a vertex of G. Then $W_0(v) = 1$, $W_1(v) = 0$, $W_2(v) = d_v$, and*

$$W_4(v) = d_v^2 + \sum_{w \neq v} c_{vw}^2 = d_v^2 + \sum_{x \in N(v)} (d_x - 1) + 2q_v. \tag{1}$$

Consequently

$$\sum_{v \in V(G)} \big(W_4(v) - d_v^2\big) = M_1(G) - 2m + 8q, \tag{2}$$

and, for every non-isolated vertex v,

$$d_v^2 \leq W_4(v) \leq \min\{\lambda_1^2 d_v,\ \Delta d_v^2\}. \tag{3}$$

Proof. The first three values are immediate. Since A^2 is symmetric, $W_4(v) = (A^2A^2)_{vv} = \sum_w \big((A^2)_{vw}\big)^2$, and $(A^2)_{vv} = d_v$, $(A^2)_{vw} = c_{vw}$ for $w \neq v$; this is the first expression in (1). For the second, write $c_{vw}^2 = c_{vw} + 2\binom{c_{vw}}{2}$. Counting pairs (x, w) with $x \in N(v) \cap N(w)$ and $w \neq v$ gives $\sum_{w \neq v} c_{vw} = \sum_{x \in N(v)} (d_x - 1)$. Every quadrangle $vxwyv$ through v is determined uniquely by the vertex w opposite to v and the unordered pair $\{x, y\} \subseteq N(v) \cap N(w)$, so $\sum_{w \neq v} \binom{c_{vw}}{2} = q_v$. This proves (1).

Summing (1) over v and using $\sum_v \sum_{x \in N(v)} (d_x - 1) = \sum_x d_x(d_x - 1) = M_1 - 2m$ and $\sum_v q_v = 4q$ gives (2).

The lower bound in (3) is obvious from (1). By Lemma 1 and $\lambda_j^2 \leq \lambda_1^2$, $W_4(v) = \sum_j p_{vj}\lambda_j^4 \leq \lambda_1^2 \sum_j p_{vj}\lambda_j^2 = \lambda_1^2 d_v$. Finally, $\sum_{x \in N(v)} (d_x - 1) \leq d_v(\Delta - 1)$ and $2q_v = \sum_{w \neq v} c_{vw}(c_{vw} - 1) \leq (d_v - 1) \sum_{w \neq v} c_{vw} \leq (d_v - 1)d_v(\Delta - 1)$, whence $W_4(v) \leq d_v^2 + d_v(\Delta - 1) + d_v(d_v - 1)(\Delta - 1) = \Delta d_v^2$. ∎

2.3 Positive and negative parts

Define the positive semidefinite matrices

$$A^+ = \sum_{\lambda_j>0} \lambda_j u_j u_j^{\mathsf{T}}, \qquad A^- = -\sum_{\lambda_j<0} \lambda_j u_j u_j^{\mathsf{T}}.$$

Then $A = A^+ - A^-$, $|A| = A^+ + A^-$ and $A^+A^- = 0$.

Lemma 3. *Let G be a graph and $u, v \in V(G)$.*

(a) $\mathcal{E}(v) = 2A^+_{vv} = 2A^-_{vv}$*; equivalently* $|A| = 2A^+ - A = 2A^- + A$*. In particular* $\mathcal{E}(G) = 2\sum_{\lambda_j>0} \lambda_j$*.*

(b) $\sum_{w\in V(G)} |A|^2_{vw} = d_v$ *and* $|A|^2_{uv} \le \mathcal{E}(u)\mathcal{E}(v)$*.*

(c) $\mathcal{E}(v) = 0$ *if and only if v is isolated; otherwise* $\mathcal{E}(v) > 0$*.*

(d) *For all u, v,*

$$\mathcal{E}(u)\mathcal{E}(v) - (|A|_{uv} + A_{uv})^2 = 4\det A^+[u,v] \ge 0,$$
$$\mathcal{E}(u)\mathcal{E}(v) - (|A|_{uv} - A_{uv})^2 = 4\det A^-[u,v] \ge 0,$$

where $M[u,v]$ denotes the 2×2 principal submatrix of M on rows and columns u, v.

Proof. (a) Since $A_{vv} = 0$, we have $A^+_{vv} = A^-_{vv}$, and $|A|_{vv} = A^+_{vv} + A^-_{vv}$. The matrix identities follow from $A = A^+ - A^-$ and $|A| = A^+ + A^-$; taking traces gives the formula for $\mathcal{E}(G)$.

(b) $\sum_w |A|^2_{vw} = (|A|^2)_{vv} = (A^2)_{vv} = d_v$. The second claim holds because every 2×2 principal submatrix of the positive semidefinite matrix $|A|$ has a nonnegative determinant.

(c) If v is isolated, the v-th row of A vanishes, hence so does the v-th row of $|A|$ (which is a polynomial in A without constant term, namely $|A| = \sum_{\lambda_j\neq 0} |\lambda_j| u_j u_j^{\mathsf{T}}$ and $u_{vj} = 0$ whenever $\lambda_j \neq 0$). Conversely, if $\mathcal{E}(v) = |A|_{vv} = 0$, then by (b) $|A|^2_{vw} \le \mathcal{E}(v)\mathcal{E}(w) = 0$ for all w, so the v-th row of $|A|$ vanishes and $d_v = \sum_w |A|^2_{vw} = 0$.

(d) By (a), $A^+ = \frac{1}{2}(|A| + A)$ and $A^- = \frac{1}{2}(|A| - A)$. The 2×2 principal submatrix of A^+ on $\{u, v\}$ is $\frac{1}{2}\begin{pmatrix} \mathcal{E}(u) & |A|_{uv}+A_{uv} \\ |A|_{uv}+A_{uv} & \mathcal{E}(v) \end{pmatrix}$, whose determinant

is $\frac{1}{4}\big(\mathcal{E}(u)\mathcal{E}(v) - (|A|_{uv} + A_{uv})^2\big)$; it is nonnegative since $A^+ \succeq 0$. The same computation applies to A^-. ∎

We shall repeatedly use the following elementary fact on Gram matrices: if $M = YY^{\mathsf{T}}$ is positive semidefinite with rows y_u of Y, then $\det M[u,v] = \|y_u\|^2\|y_v\|^2 - \langle y_u, y_v\rangle^2$ vanishes if and only if y_u and y_v are linearly dependent, in which case also Me_u and Me_v are linearly dependent, since $Me_u = Yy_u$.

2.4 Perron–Frobenius facts and two structural lemmas

Lemma 4 ([9,11])**.** *Let G be connected with $n \geq 2$. Then λ_1 is a simple eigenvalue with an eigenvector x having positive entries; hence $p_{v1} = x_v^2 > 0$ for every v when x is normalized. Moreover $\sqrt{\Delta} \leq \lambda_1 \leq \Delta$, with $\lambda_1 = \Delta$ if and only if G is regular and $\lambda_1 = \sqrt{\Delta}$ if and only if $G \cong K_{1,\Delta}$; and $-\lambda_1$ is an eigenvalue of G if and only if G is bipartite.*

Lemma 5. *Let G be a connected graph with $n \geq 2$ vertices whose spectrum is contained in $\{0, \lambda_1, -\lambda_1\}$. Then $G \cong K_{a,b}$ for some $a, b \geq 1$. Conversely, the spectrum of $K_{a,b}$ is $\{\pm\sqrt{ab}, 0^{(a+b-2)}\}$.*

Proof. If $-\lambda_1$ were not an eigenvalue, then $0 = \operatorname{tr} A = \lambda_1 \cdot \operatorname{mult}(\lambda_1) > 0$, a contradiction. Hence $-\lambda_1$ is an eigenvalue and G is bipartite by Lemma 4; write $A = \left(\begin{smallmatrix} 0 & B \\ B^{\mathsf{T}} & 0 \end{smallmatrix}\right)$ with respect to the bipartition $X \cup Y$. The polynomial $t^3 - \lambda_1^2 t$ vanishes on the spectrum and A is diagonalizable, so $A^3 = \lambda_1^2 A$, that is, $BB^{\mathsf{T}}B = \lambda_1^2 B$. Consequently $(BB^{\mathsf{T}})^2 = \lambda_1^2 BB^{\mathsf{T}}$, and every eigenvalue of BB^{T} belongs to $\{0, \lambda_1^2\}$.

The matrix BB^{T} is nonnegative, and $(BB^{\mathsf{T}})_{xx'} > 0$ if and only if $x, x' \in X$ have a common neighbour. Since G is connected, any two vertices of X are joined by a path whose vertices alternate between X and Y, so BB^{T} is irreducible. By the Perron–Frobenius theorem its spectral radius λ_1^2 is a simple eigenvalue. Hence $\operatorname{rank}(B) = \operatorname{rank}(BB^{\mathsf{T}}) = 1$. A 0/1 matrix of rank one with no zero row has all rows equal to a single 0/1 vector r; since B has no zero column either, r is the all-ones vector. Thus $B = J$ and $G \cong K_{|X|,|Y|}$. The converse is standard. ∎

Lemma 6 ([48]). *A graph without isolated vertices has exactly one positive eigenvalue if and only if it is a complete multipartite graph.*

Lemma 7. *Let G be bipartite with parts X, Y. Then $|A|_{uv} = 0$ whenever $u \in X$, $v \in Y$; in particular $|A|_{uv} = 0$ for every edge uv, and*

$$\sum_{v \in X} \mathcal{E}(v) = \sum_{v \in Y} \mathcal{E}(v) = \tfrac{1}{2}\mathcal{E}(G).$$

Proof. With $A = \left(\begin{smallmatrix} 0 & B \\ B^{\mathsf{T}} & 0 \end{smallmatrix}\right)$ we have $A^2 = BB^{\mathsf{T}} \oplus B^{\mathsf{T}}B$. The positive semidefinite square root of a block-diagonal positive semidefinite matrix is block diagonal, so $|A| = (BB^{\mathsf{T}})^{1/2} \oplus (B^{\mathsf{T}}B)^{1/2}$. Since BB^{T} and $B^{\mathsf{T}}B$ have the same nonzero eigenvalues, their square roots have equal traces. This is also [4, Prop. 3.9]. ■

3 Vertex-energy topological indices

By Lemma 3(c) both endpoints of an edge have positive energy, so Definition 1 makes sense for every symmetric $f : (0, \infty)^2 \to \mathbb{R}$. We shall also use vertex sums of the form $\sum_v g(d_v, \mathcal{E}(v))$.

Definition 2. For a graph G we define the *first vertex-energy Zagreb index*, the *energy-degree index*, the *second vertex-energy Zagreb index*, the *general vertex-energy Randić index* ($\alpha \in \mathbb{R}$), the *vertex-energy Randić index* and the *vertex-energy Sombor index*, respectively, by

$$\begin{aligned}
\mathrm{EM}_1(G) &= \sum_{v \in V(G)} \mathcal{E}(v)^2, \\
\mathrm{ED}(G) &= \sum_{v \in V(G)} d_v \mathcal{E}(v) = \sum_{uv \in E(G)} \big(\mathcal{E}(u) + \mathcal{E}(v)\big), \\
\mathrm{EM}_2(G) &= \sum_{uv \in E(G)} \mathcal{E}(u)\mathcal{E}(v), \\
\mathrm{ER}_\alpha(G) &= \sum_{uv \in E(G)} \big(\mathcal{E}(u)\mathcal{E}(v)\big)^\alpha,
\end{aligned}$$

$$\mathrm{ER}(G) = \mathrm{ER}_{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\mathcal{E}(u)\mathcal{E}(v)}},$$
$$\mathrm{ESO}(G) = \sum_{uv \in E(G)} \sqrt{\mathcal{E}(u)^2 + \mathcal{E}(v)^2}.$$

The names reflect the degree-based prototypes $M_1 = \sum_v d_v^2 = \sum_{uv}(d_u + d_v)$, M_2, R_α, R and SO. Note that ED is the edge form of the first Zagreb index with degrees replaced by energies, while EM_1 is its vertex form with d_v replaced by $\mathcal{E}(v)$; unlike the degree case, these two indices differ. The graph energy itself belongs to the same circle of ideas: as observed in [1, 50], for a graph without isolated vertices

$$\mathcal{E}(G) = \sum_{uv \in E(G)} \Big(\frac{\mathcal{E}(u)}{d_u} + \frac{\mathcal{E}(v)}{d_v} \Big), \tag{4}$$

because every vertex v occurs in exactly d_v edges.

Proposition 1. *Let* I *be any of the indices of Definition 2 or, more generally, any* VE_f.

(a) I *is a graph invariant, and* $\mathrm{I}(G_1 \cup G_2) = \mathrm{I}(G_1) + \mathrm{I}(G_2)$ *for disjoint unions.*

(b) *If all vertices of a connected graph* G *have the same energy* $\varepsilon_0 = \mathcal{E}(G)/n$ *(for example if* G *is vertex-transitive or, more generally, walk-regular), then*

$$\mathrm{VE}_f(G) = m\, f(\varepsilon_0, \varepsilon_0), \qquad \mathrm{EM}_1(G) = \frac{\mathcal{E}(G)^2}{n},$$
$$\mathrm{EM}_2(G) = \frac{m\,\mathcal{E}(G)^2}{n^2}, \quad \mathrm{ER}(G) = \frac{mn}{\mathcal{E}(G)}, \quad \mathrm{ESO}(G) = \frac{\sqrt{2}\,m\,\mathcal{E}(G)}{n}.$$

Proof. (a) An isomorphism $\sigma : G \to H$ corresponds to a permutation matrix Q with $A(H) = QA(G)Q^{\mathsf{T}}$; then $|A(H)| = Q|A(G)|Q^{\mathsf{T}}$, so $\mathcal{E}_H(\sigma v) = \mathcal{E}_G(v)$. For a disjoint union, $A(G_1 \cup G_2) = A(G_1) \oplus A(G_2)$ and $|A(G_1) \oplus A(G_2)| = |A(G_1)| \oplus |A(G_2)|$, so vertex energies are computed componentwise and the sums split.

(b) The first assertion is immediate. A graph is walk-regular if $W_k(v)$ does not depend on v for every k [17]; then all spectral measures μ_v have the same moments, hence coincide (they are supported on the finite spectrum), and so all $\mathcal{E}(v)$ coincide. Vertex-transitive graphs are walk-regular. ∎

Example 1. K_n has spectrum $\{n-1, (-1)^{(n-1)}\}$, so with $P = \frac{1}{n}J$ we get $A = (n-1)P - (I-P)$ and $|A| = (n-1)P + (I-P) = I + \frac{n-2}{n}J$. Hence

$$\mathcal{E}(v) = \frac{2(n-1)}{n}, \qquad |A|_{uv} = \frac{n-2}{n} \ (u \neq v),$$

and

$$\mathrm{EM}_1(K_n) = \frac{4(n-1)^2}{n}, \qquad \mathrm{EM}_2(K_n) = \frac{2(n-1)^3}{n},$$
$$\mathrm{ER}(K_n) = \frac{n^2}{4}, \qquad \mathrm{ESO}(K_n) = \sqrt{2}\,(n-1)^2.$$

Example 2. Let $G = K_{a,b}$ with parts X, $|X| = a$, and Y, $|Y| = b$. By [4, (5.6)], $\mathcal{E}(v) = \sqrt{b/a}$ for $v \in X$ and $\mathcal{E}(v) = \sqrt{a/b}$ for $v \in Y$ (this also follows from Proposition 7 below). Hence $\mathcal{E}(u)\mathcal{E}(v) = 1$ on every edge and

$$\mathrm{EM}_1(K_{a,b}) = a + b, \qquad \mathrm{ED}(K_{a,b}) = ab\Big(\sqrt{\tfrac{b}{a}} + \sqrt{\tfrac{a}{b}}\Big) = \sqrt{ab}\,(a+b),$$

$$\mathrm{EM}_2(K_{a,b}) = \mathrm{ER}(K_{a,b}) = ab, \qquad \mathrm{ESO}(K_{a,b}) = \sqrt{ab\,(a^2+b^2)}.$$

For the star $K_{1,k}$ this gives $\mathcal{E}(\text{centre}) = \sqrt{k}$, $\mathcal{E}(\text{leaf}) = 1/\sqrt{k}$ and $\mathrm{ESO}(K_{1,k}) = \sqrt{k^3 + k}$.

Example 3. Cycles are vertex-transitive, and $\mathcal{E}(C_n)$ equals $4\cot(\pi/n)$, $4\csc(\pi/n)$ or $2\csc(\pi/2n)$ according as $n \equiv 0 \pmod 4$, $n \equiv 2 \pmod 4$ or n is odd [36]. By Proposition 1(b), $\mathcal{E}(v) = \mathcal{E}(C_n)/n \to 4/\pi$ and

$$\mathrm{EM}_1(C_n) = \mathrm{EM}_2(C_n) = \frac{\mathcal{E}(C_n)^2}{n},$$
$$\mathrm{ER}(C_n) = \frac{n^2}{\mathcal{E}(C_n)}, \qquad \mathrm{ESO}(C_n) = \sqrt{2}\,\mathcal{E}(C_n).$$

4 Pointwise bounds for vertex energy

In this section we establish two-sided bounds for $\mathcal{E}(v)$ in terms of local walk counts and λ_1. They are the engine of all later estimates.

Theorem 2. *Let G be a graph with spectral radius λ_1 and maximum degree Δ, and let v be a non-isolated vertex. Then*

$$\mathcal{E}(v) \;\geq\; \frac{d_v^{3/2}}{\sqrt{W_4(v)}} \;\geq\; \max\Big\{\frac{d_v}{\lambda_1},\; \sqrt{\frac{d_v}{\Delta}}\Big\}. \tag{5}$$

Assume moreover that G is connected. Then the following are equivalent:

(i) $\mathcal{E}(v) = d_v^{3/2}/\sqrt{W_4(v)}$;

(ii) *every eigenvalue λ_j with $p_{vj} > 0$ belongs to $\{0, \lambda_1, -\lambda_1\}$;*

(iii) $\mathcal{E}(v) = d_v/\lambda_1$;

(iv) $A^3 e_v = \lambda_1^2 A e_v$, *i.e., for every vertex w the number of v–w walks of length three equals $\lambda_1^2 A_{vw}$.*

Finally, equality $\mathcal{E}(v) = d_v/\lambda_1$ holds for every *vertex of a connected graph G with $n \geq 2$ if and only if $G \cong K_{a,b}$ for some $a, b \geq 1$.*

Proof. The Hölder bound. Write $p_j = p_{vj}$. By Lemmas 1 and 2,

$$d_v = \sum_j p_j \lambda_j^2 = \sum_j \big(p_j^{2/3}|\lambda_j|^{2/3}\big)\big(p_j^{1/3}|\lambda_j|^{4/3}\big).$$

Apply Hölder's inequality with the conjugate exponents $r = 3/2$ and $s = 3$ to the vectors $a_j = p_j^{2/3}|\lambda_j|^{2/3}$ and $b_j = p_j^{1/3}|\lambda_j|^{4/3}$:

$$\begin{aligned} d_v &\leq \Big(\sum_j a_j^{3/2}\Big)^{2/3}\Big(\sum_j b_j^3\Big)^{1/3} \\ &= \Big(\sum_j p_j|\lambda_j|\Big)^{2/3}\Big(\sum_j p_j\lambda_j^4\Big)^{1/3} = \mathcal{E}(v)^{2/3} W_4(v)^{1/3}. \end{aligned}$$

Cubing gives $d_v^3 \leq \mathcal{E}(v)^2 W_4(v)$. As $d_v \geq 1$, $W_4(v) \geq d_v^2 > 0$ and we obtain the first inequality in (5).

Comparison with the other bounds. By (3), $W_4(v) \le \lambda_1^2 d_v$ and $W_4(v) \le \Delta d_v^2$. Therefore

$$\frac{d_v^{3/2}}{\sqrt{W_4(v)}} \ge \frac{d_v^{3/2}}{\lambda_1\sqrt{d_v}} = \frac{d_v}{\lambda_1} \qquad \text{and} \qquad \frac{d_v^{3/2}}{\sqrt{W_4(v)}} \ge \frac{d_v^{3/2}}{d_v\sqrt{\Delta}} = \sqrt{\frac{d_v}{\Delta}}.$$

Equality. Let G be connected, so $p_{v1} > 0$ by Lemma 4.

(i)⇒(ii). Equality in Hölder's inequality for the nonzero vectors a, b forces $a^{3/2}$ and b^3 to be proportional: there are $\alpha, \beta > 0$ with $\alpha p_j|\lambda_j| = \beta p_j \lambda_j^4$ for all j. Hence $|\lambda_j|^3 = \alpha/\beta$ for every j with $p_j > 0$ and $\lambda_j \neq 0$. Taking $j = 1$ shows that this common value is λ_1^3, which is (ii).

(ii)⇒(iii) and (ii)⇒(i). If (ii) holds, set $s = \sum_{j:\,\lambda_j \neq 0} p_j$. Then $\mathcal{E}(v) = \lambda_1 s$, $d_v = \lambda_1^2 s$ and $W_4(v) = \lambda_1^4 s$, so $\mathcal{E}(v) = d_v/\lambda_1 = d_v^{3/2}/\sqrt{W_4(v)}$.

(iii)⇒(ii). For $t \in [-\lambda_1, \lambda_1]$ we have $|t| - t^2/\lambda_1 = |t|(\lambda_1 - |t|)/\lambda_1 \ge 0$, with equality if and only if $t \in \{0, \pm\lambda_1\}$. Hence

$$\mathcal{E}(v) - \frac{d_v}{\lambda_1} = \sum_j p_j\Big(|\lambda_j| - \frac{\lambda_j^2}{\lambda_1}\Big) \ge 0,$$

and equality forces $\lambda_j \in \{0, \pm\lambda_1\}$ whenever $p_j > 0$.

(ii)⇔(iv). Let $\pi(t) = t^3 - \lambda_1^2 t$. Then $\|\pi(A)e_v\|^2 = (\pi(A)^2)_{vv} = \sum_j p_j \pi(\lambda_j)^2$, which vanishes if and only if $\pi(\lambda_j) = 0$ whenever $p_j > 0$, i.e., if and only if (ii) holds. The walk interpretation of $\pi(A)e_v = 0$ is clear.

Global equality. Suppose $\mathcal{E}(v) = d_v/\lambda_1$ for every vertex. Given an eigenvalue λ_j, the j-th column of the doubly stochastic matrix P sums to 1, so $p_{vj} > 0$ for some vertex v; applying (iii)⇒(ii) at that vertex shows $\lambda_j \in \{0, \pm\lambda_1\}$. Thus the spectrum of G is contained in $\{0, \pm\lambda_1\}$, and $G \cong K_{a,b}$ by Lemma 5. Conversely, for $K_{a,b}$ the spectrum is $\{\pm\sqrt{ab}, 0\}$, so (ii) holds at every vertex. ∎

Remark. Theorem 2 unifies and sharpens the two lower bounds $\mathcal{E}(v) \ge d_v/\Delta$ and $\mathcal{E}(v) \ge \sqrt{d_v/\Delta}$ of [4, Thms. 3.3, 3.6]. Since $\lambda_1 \le \Delta$, the bound d_v/λ_1 is better than d_v/Δ; moreover its equality class is the whole family $\{K_{a,b}\}$ rather than only the regular members $K_{d,d}$. The walk-count bound $d_v^{3/2} W_4(v)^{-1/2}$ is purely combinatorial by (1) and dominates both.

Corollary 1. For every graph G with m edges,

$$\mathcal{E}(G) \geq \sum_v d_v^{3/2} W_4(v)^{-1/2} \geq 2m/\lambda_1.$$

If G is connected with $n \geq 2$, then $\mathcal{E}(G) = 2m/\lambda_1$ if and only if G is complete bipartite.

Proof. Sum (5) over the non-isolated vertices and use $\sum_v d_v = 2m$; the equality case is the last part of Theorem 2. ∎

We now turn to upper bounds. The inequality $\mathcal{E}(v) \leq \sqrt{d_v}$ of [4] is an immediate consequence of the Cauchy–Schwarz inequality $\left(\sum_j p_j|\lambda_j|\right)^2 \leq \sum_j p_j\lambda_j^2$. The following theorem quantifies the defect $d_v - \mathcal{E}(v)^2$ in terms of the common neighbours of v, and gives an independent proof of the equality case.

Theorem 3. *Let G be a graph with spectral radius λ_1 and let v be a vertex with $d_v \geq 1$. Then*

$$\left(d_v - \mathcal{E}(v)^2\right)\left(\mathcal{E}(v) + \lambda_1\right)^2 \;\geq\; W_4(v) - d_v^2 \;=\; \sum_{w \neq v} c_{vw}^2, \tag{6}$$

and consequently

$$\mathcal{E}(v) \;\leq\; \sqrt{d_v - \frac{W_4(v) - d_v^2}{(\sqrt{d_v} + \lambda_1)^2}} \;\leq\; \sqrt{d_v}. \tag{7}$$

Moreover, $\mathcal{E}(v) = \sqrt{d_v}$ if and only if every neighbour of v is a pendant vertex, i.e., the component of v is the star K_{1,d_v} with centre v (for $d_v = 1$ this means that the component is K_2).

Proof. Put $B = |A|$ and $b = Be_v$ (the v-th column of B). Then $b_v = \mathcal{E}(v)$ and $\|b\|^2 = (B^2)_{vv} = (A^2)_{vv} = d_v$. Decompose $b = \mathcal{E}(v)e_v + b'$ with $b' \perp e_v$; then

$$\|b'\|^2 = d_v - \mathcal{E}(v)^2 =: o_v \;\geq 0,$$

the "off-diagonal energy mass" of v. Since $B^2 = A^2$,

$$A^2 e_v = B^2 e_v = Bb = \mathcal{E}(v)\, b + Bb' = \mathcal{E}(v)^2 e_v + \mathcal{E}(v)\, b' + Bb'.$$

Let $\Pi = I - e_v e_v^{\mathsf{T}}$ be the orthogonal projection onto $e_v^{\perp}$. Applying Π and using $\Pi b' = b'$,

$$\Pi A^2 e_v = \mathcal{E}(v)\, b' + \Pi B b'.$$

The left-hand side is the vector $\big((A^2)_{wv}\big)_{w\neq v} = (c_{vw})_{w\neq v}$ padded by a zero, so by (1) its squared norm is $\sum_{w\neq v} c_{vw}^2 = W_4(v) - d_v^2$. On the right-hand side, $\|\Pi B b'\| \le \|B\|\,\|b'\| = \lambda_1\sqrt{o_v}$, because the operator norm of $B = |A|$ equals $\max_j |\lambda_j| = \lambda_1$. The triangle inequality therefore gives

$$\sqrt{W_4(v) - d_v^2} \le \mathcal{E}(v)\sqrt{o_v} + \lambda_1\sqrt{o_v} = (\mathcal{E}(v) + \lambda_1)\sqrt{o_v},$$

which is (6). Since $\mathcal{E}(v) \le \sqrt{d_v}$ (Cauchy–Schwarz, as recalled above), we have $(\mathcal{E}(v)+\lambda_1)^2 \le (\sqrt{d_v}+\lambda_1)^2$, and (6) yields $o_v \ge (W_4(v) - d_v^2)/(\sqrt{d_v}+\lambda_1)^2$, i.e. (7). The last inequality in (7) is (3).

Equality. If some neighbour x of v has a neighbour $w \neq v$, then $c_{vw} \ge 1$, so $W_4(v) - d_v^2 \ge 1$ and (7) gives $\mathcal{E}(v) < \sqrt{d_v}$. Otherwise all neighbours of v are pendant, the component of v is K_{1,d_v} centred at v, and $\mathcal{E}(v) = \sqrt{d_v}$ by Example 2. ∎

Remark. The implicit inequality (6) carries more information than (7), since in (7) the unknown $\mathcal{E}(v)$ in the factor $(\mathcal{E}(v)+\lambda_1)^2$ has been replaced by its trivial upper bound $\sqrt{d_v}$. Note also that (7) is a genuinely *local* refinement: the correction term only involves the numbers c_{vw} of common neighbours of v and other vertices, together with the global quantity λ_1 (which may be replaced by Δ).

For pendant vertices the walk counts are explicit and we obtain a sharp two-sided estimate.

Corollary 2. Let v be a pendant vertex of a graph G and let x be its neighbour. Then

$$\frac{1}{\sqrt{d_x}} \;\le\; \mathcal{E}(v) \;\le\; \sqrt{1 - \frac{d_x - 1}{(1+\lambda_1)^2}}.$$

The left inequality is an equality if and only if the component of v is the star K_{1,d_x}; the right one is an equality if and only if the component of v is K_2.

Proof. A pendant vertex lies on no quadrangle and $N(v) = \{x\}$, so $W_4(v) = 1 + (d_x - 1) = d_x$ by (1). The two inequalities are Theorems 2 and 3 with $d_v = 1$. Let C be the component of v (all quantities are unchanged if G is replaced by C, see Proposition 1(a)). If equality holds on the left, Theorem 2 (i)⇒(iii) applied to C gives $1/\sqrt{d_x} = \mathcal{E}(v) = 1/\lambda_1(C)$, so $\lambda_1(C) = \sqrt{d_x} \le \sqrt{\Delta(C)} \le \lambda_1(C)$; hence $\lambda_1(C) = \sqrt{\Delta(C)}$ and $C \cong K_{1,\Delta(C)}$ by Lemma 4. Conversely, for a leaf of $K_{1,k}$ both sides equal $1/\sqrt{k}$. On the right: if $d_x = 1$, the component of v is K_2 and both sides equal 1. If $d_x \ge 2$, then x has a neighbour $w \ne v$, so v is not the centre of a star component and $\mathcal{E}(v) < 1 = \sqrt{d_v}$ by Theorem 3; hence $(\mathcal{E}(v) + \lambda_1)^2 < (1 + \lambda_1)^2$, and (6) with $W_4(v) - d_v^2 = d_x - 1 > 0$ gives $1 - \mathcal{E}(v)^2 = o_v > (d_x - 1)/(1 + \lambda_1)^2$, a strict inequality. ∎

The pointwise bounds transfer to every monotone vertex-energy index.

Theorem 4. *Let $f : (0, \infty)^2 \to \mathbb{R}$ be symmetric and nondecreasing in each variable, and let G be a graph with $m \ge 1$ edges. Put $h_v = d_v^{3/2} W_4(v)^{-1/2}$ for non-isolated v. Then*

$$\sum_{uv \in E} f\Big(\frac{d_u}{\lambda_1}, \frac{d_v}{\lambda_1}\Big) \;\le\; \sum_{uv \in E} f(h_u, h_v) \;\le\; \mathrm{VE}_f(G) \;\le\; \sum_{uv \in E} f\big(\sqrt{d_u}, \sqrt{d_v}\big). \tag{8}$$

If f is nonincreasing in each variable, all inequalities are reversed. If f is strictly monotone in each variable and G is connected, then equality holds in the first or in the second inequality if and only if $G \cong K_{a,b}$, and in the third inequality if and only if $G \cong K_2$. In particular, if f is moreover homogeneous of degree k, the leftmost term equals $\lambda_1^{-k}\mathrm{BID}_f(G)$.

Proof. The chain $d_u/\lambda_1 \le h_u \le \mathcal{E}(u) \le \sqrt{d_u}$ from Theorems 2 and 3 holds at both endpoints of every edge; monotonicity of f gives (8) termwise, and the reversed version for nonincreasing f.

Let f be strictly monotone and G connected. Equality in the second inequality of (8) holds if and only if $f(h_u, h_v) = f(\mathcal{E}(u), \mathcal{E}(v))$ for every edge; as $h_u \le \mathcal{E}(u)$, $h_v \le \mathcal{E}(v)$ and f is strictly monotone in each variable, this means $h_u = \mathcal{E}(u)$ for every vertex (every vertex lies on an edge), i.e., by Theorem 2, $\mathcal{E}(u) = d_u/\lambda_1$ for all u, i.e., $G \cong K_{a,b}$. Equality in the first

inequality similarly means $h_u = d_u/\lambda_1$, i.e., $W_4(u) = \lambda_1^2 d_u$, for all u; by the proof of Theorem 2 this is again condition (ii) at every vertex, hence $G \cong K_{a,b}$. Equality in the third inequality means $\mathcal{E}(u) = \sqrt{d_u}$ for all u, i.e., every vertex is the centre of the star G; a star $K_{1,k}$ with $k \geq 2$ has non-central vertices, so $G \cong K_2$. Conversely, $K_{a,b}$ and K_2 give equality by Theorems 2 and 3. The last statement is obvious. ∎

Corollary 3. For every graph G and every $\alpha > 0$,

$$\lambda_1^{-2\alpha} R_\alpha(G) \leq \mathrm{ER}_\alpha(G) \leq R_{\alpha/2}(G),$$

and for $\alpha < 0$ both inequalities are reversed. For connected G and $\alpha \neq 0$, equality on the λ_1-side holds if and only if G is complete bipartite, and on the other side if and only if $G \cong K_2$.

Proof. Apply Theorem 4 to $f(x, y) = (xy)^\alpha$, which is homogeneous of degree 2α and strictly increasing (decreasing) in each variable for $\alpha > 0$ ($\alpha < 0$); note $f(\sqrt{d_u}, \sqrt{d_v}) = (d_u d_v)^{\alpha/2}$. ∎

5 Energies of adjacent vertices

The following theorem strengthens the inequality $\mathcal{E}(u)\mathcal{E}(v) \geq 1$ of G. Arizmendi and O. Arizmendi [1, Thm. 3] and describes the extremal edges.

Theorem 5. *Let uv be an edge of a graph G and put $t = |A|_{uv}$. Then:*

(a) $\mathcal{E}(u)\mathcal{E}(v) - (1+t)^2 = 4 \det A^+[u, v] \geq 0$ *and* $\mathcal{E}(u)\mathcal{E}(v) - (1-t)^2 = 4 \det A^-[u, v] \geq 0$*; consequently*

$$\sqrt{\mathcal{E}(u)\mathcal{E}(v)} \;\geq\; 1 + ||A|_{uv}| \;\geq\; 1, \qquad \mathcal{E}(u) + \mathcal{E}(v) \geq 2\big(1 + ||A|_{uv}|\big). \tag{9}$$

(b) $\mathcal{E}(u)\mathcal{E}(v) = 1$ *if and only if*

$$|A| e_u = \mathcal{E}(u)\, A e_v. \tag{10}$$

In this case $|A|_{uv} = 0$, $\mathcal{E}(u)^2 = d_u/d_v$, and the u-th column of $|A|$ is supported exactly on $N(v)$, where all its entries are equal to $\mathcal{E}(u)$.

(c) *Let G be connected with $n \geq 2$. Then $\mathcal{E}(u)\mathcal{E}(v) = 1$ for every edge uv if and only if G is complete bipartite.*

Proof. (a) Since $A_{uv} = 1$, the two identities are Lemma 3(d). Both determinants are nonnegative, so $\mathcal{E}(u)\mathcal{E}(v) \geq \max\{(1+t)^2, (1-t)^2\} = (1+|t|)^2$. The second inequality in (9) is the AM–GM inequality.

(b) Suppose $\mathcal{E}(u)\mathcal{E}(v) = 1$. By (a), $(1 + |t|)^2 \leq 1$, so $t = 0$, and both $\det A^+[u, v]$ and $\det A^-[u, v]$ vanish. Write $A^+ = Y_+ Y_+^{\mathsf{T}}$ (e.g. $Y_+ = (A^+)^{1/2}$) with rows y_u, y_v. The vanishing of the Gram determinant means that y_u and y_v are linearly dependent; since $\|y_v\|^2 = A^+_{vv} = \mathcal{E}(v)/2 > 0$, we can write $y_u = cy_v$, and then $A^+e_u = Y_+y_u = cA^+e_v$. Comparing the u-th coordinates, $\mathcal{E}(u)/2 = A^+_{uu} = cA^+_{uv} = c(t + 1)/2 = c/2$, so $c = \mathcal{E}(u)$ and $A^+e_u = \mathcal{E}(u)A^+e_v$. In exactly the same way, $A^-e_u = c'A^-e_v$ and the u-th coordinate gives $\mathcal{E}(u)/2 = c'A^-_{uv} = c'(t - 1)/2 = -c'/2$, so $A^-e_u = -\mathcal{E}(u)A^-e_v$. Adding, $|A|e_u = (A^+ + A^-)e_u = \mathcal{E}(u)(A^+ - A^-)e_v = \mathcal{E}(u)Ae_v$.

Conversely, assume (10). Let Π_+ be the orthogonal projection onto the sum of the eigenspaces of A with positive eigenvalues. Then $\Pi_+|A| = A^+ = \Pi_+A$, so applying Π_+ to (10) gives $A^+e_u = \mathcal{E}(u)A^+e_v$. Reading this identity in the coordinates u and v:

$$\tfrac{1}{2}\mathcal{E}(u) = A^+_{uu} = \mathcal{E}(u)A^+_{uv} = \tfrac{1}{2}\mathcal{E}(u)(1 + t),$$
$$\tfrac{1}{2}(1 + t) = A^+_{vu} = \mathcal{E}(u)A^+_{vv} = \tfrac{1}{2}\mathcal{E}(u)\mathcal{E}(v).$$

As $\mathcal{E}(u) > 0$, the first identity gives $t = 0$ and then the second gives $\mathcal{E}(u)\mathcal{E}(v) = 1$.

Finally, under (10) the u-th column of $|A|$ equals $\mathcal{E}(u)$ times the indicator vector of $N(v)$; taking squared norms and using Lemma 3(b), $d_u = \||A|e_u\|^2 = \mathcal{E}(u)^2 d_v$.

(c) If $G = K_{a,b}$, then $\mathcal{E}(u)\mathcal{E}(v) = \sqrt{b/a}\sqrt{a/b} = 1$ on every edge (Example 2). Conversely, assume $\mathcal{E}(u)\mathcal{E}(v) = 1$ on every edge. By (b), for every edge ij the support of $|A|e_i$ is $N(j)$. Consequently, *any two vertices j, j' having a common neighbour i satisfy* $N(j) = N(j')$, both being equal to the support of $|A|e_i$.

Fix an edge uv and put $X = N(v) \ni u$ and $Y = N(u) \ni v$. Every

$x \in X$ has the common neighbour v with u, hence $N(x) = N(u) = Y$; every $y \in Y$ has the common neighbour u with v, hence $N(y) = N(v) = X$. Thus the set $X \cup Y$ is closed under taking neighbours, and connectivity gives $V(G) = X \cup Y$. If $z \in X \cap Y$, then $N(z) = Y$ and $N(z) = X$, so $z \in Y = N(z)$, which is impossible in a simple graph. Therefore $X \cap Y = \emptyset$, every vertex of X is adjacent to every vertex of Y, and there are no edges inside X or inside Y. Hence $G \cong K_{|X|,|Y|}$. ■

Remark. Part (b) shows that, locally, an edge with $\mathcal{E}(u)\mathcal{E}(v) = 1$ "looks complete bipartite": the energies are $\mathcal{E}(u) = \sqrt{d_u/d_v}$ and $\mathcal{E}(v) = \sqrt{d_v/d_u}$, exactly as in K_{d_v,d_u}. By Lemma 7, $|A|_{uv} = 0$ on every edge of a bipartite graph, so for bipartite graphs (9) reduces to the inequality of [1]; the improvement is relevant for non-bipartite graphs.

We next identify the graphs for which the first identity in Theorem 5(a) is an equality on all edges. Recall that a complete multipartite graph $K_{n_1,\dots,n_k}$ ($k \geq 2$) is the complement of a disjoint union of cliques.

Theorem 6. *Let G be a connected graph with $n \geq 2$ vertices and Perron vector x (positive, $\|x\| = 1$). The following statements are equivalent.*

(i) *G is a complete multipartite graph.*

(ii) *G has exactly one positive eigenvalue.*

(iii) $|A| = 2\lambda_1 xx^{\mathsf{T}} - A$.

(iv) *For every edge uv of G, $|A|_{uv} \geq 0$ and $\mathcal{E}(u)\mathcal{E}(v) = (1 + |A|_{uv})^2$.*

If these conditions hold, then $\mathcal{E}(v) = 2\lambda_1 x_v^2$ for every vertex v, $\mathcal{E}(G) = 2\lambda_1$, and $|A|_{uv} = 2\lambda_1 x_u x_v - 1$ for every edge uv.

Proof. (i)⇔(ii) is Smith's theorem (Lemma 6).

(ii)⇒(iii). If λ_1 is the only positive eigenvalue, then $A^+ = \lambda_1 xx^{\mathsf{T}}$, and $|A| = 2A^+ - A$ by Lemma 3(a).

(iii)⇒(iv). By (iii), $\mathcal{E}(v) = |A|_{vv} = 2\lambda_1 x_v^2$ and, for an edge uv, $t := |A|_{uv} = 2\lambda_1 x_u x_v - 1$. Hence

$$\mathcal{E}(u)\mathcal{E}(v) = 4\lambda_1^2 x_u^2 x_v^2 = (1 + t)^2.$$

On the other hand $\mathcal{E}(u)\mathcal{E}(v) \geq (1+|t|)^2$ by Theorem 5(a). Therefore $(1+t)^2 \geq (1+|t|)^2$; since $1+t = 2\lambda_1 x_u x_v > 0$, this gives $1+t \geq 1+|t|$, i.e. $t \geq 0$.

(iv)⇒(ii). Write $A^+ = YY^{\mathsf{T}}$ and let y_w denote the rows of Y. For an edge uv with $t = |A|_{uv} \geq 0$ and $\mathcal{E}(u)\mathcal{E}(v) = (1+t)^2$ we have $\det A^+[u,v] = 0$ by Lemma 3(d), so y_u and y_v are linearly dependent. Both are nonzero because $\|y_w\|^2 = A^+_{ww} = \mathcal{E}(w)/2 > 0$, hence $y_u = c_{uv} y_v$ with $c_{uv} \neq 0$ (in fact $c_{uv} > 0$, since $\langle y_u, y_v \rangle = A^+_{uv} = (1+t)/2 > 0$). Fix a vertex w_0. As G is connected, following a path from w_0 to any vertex w we obtain $y_w = c_w y_{w_0}$ for some scalar c_w. Hence Y has rank at most one, and so has $A^+ = YY^{\mathsf{T}}$. Since $A^+ \neq 0$ (because $\operatorname{tr} A^+ = \mathcal{E}(G)/2 > 0$), $\operatorname{rank} A^+ = 1$, i.e., A has exactly one positive eigenvalue.

The final assertions were obtained in the proof of (iii)⇒(iv), together with $\mathcal{E}(G) = \operatorname{tr}|A| = 2\lambda_1 \|x\|^2 - \operatorname{tr} A = 2\lambda_1$. ∎

Remark. The sign condition $|A|_{uv} \geq 0$ in (iv) cannot be dropped. For the triangular prism $C_3 \,\square\, K_2$ (spectrum $\{3, 1, 0^{(2)}, (-2)^{(2)}\}$, two positive eigenvalues) all vertex energies equal $4/3$, $||A|_{uv}| = 1/3$ on every edge, and so $\mathcal{E}(u)\mathcal{E}(v) = (1+||A|_{uv}|)^2$ on every edge; however $|A|_{uv} = -1/3$ on the three edges of the perfect matching between the two triangles. An exhaustive search over the 995 connected graphs on $2 \leq n \leq 7$ vertices shows that the prism is the *only* one among them that is not complete multipartite but satisfies $\mathcal{E}(u)\mathcal{E}(v) = (1+||A|_{uv}|)^2$ on all edges.

Theorem 6 yields explicit vertex energies for all complete multipartite graphs.

Proposition 7. *Let $G = K_{n_1,\ldots,n_k}$ with $k \geq 2$ and $n = n_1 + \cdots + n_k$. Then λ_1 is the unique positive root of*

$$\sum_{i=1}^{k} \frac{n_i}{\lambda + n_i} = 1,$$

and for every vertex v in the i-th part

$$\mathcal{E}(v) = \frac{2\lambda_1}{(\lambda_1 + n_i)^2 \sum_{j=1}^{k} \frac{n_j}{(\lambda_1 + n_j)^2}}.$$

In particular, for the regular complete multipartite graph $K_{r,\dots,r}$ with k parts, $\mathcal{E}(v) = 2(k-1)/k$ for all v.

Proof. By symmetry the Perron vector is constant on each part, say $x_v = \xi_i$ for v in part i. The eigenvalue equation at such v reads $\lambda_1 \xi_i = s - n_i \xi_i$, where $s = \sum_j n_j \xi_j > 0$. Hence $\xi_i = s/(\lambda_1 + n_i)$, and substituting into the definition of s gives $\sum_j n_j/(\lambda_1 + n_j) = 1$. The function $\lambda \mapsto \sum_j n_j/(\lambda + n_j)$ decreases strictly on $[0, \infty)$ from $k \geq 2$ to 0, so this equation has a unique positive root. The normalisation $\sum_j n_j \xi_j^2 = 1$ gives $s^2 = \big(\sum_j n_j (\lambda_1 + n_j)^{-2}\big)^{-1}$, and $\mathcal{E}(v) = 2\lambda_1 \xi_i^2$ by Theorem 6. For $n_1 = \cdots = n_k = r$ the root is $\lambda_1 = (k-1)r$ and the formula gives $2(k-1)r \cdot \frac{1}{kr} = \frac{2(k-1)}{k}$. ∎

Example 4. For $K_{a,b}$, $\lambda_1 = \sqrt{ab}$ and Proposition 7 gives $\mathcal{E}(v) = \sqrt{b/a}$ on the part of size a, recovering Example 2. For $K_{1,1,2} = K_4 - e$ we get $\lambda_1 = (1 + \sqrt{17})/2$, $\mathcal{E}(G) = 1 + \sqrt{17} \approx 5.1231$, and the vertex energies are approximately 1.5914 (the two vertices of degree 3) and 0.9701 (the two vertices of degree 2). Note that $\mathcal{E}(v) < 1$ for a vertex of degree 2 in this non-bipartite graph.

As a consequence of Theorem 5 we obtain a refinement of the energy–Randić inequality $\mathcal{E}(G) \geq 2R(G)$ of [1].

Corollary 4. For every graph G,

$$\mathcal{E}(G) \;\geq\; 2 \sum_{uv \in E(G)} \frac{1 + ||A|_{uv}|}{\sqrt{d_u d_v}} \;\geq\; 2R(G). \tag{11}$$

Equality holds in the first inequality if and only if $\mathcal{E}(u)/d_u = \mathcal{E}(v)/d_v$ and $\mathcal{E}(u)\mathcal{E}(v) = (1 + ||A|_{uv}|)^2$ for every edge uv. It holds, for instance, for all complete bipartite graphs, all regular complete multipartite graphs $K_{r,\dots,r}$ (including all complete graphs K_n) and the prism $C_3 \square K_2$. The second inequality is strict as soon as some edge has $|A|_{uv} \neq 0$.

Proof. Discarding isolated vertices, by (4), the AM–GM inequality and (9),

$$\mathcal{E}(G) = \sum_{uv \in E} \Big(\frac{\mathcal{E}(u)}{d_u} + \frac{\mathcal{E}(v)}{d_v} \Big) \geq 2 \sum_{uv \in E} \sqrt{\frac{\mathcal{E}(u)\mathcal{E}(v)}{d_u d_v}} \geq 2 \sum_{uv \in E} \frac{1 + ||A|_{uv}|}{\sqrt{d_u d_v}}.$$

Equality requires equality in AM–GM and in (9) on every edge, and conversely. For $K_{a,b}$ both conditions hold because $\mathcal{E}(u)/d_u = 1/\sqrt{ab}$ for all u and $\mathcal{E}(u)\mathcal{E}(v) = 1$, $|A|_{uv} = 0$. For a regular graph with constant vertex energy the first condition is automatic; $K_{r,\dots,r}$ satisfies the second by Theorem 6 and the prism by the preceding remark. ∎

Remark. For the complete graph, $2R(K_n) = n$ whereas $\mathcal{E}(K_n) = 2n - 2$; (11) is exact: $2\binom{n}{2}\frac{1+(n-2)/n}{n-1} = 2n - 2$. Thus the refinement closes the gap between $\mathcal{E}(G)$ and $2R(G)$ completely for complete graphs, and it is strictly stronger than $\mathcal{E}(G) \geq 2R(G)$ for many non-bipartite graphs (see Table 3).

6 The first vertex-energy Zagreb index

Theorem 8. *Let G be a graph with n vertices, $n_0 \geq 1$ non-isolated vertices, m edges, q quadrangles, maximum degree Δ and spectral radius λ_1. Then:*

(a) $\mathrm{EM}_1(G) = 2m - \sum_{u \neq w} |A|_{uw}^2$.

(b) $\dfrac{M_1(G)}{\lambda_1^2} \leq \sum_{d_v > 0} \dfrac{d_v^3}{W_4(v)} \leq \mathrm{EM}_1(G) \leq 2m - \dfrac{M_1(G) - 2m + 8q}{(\sqrt{\Delta} + \lambda_1)^2} \leq 2m$.

(c) $\dfrac{\mathcal{E}(G)^2}{n_0} \leq \mathrm{EM}_1(G)$.

Moreover, for connected G with $n \geq 2$: each of the first two inequalities in (b) is an equality if and only if $G \cong K_{a,b}$; each of the last two inequalities in (b) is an equality if and only if $G \cong K_2$; and equality in (c) holds if and only if all vertices of G have the same energy.

Proof. (a) By Lemma 3(b), $\sum_w |A|_{vw}^2 = d_v$ for each v. Summing over v gives $\sum_{v,w} |A|_{vw}^2 = 2m$, and the diagonal part of this double sum is $\sum_v |A|_{vv}^2 = \mathrm{EM}_1(G)$.

(b) Squaring the chain of Theorem 2 and summing over non-isolated vertices gives the first two inequalities (note $d_v^2/\lambda_1^2 \leq d_v^3/W_4(v)$ is (3)).

For the third, square (7), use $\sqrt{d_v} \le \sqrt{\Delta}$, and sum:

$$\begin{aligned}\mathrm{EM}_1(G) &\le \sum_{d_v>0} \Big(d_v - \frac{W_4(v) - d_v^2}{(\sqrt{d_v} + \lambda_1)^2} \Big) \le 2m - \frac{\sum_v (W_4(v) - d_v^2)}{(\sqrt{\Delta} + \lambda_1)^2} \\ &= 2m - \frac{M_1 - 2m + 8q}{(\sqrt{\Delta} + \lambda_1)^2},\end{aligned}$$

where (2) was used (isolated vertices contribute zero to that sum). The last inequality holds because $M_1 - 2m = \sum_v d_v(d_v - 1) \ge 0$.

(c) By the Cauchy–Schwarz inequality over the n_0 non-isolated vertices, $\mathcal{E}(G)^2 = \big(\sum_{d_v>0} \mathcal{E}(v)\big)^2 \le n_0 \sum_{d_v>0} \mathcal{E}(v)^2 = n_0 \mathrm{EM}_1(G)$.

Equality cases. Let G be connected, $n \ge 2$, so $n_0 = n$. Equality in the second inequality of (b) holds if and only if $\mathcal{E}(v) = h_v$ for all v, and in the first if and only if $W_4(v) = \lambda_1^2 d_v$ for all v; by Theorem 2 and its proof, both mean that condition (ii) of Theorem 2 holds at every vertex, i.e. $G \cong K_{a,b}$. For the last inequality of (b): $M_1 - 2m + 8q = 0$ forces $d_v \le 1$ for all v, so the connected graph G is K_2; conversely K_2 gives equality everywhere. If equality holds in the third inequality of (b), then in particular $\mathcal{E}(v)^2 = d_v - (W_4(v) - d_v^2)/(\sqrt{d_v} + \lambda_1)^2$ for every v and $\sqrt{d_v} = \sqrt{\Delta}$ whenever $W_4(v) > d_v^2$. Suppose $G \ncong K_2$; since G is connected with $n \ge 3$, it has a vertex v with a neighbour of degree at least 2, so $W_4(v) > d_v^2$ and, as in the proof of Corollary 2, $\mathcal{E}(v) < \sqrt{d_v}$; then $(\mathcal{E}(v) + \lambda_1)^2 < (\sqrt{d_v} + \lambda_1)^2$ and (6) gives a strict inequality in (7) at v, a contradiction. Hence $G \cong K_2$. Finally, equality in the Cauchy–Schwarz inequality of (c) holds if and only if all $\mathcal{E}(v)$ are equal. ■

Corollary 5. For every graph G with n_0 non-isolated vertices,

$$\mathcal{E}(G) \;\le\; \sqrt{n_0\, \mathrm{EM}_1(G)} \;\le\; \sqrt{n_0 \Big(2m - \frac{M_1(G) - 2m + 8q}{(\sqrt{\Delta} + \lambda_1)^2} \Big)} \;\le\; \sqrt{2mn}.$$

For a connected graph G with $n \ge 3$ the second and third inequalities are strict.

Proof. Combine (b) and (c) of Theorem 8, and use $n_0 \le n$; strictness follows from the equality cases of Theorem 8(b). ■

Remark. Part (a) of Theorem 8 has a transparent meaning: $2m = \|A\|_F^2 = \||A|\|_F^2$ is the total "energy mass", of which $\mathrm{EM}_1(G)$ is the part carried by the diagonal of $|A|$. In particular $\mathrm{EM}_1(G) = 2m$ if and only if $|A|$ is diagonal, if and only if $A^2 = |A|^2$ is diagonal, i.e., if and only if no two distinct vertices have a common neighbour; for graphs without isolated vertices this means that G is a perfect matching mK_2.

7 The second vertex-energy Zagreb index and the vertex-energy Randić index

Theorem 9. *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then:*

(a) $$\mathrm{EM}_2(G) \;\geq\; \sum_{uv\in E} \max\Big\{(1+||A|_{uv}|)^2,\; \frac{d_u d_v}{\lambda_1^2}\Big\} \;\geq\; \max\Big\{m,\; \frac{M_2(G)}{\lambda_1^2}\Big\};$$

(b) $$\mathrm{EM}_2(G) \;\leq\; \min\Big\{R_{1/2}(G),\; \tfrac{1}{2}\sum_v d_v \mathcal{E}(v)^2\Big\}$$
$$\leq\; \min\Big\{\tfrac{1}{2}M_1(G),\; \tfrac{\Delta}{2}\mathrm{EM}_1(G)\Big\};$$

(c) $$R_{-1/4}(G) \;\leq\; \mathrm{ER}(G) \;\leq\; \min\Big\{\sum_{uv\in E} \frac{1}{1+||A|_{uv}|},\; \lambda_1 R(G)\Big\} \;\leq\; m;$$

(d) $$\mathrm{ER}(G) \;\geq\; \frac{m^{3/2}}{\sqrt{\mathrm{EM}_2(G)}}.$$

Moreover: $\mathrm{EM}_2(G) = m \iff \mathrm{EM}_2(G) = M_2(G)/\lambda_1^2 \iff \mathrm{ER}(G) = m \iff \mathrm{ER}(G) = \lambda_1 R(G) \iff$ *G is complete bipartite;* $\mathrm{EM}_2(G) = R_{1/2}(G) \iff \mathrm{ER}(G) = R_{-1/4}(G) \iff G \cong K_2$*; and equality holds in (d) if and only if $\mathcal{E}(u)\mathcal{E}(v)$ is the same for all edges uv.*

Proof. (a) For every edge, $\mathcal{E}(u)\mathcal{E}(v) \geq (1 + ||A|_{uv}|)^2 \geq 1$ by Theorem 5, and $\mathcal{E}(u)\mathcal{E}(v) \geq d_u d_v/\lambda_1^2$ by Theorem 2. Summing the larger of the two bounds over the edges gives the first inequality; the second follows from $\sum_{uv} \max\{a_{uv}, b_{uv}\} \geq \max\{\sum a_{uv}, \sum b_{uv}\}$.

(b) By Theorem 3, $\mathcal{E}(u)\mathcal{E}(v) \leq \sqrt{d_u d_v}$, whence $\mathrm{EM}_2 \leq R_{1/2}$; and $\sqrt{d_u d_v} \leq (d_u + d_v)/2$ gives $R_{1/2} \leq \frac{1}{2}\sum_{uv}(d_u + d_v) = \frac{1}{2}M_1$. Also

$\mathcal{E}(u)\mathcal{E}(v) \le \frac{1}{2}(\mathcal{E}(u)^2 + \mathcal{E}(v)^2)$, and summing over edges, each vertex v occurs d_v times: $\mathrm{EM}_2 \le \frac{1}{2}\sum_v d_v \mathcal{E}(v)^2 \le \frac{\Delta}{2}\mathrm{EM}_1$.

(c) The lower bound is Corollary 3 with $\alpha = -1/2$. For the upper bounds, $1/\sqrt{\mathcal{E}(u)\mathcal{E}(v)} \le 1/(1 + ||A|_{uv}|) \le 1$ by Theorem 5, and $1/\sqrt{\mathcal{E}(u)\mathcal{E}(v)} \le \lambda_1/\sqrt{d_u d_v}$ by Theorem 2.

(d) Put $s_{uv} = \sqrt{\mathcal{E}(u)\mathcal{E}(v)} > 0$. By the power-mean inequality and the arithmetic–harmonic mean inequality,

$$\sqrt{\frac{\mathrm{EM}_2(G)}{m}} = \Big(\frac{1}{m}\sum_{uv} s_{uv}^2\Big)^{1/2} \ge \frac{1}{m}\sum_{uv} s_{uv} \ge \frac{m}{\sum_{uv} s_{uv}^{-1}} = \frac{m}{\mathrm{ER}(G)},$$

which rearranges to (d); equality holds throughout if and only if all s_{uv} are equal.

Equality cases. $\mathrm{EM}_2(G) = m$ holds if and only if $\mathcal{E}(u)\mathcal{E}(v) = 1$ on every edge, i.e., by Theorem 5(c), if and only if G is complete bipartite; the same condition characterizes $\mathrm{ER}(G) = m$. By Corollary 3 (with $\alpha = 1$ and $\alpha = -1/2$), $\mathrm{EM}_2(G) = M_2/\lambda_1^2$ and $\mathrm{ER}(G) = \lambda_1 R(G)$ both characterize $K_{a,b}$, and $\mathrm{EM}_2(G) = R_{1/2}(G)$ and $\mathrm{ER}(G) = R_{-1/4}(G)$ both characterize K_2. Conversely, for $K_{a,b}$ all these quantities equal ab, and for K_2 they equal 1. ∎

Remark. For $K_{a,b}$ the two lower bounds in Theorem 9(a) coincide: $m = ab = M_2/\lambda_1^2$, and for every regular graph $M_2/\lambda_1^2 = m$. For non-regular graphs neither of them dominates the other: for P_4 we have $M_2/\lambda_1^2 = 8/\varphi^2 \approx 3.056 > 3 = m$ (φ the golden ratio), whereas for the graph obtained from K_4 by attaching a pendant path of length three, $M_2/\lambda_1^2 \approx 0.892\,m$. The edgewise maximum in (a) is in general strictly larger than both.

8 The vertex-energy Sombor index

We now study ESO, the vertex-energy analogue of the Sombor index, and compare it with the results of [50, 51].

Theorem 10. *Let G be a connected graph with $n \ge 2$ vertices, m edges, minimum degree δ, maximum degree Δ and spectral radius λ_1. Then:*

(a) $\sqrt{2}\,m \;\le\; \sqrt{2}\sum_{uv\in E}\big(1+||A|_{uv}|\big) \;\le\; \mathrm{ESO}(G)$, *and* $\mathrm{ESO}(G)=\sqrt{2}\,m$ *if and only if* $G\cong K_{a,a}$ *for some* $a\ge 1$*;*

(b) $\dfrac{\mathrm{SO}(G)}{\lambda_1} \;\le\; \mathrm{ESO}(G) \;\le\; \chi_{1/2}(G)=\sum_{uv\in E}\sqrt{d_u+d_v} \;\le\; \mathrm{SO}(G)$, *where the first inequality is an equality if and only if* G *is complete bipartite, and each of the other two is an equality if and only if* $G\cong K_2$*;*

(c) $\dfrac{\delta}{\sqrt{2}}\,\mathcal{E}(G) \;\le\; \dfrac{1}{\sqrt{2}}\mathrm{ED}(G) \;\le\; \mathrm{ESO}(G) \;<\; \mathrm{ED}(G) \;\le\; \Delta\,\mathcal{E}(G)$. *Here the first and the last inequalities are equalities if and only if* G *is regular, and the second one if and only if all vertices of* G *have the same energy. Consequently* $\mathrm{ESO}(G)=\frac{\delta}{\sqrt{2}}\mathcal{E}(G)$ *if and only if* G *is regular and all its vertex energies coincide (e.g.* G *walk-regular).*

Proof. (a) For an edge uv, $\sqrt{\mathcal{E}(u)^2+\mathcal{E}(v)^2} \ge \sqrt{2\mathcal{E}(u)\mathcal{E}(v)} \ge \sqrt{2}\,(1+||A|_{uv}|) \ge \sqrt{2}$ by Theorem 5. Summation gives the two inequalities. If $\mathrm{ESO}(G)=\sqrt{2}m$, then on every edge $\mathcal{E}(u)=\mathcal{E}(v)$ and $\mathcal{E}(u)\mathcal{E}(v)=1$. By Theorem 5(c), $G\cong K_{a,b}$, and then $\sqrt{b/a}=\sqrt{a/b}$ forces $a=b$. Conversely, all vertex energies of $K_{a,a}$ equal 1.

(b) The function $f(x,y)=\sqrt{x^2+y^2}$ is symmetric, homogeneous of degree one and strictly increasing in each variable on $(0,\infty)^2$, and $f(\sqrt{d_u},\sqrt{d_v})=\sqrt{d_u+d_v}$. Hence the first two inequalities and their equality cases are Theorem 4. The third follows from $d\le d^2$ for positive integers d, with equality for an edge uv if and only if $d_u=d_v=1$, which for a connected graph means $G\cong K_2$.

(c) Since $\mathcal{E}(v)>0$ for all v, $\mathrm{ED}(G)=\sum_v d_v\mathcal{E}(v)$ satisfies $\delta\mathcal{E}(G)\le \mathrm{ED}(G)\le \Delta\mathcal{E}(G)$, and each of these is an equality if and only if d_v is constant, i.e. G is regular. For every edge, the quadratic-mean inequality gives $\sqrt{\mathcal{E}(u)^2+\mathcal{E}(v)^2}\ge\frac{1}{\sqrt{2}}(\mathcal{E}(u)+\mathcal{E}(v))$ with equality if and only if $\mathcal{E}(u)=\mathcal{E}(v)$, while $\sqrt{x^2+y^2}<x+y$ for $x,y>0$. Summing over the edges and using $\mathrm{ED}(G)=\sum_{uv\in E}(\mathcal{E}(u)+\mathcal{E}(v))$ gives the middle inequalities. Equality in the second inequality means $\mathcal{E}(u)=\mathcal{E}(v)$ for all edges, which for a connected graph means that all vertex energies coincide. The final statement combines the equality cases of the first two inequalities, and walk-regular graphs have constant vertex energy by Proposition 1(b). ■

Corollary 6. Let G be a connected graph with $n \geq 2$ vertices.

(i) If $\delta \geq 2$, then

$$\mathcal{E}(G) \;\leq\; \frac{\sqrt{2}}{\delta}\,\mathrm{ESO}(G) \;\leq\; \frac{1}{\sqrt{2}}\mathrm{ESO}(G) \;\leq\; \frac{1}{\sqrt{2}}\chi_{1/2}(G) \;<\; \frac{1}{\sqrt{2}}\mathrm{SO}(G),$$

and $\mathcal{E}(G) = \mathrm{ESO}(G)/\sqrt{2}$ if and only if G is a cycle.

(ii) $\mathrm{SO}(G) \;\leq\; \dfrac{\lambda_1\Delta}{\sqrt{2}}\,\mathcal{E}(G) \;\leq\; \dfrac{\Delta^2}{\sqrt{2}}\,\mathcal{E}(G)$. The first inequality is an equality if and only if $G \cong K_{a,a}$, and the second one if and only if G is regular.

(iii) If G is r-regular, then $\frac{r}{\sqrt{2}}\mathcal{E}(G) \leq \mathrm{ESO}(G) < r\mathcal{E}(G)$ and $\mathrm{ESO}(G) \leq \sqrt{2r}\,m$.

Proof. (i) By Theorem 10(c), $\mathrm{ESO}(G) \geq \frac{\delta}{\sqrt{2}}\mathcal{E}(G)$, i.e. $\mathcal{E}(G) \leq \frac{\sqrt{2}}{\delta}\mathrm{ESO}(G)$, and $\frac{\sqrt{2}}{\delta} \leq \frac{1}{\sqrt{2}}$ for $\delta \geq 2$. The remaining inequalities are Theorem 10(b) ($G \ncong K_2$ since $\delta \geq 2$). If $\mathcal{E}(G) = \mathrm{ESO}(G)/\sqrt{2}$, then $\delta = 2$ and, by Theorem 10(c), G is 2-regular, i.e. a cycle; conversely cycles are vertex-transitive, so equality holds.

(ii) We have $\mathrm{SO}(G) = \sum_{uv}\sqrt{d_u^2 + d_v^2} \leq \sqrt{2}\,\Delta m$, with equality if and only if G is regular, and $\mathcal{E}(G) \geq 2m/\lambda_1$ by Corollary 1, with equality if and only if G is complete bipartite. Therefore $\mathrm{SO}(G) \leq \sqrt{2}\Delta \cdot \frac{\lambda_1}{2}\mathcal{E}(G) = \frac{\lambda_1\Delta}{\sqrt{2}}\mathcal{E}(G)$, with equality if and only if G is a regular complete bipartite graph $K_{a,a}$. The second inequality is $\lambda_1 \leq \Delta$, with equality exactly for regular graphs (Lemma 4).

(iii) The first claim is Theorem 10(c) with $\delta = \Delta = r$; the second is Theorem 10(b), as $\chi_{1/2}(G) = \sqrt{2r}\,m$. ∎

Remark. Corollary 6(i) improves the inequality $\mathcal{E}(G) \leq \mathrm{SO}(G)$ for $\delta \geq 2$ of [50, Thm. 3.4] by the factor $\sqrt{2}$ and passes through the much smaller quantity $\chi_{1/2}(G)$; for graphs with large minimum degree it gives $\mathcal{E}(G) = O(\mathrm{SO}(G)/\delta)$. Corollary 6(ii) improves $\mathrm{SO}(G) \leq \frac{\Delta^2}{\sqrt{2}}\mathcal{E}(G)$ of [51, Thm. 4.1] (which in turn improved $\mathrm{SO}(G) \leq \Delta^3\mathcal{E}(G)$ of [50]), strictly for every non-regular connected graph. Note also that for regular graphs the upper constant $\Delta/\sqrt{2}$ is *not* valid for $\mathrm{ESO}(G)/\mathcal{E}(G)$ in general: for an r-regular

graph $\mathrm{ESO}(G) \geq \frac{r}{\sqrt{2}}\mathcal{E}(G)$, with strict inequality whenever the vertex energies are not all equal (such 4-regular graphs on 7 vertices exist, cf. [4, Ex. 5.1]).

9 Tensor products

We show that vertex energy is multiplicative with respect to the tensor product. This yields product formulas for all indices built from multiplicative functions and a simple way to construct graphs with prescribed extremal behaviour.

Theorem 11. *Let G and H be graphs. For all $g \in V(G)$ and $h \in V(H)$,*

$$\mathcal{E}_{G\times H}\big((g,h)\big) = \mathcal{E}_G(g)\,\mathcal{E}_H(h). \tag{12}$$

Consequently:

(a) $\mathcal{E}(G \times H) = \mathcal{E}(G)\mathcal{E}(H)$, $\mathrm{EM}_1(G \times H) = \mathrm{EM}_1(G)\mathrm{EM}_1(H)$ *and* $\mathrm{ED}(G \times H) = \mathrm{ED}(G)\mathrm{ED}(H)$*;*

(b) *if $f : (0,\infty)^2 \to \mathbb{R}$ is symmetric and multiplicative in the sense that $f(xy, x'y') = f(x,x')f(y,y')$ for all positive x, x', y, y', then*

$$\mathrm{VE}_f(G \times H) = 2\,\mathrm{VE}_f(G)\,\mathrm{VE}_f(H);$$

in particular $\mathrm{EM}_2(G \times H) = 2\mathrm{EM}_2(G)\mathrm{EM}_2(H)$ and $\mathrm{ER}_\alpha(G \times H) = 2\mathrm{ER}_\alpha(G)\mathrm{ER}_\alpha(H)$ for every $\alpha \in \mathbb{R}$;

(c) *if G and H have at least one edge each, then*

$$\frac{1}{\sqrt{2}}\mathrm{ED}(G)\mathrm{ED}(H) \;\leq\; \mathrm{ESO}(G \times H) \;<\; 2\,\mathrm{ESO}(G)\,\mathrm{ESO}(H).$$

Proof. Let $A = A(G) = U\Lambda U^{\mathsf{T}}$ and $B = A(H) = VMV^{\mathsf{T}}$ be spectral decompositions. With the lexicographic ordering of $V(G) \times V(H)$, $A(G \times H) = A \otimes B$ [52]. By the mixed-product rule,

$$A \otimes B = (U \otimes V)(\Lambda \otimes M)(U \otimes V)^{\mathsf{T}},$$

where $U \otimes V$ is orthogonal and $\Lambda \otimes M$ is diagonal with entries $\lambda_i \mu_k$. Hence

$$\begin{aligned} |A \otimes B| &= (U \otimes V)\, |\Lambda \otimes M|\, (U \otimes V)^{\mathsf{T}} \\ &= (U \otimes V)(|\Lambda| \otimes |M|)(U \otimes V)^{\mathsf{T}} = |A| \otimes |B|, \end{aligned}$$

because $|\lambda_i \mu_k| = |\lambda_i|\,|\mu_k|$. The diagonal entry of $|A| \otimes |B|$ at $((g,h),(g,h))$ equals $|A|_{gg} |B|_{hh}$, which is (12).

(a) Summing (12), its square, and (12) multiplied by $d_{(g,h)} = d_g d_h$ over all (g,h) gives the three identities.

(b) The map $\big((g,g'),(h,h')\big) \mapsto \big((g,h),(g',h')\big)$ is a bijection between pairs consisting of an ordered adjacent pair of G and an ordered adjacent pair of H, and ordered adjacent pairs of $G \times H$. For symmetric f, the sum of f over ordered adjacent pairs is twice the sum over edges. Therefore, using (12) and multiplicativity,

$$\begin{aligned} 2\mathrm{VE}_f(G \times H) &= \sum_{(g,g')} \sum_{(h,h')} f\big(\mathcal{E}(g)\mathcal{E}(h), \mathcal{E}(g')\mathcal{E}(h')\big) \\ &= \Big(\sum_{(g,g')} f(\mathcal{E}(g), \mathcal{E}(g'))\Big)\Big(\sum_{(h,h')} f(\mathcal{E}(h), \mathcal{E}(h'))\Big), \end{aligned}$$

which equals $4\mathrm{VE}_f(G)\mathrm{VE}_f(H)$. The functions $f(x,y) = xy$ and $f(x,y) = (xy)^{\alpha}$ are multiplicative.

(c) The lower bound is Theorem 10(c) (whose second inequality does not need connectivity) applied to $G \times H$, together with (a). For the upper bound, for positive a, c, b, e we have

$$a^2 b^2 + c^2 e^2 < (a^2 + c^2)(b^2 + e^2),$$

the difference being $a^2 e^2 + c^2 b^2 > 0$. Applying this with $a = \mathcal{E}(g)$, $c = \mathcal{E}(g')$, $b = \mathcal{E}(h)$, $e = \mathcal{E}(h')$ and summing over ordered adjacent pairs as in (b),

$$\begin{aligned} 2\mathrm{ESO}(G \times H) &< \Big(\sum_{(g,g')} \sqrt{\mathcal{E}(g)^2 + \mathcal{E}(g')^2}\Big)\Big(\sum_{(h,h')} \sqrt{\mathcal{E}(h)^2 + \mathcal{E}(h')^2}\Big) \\ &= 4\mathrm{ESO}(G)\mathrm{ESO}(H). \end{aligned}$$

■

Corollary 7. Let $G^{(2)} = G \times K_2$ be the bipartite double cover of G. Then $\mathcal{E}_{G^{(2)}}((g,i)) = \mathcal{E}_G(g)$ for $i = 1, 2$, and

$$\mathcal{E}(G^{(2)}) = 2\mathcal{E}(G), \qquad \mathrm{EM}_1(G^{(2)}) = 2\mathrm{EM}_1(G),$$
$$\mathrm{EM}_2(G^{(2)}) = 2\mathrm{EM}_2(G), \qquad \mathrm{ER}(G^{(2)}) = 2\mathrm{ER}(G),$$
$$\mathrm{ESO}(G^{(2)}) = 2\mathrm{ESO}(G).$$

Proof. Both vertices of K_2 have energy 1, so (12) gives the vertex energies. Each edge gg' of G gives rise to the two edges $(g,1)(g',2)$ and $(g,2)(g',1)$ of $G^{(2)}$, whose endpoints have energies $\mathcal{E}(g)$ and $\mathcal{E}(g')$; hence every edge-additive vertex-energy index doubles. ■

The invariance of vertex energies under the bipartite double cover, and its extension to double graphs, has been studied independently by Dede and Popat [14]; Theorem 11 shows that it is a special case of the multiplicativity of vertex energy under arbitrary tensor products.

Example 5. (1) The crown graph $K_n \times K_2$ ($K_{n,n}$ minus a perfect matching) has all vertex energies equal to $2(n-1)/n$. For $n = 3$ it is C_6, and indeed $\mathcal{E}(C_6)/6 = 4/3$. (2) $K_{a,b} \times K_{c,d} \cong K_{ac,bd} \cup K_{ad,bc}$. By (12) a vertex in the part of size ac has energy $\sqrt{b/a}\sqrt{d/c} = \sqrt{bd/(ac)}$, in accordance with Example 2; $\mathcal{E}(u)\mathcal{E}(v) = 1$ on all edges, as predicted by Theorem 5(c) applied to each component. (3) The Desargues graph (the bipartite double cover of the Petersen graph) has all vertex energies equal to 1.6, because the Petersen graph has spectrum $\{3, 1^{(5)}, (-2)^{(4)}\}$, energy 16 and is vertex-transitive. (4) For the k-fold tensor power $G^{\times k}$, $\mathrm{EM}_1(G^{\times k}) = \mathrm{EM}_1(G)^k$ and $\mathrm{EM}_2(G^{\times k}) = 2^{k-1}\mathrm{EM}_2(G)^k$.

Remark. Recall [52] that $G \times H$ is connected if and only if G and H are connected and at least one of them is non-bipartite. Thus Theorem 11 produces connected graphs whose vertex-energy indices are completely determined by those of the factors.

10 Quadrangle-free graphs and trees

For graphs without quadrangles the walk count $W_4(v)$ depends only on the degrees in the closed neighbourhood of v, and the bounds of Section 4 become explicit degree-based expressions. For a vertex v let

$$S_v = \sum_{x \in N(v)} d_x$$

be the sum of the degrees of its neighbours.

Theorem 12. *Let G be a graph without quadrangles, and let v be a vertex with $d_v \geq 1$. Then*

$$\frac{d_v^{3/2}}{\sqrt{d_v^2 - d_v + S_v}} \;\leq\; \mathcal{E}(v) \;\leq\; \sqrt{d_v - \frac{S_v - d_v}{(\sqrt{d_v} + \lambda_1)^2}}. \tag{13}$$

Consequently, writing $\Phi(G) = \sum_{d_v > 0} d_v^{3/2}(d_v^2 - d_v + S_v)^{-1/2}$ and $\Psi(G) = \sum_{d_v > 0} \bigl(d_v - \frac{S_v - d_v}{(\sqrt{d_v} + \lambda_1)^2}\bigr)^{1/2}$:

(a) $\Phi(G) \leq \mathcal{E}(G) \leq \Psi(G)$;

(b) $\displaystyle\sum_{d_v > 0} \frac{d_v^3}{d_v^2 - d_v + S_v} \leq \mathrm{EM}_1(G) \leq 2m - \frac{M_1(G) - 2m}{(\sqrt{\Delta} + \lambda_1)^2}$;

(c) *if G is bipartite with parts X and Y, then with $\Phi_X = \sum_{v \in X} d_v^{3/2}(d_v^2 - d_v + S_v)^{-1/2}$ and similarly Φ_Y, Ψ_X, Ψ_Y,*

$$2\max\{\Phi_X, \Phi_Y\} \;\leq\; \mathcal{E}(G) \;\leq\; 2\min\{\Psi_X, \Psi_Y\}.$$

If G is connected with $n \geq 2$, then $\mathcal{E}(G) = \Phi(G)$ if and only if G is a star $K_{1,n-1}$, and $\mathcal{E}(G) = \Psi(G)$ if and only if $G \cong K_2$.

Proof. Without quadrangles $q_v = 0$, and (1) reads $W_4(v) = d_v^2 + \sum_{x \in N(v)}(d_x - 1) = d_v^2 - d_v + S_v$. Hence (13) is the combination of Theorem 2 and Theorem 3, and (a) follows by summation. Part (b) is Theorem 8(b) with $q = 0$ together with the squared, summed left inequality of (13). For (c), $\mathcal{E}(G) = 2\sum_{v \in X} \mathcal{E}(v) = 2\sum_{v \in Y} \mathcal{E}(v)$ by Lemma 7; apply (13) to the vertices of X and of Y separately.

Let G be connected. If $\mathcal{E}(G) = \Phi(G)$, then $\mathcal{E}(v) = d_v^{3/2} W_4(v)^{-1/2}$ for all v, and by Theorem 2 $G \cong K_{a,b}$. Since $K_{a,b}$ contains a quadrangle whenever $a, b \geq 2$, we get $\min\{a,b\} = 1$, i.e. G is a star. Conversely, for $K_{1,k}$: the centre has $d = k$, $S = k$ and the bound equals $k^{3/2}/k = \sqrt{k}$; a leaf has $d = 1$, $S = k$ and the bound equals $1/\sqrt{k}$; these are the exact energies (Example 2). If $\mathcal{E}(G) = \Psi(G)$, then equality holds in the right inequality of (13) at every vertex; as in the proof of Theorem 8, a vertex having a neighbour of degree at least two gives a strict inequality, so all degrees are 1 and $G \cong K_2$. ∎

Corollary 8. Let T be a tree with $n \geq 2$ vertices. Then $\Phi(T) \leq \mathcal{E}(T) \leq \Psi(T)$, with equality on the left if and only if T is a star. Moreover

$$\mathrm{EM}_2(T) \;\geq\; n-1 \qquad \text{and} \qquad \mathrm{ER}(T) \;\leq\; n-1,$$

and each of these is an equality if and only if $T \cong K_{1,n-1}$.

Proof. Trees have no cycles, so Theorem 12 applies. By Theorem 9, $\mathrm{EM}_2(T) \geq m = n-1$ and $\mathrm{ER}(T) \leq m$, with equality if and only if T is complete bipartite, i.e. a star. ∎

Example 6. For the path P_n ($n \geq 5$) the two end vertices have $(d,S) = (1,2)$, their neighbours have $(d,S) = (2,3)$, and the remaining $n-4$ vertices have $(d,S) = (2,4)$. Theorem 12 gives

$$\mathcal{E}(P_n) \;\geq\; \Phi(P_n) = \sqrt{2} + 4\sqrt{\tfrac{2}{5}} + \frac{2}{\sqrt{3}}(n-4) \approx 1.1547\,n - 0.675.$$

Since $\mathcal{E}(P_n) \sim \frac{4}{\pi} n \approx 1.2732\,n$ [36], the bound captures more than 90% of the energy asymptotically; by comparison, $2R(P_n) = n - 3 + 2\sqrt{2}$ and $2m/\lambda_1 = (n-1)/\cos\frac{\pi}{n+1} \sim n$. For $n = 5$: $\Phi(P_5) \approx 5.099$, $2R(P_5) \approx 4.828$, while $\mathcal{E}(P_5) = 2 + 2\sqrt{3} \approx 5.464$.

11 A Perron-refined two-sided bound and a vertex Koolen–Moulton inequality

The bounds of Section 4 treat the spectral measure μ_v as a whole. For a connected graph the atom of μ_v at λ_1 is explicitly known, namely $p_{v1} = x_v^2$, where x is the unit Perron vector, and removing it before applying Hölder's and Cauchy's inequalities gives strictly better estimates. Summed over the vertices, the upper estimate becomes a vertex decomposition of the inequality behind the Koolen–Moulton bound [35].

Throughout this section G is connected with $n \geq 2$ vertices and x denotes the unit Perron vector of A (Lemma 4). For $v \in V(G)$ put

$$\rho_v = 1 - x_v^2, \qquad \sigma_v = d_v - \lambda_1^2 x_v^2, \qquad \tau_v = W_4(v) - \lambda_1^4 x_v^2.$$

Lemma 8. *Let $\mu_v^\circ = \sum_{j \geq 2} p_{vj} \delta_{\lambda_j}$ be the spectral measure of v with the Perron atom removed. Then ρ_v, σ_v and τ_v are the moments of order 0, 2 and 4 of μ_v°, and $\mathcal{E}(v) - \lambda_1 x_v^2$ is its first absolute moment. In particular $\rho_v, \sigma_v, \tau_v \geq 0$, $\sigma_v \leq \lambda_1^2 \rho_v$, $\sigma_v^2 \leq \rho_v \tau_v$, and $\tau_v = 0$ implies $\sigma_v = 0$. Moreover*

$$\sum_v \rho_v = n - 1, \qquad \sum_v \sigma_v = 2m - \lambda_1^2.$$

Proof. By Lemma 4 the eigenvalue λ_1 is simple, so we may take $u_1 = x$; then $p_{v1} = x_v^2$ and all assertions about moments follow from Lemma 1 with $\varphi(t) = 1, t^2, t^4, |t|$. The inequality $\sigma_v \leq \lambda_1^2 \rho_v$ holds because $\lambda_j^2 \leq \lambda_1^2$, and $\sigma_v^2 \leq \rho_v \tau_v$ is the Cauchy–Schwarz inequality for μ_v°; the latter shows that $\tau_v = 0$ forces $\sigma_v = 0$. Finally $\sum_v x_v^2 = 1$ and $\sum_v d_v = 2m$. ∎

Theorem 13. *Let G be a connected graph with $n \geq 2$ vertices and let $v \in V(G)$. Put*

$$L_v = \lambda_1 x_v^2 + \frac{\sigma_v^{3/2}}{\tau_v^{1/2}}, \qquad U_v = \lambda_1 x_v^2 + \sqrt{\rho_v \sigma_v},$$

with the convention $\sigma_v^{3/2}\tau_v^{-1/2} = 0$ *if* $\tau_v = 0$. *Then*

$$\frac{d_v^{3/2}}{\sqrt{W_4(v)}} \;\le\; L_v \;\le\; \mathcal{E}(v) \;\le\; U_v \;\le\; \sqrt{d_v}. \tag{14}$$

Moreover:

(a) $\mathcal{E}(v) = L_v$ *if and only if the nonzero numbers among* $|\lambda_j|$, $j \ge 2$, $p_{vj} > 0$, *all coincide;*

(b) $\mathcal{E}(v) = U_v$ *if and only if there is* $\theta \ge 0$ *with* $|\lambda_j| = \theta$ *for all* $j \ge 2$ *with* $p_{vj} > 0$; *in that case* $\mathcal{E}(v) = \lambda_1 x_v^2 + \theta(1 - x_v^2)$;

(c) *the first inequality in* (14) *is an equality if and only if* $\lambda_j \in \{0, -\lambda_1\}$ *for every* $j \ge 2$ *with* $p_{vj} > 0$;

(d) *the last inequality in* (14) *is the identity*

$$d_v - U_v^2 = x_v^2\big(\sqrt{\sigma_v} - \lambda_1\sqrt{\rho_v}\big)^2, \tag{15}$$

so $U_v = \sqrt{d_v}$ *if and only if* $d_v = \lambda_1^2$, *i.e. if and only if* $G \cong K_{1,\Delta}$ *and* v *is its centre (or* $G \cong K_2$*).*

Proof. Write $E^\circ = \mathcal{E}(v) - \lambda_1 x_v^2 = \sum_{j\ge2} p_{vj}|\lambda_j|$.

Upper bound and (b). By the Cauchy–Schwarz inequality,

$$(E^\circ)^2 = \Big(\sum_{j\ge2} \sqrt{p_{vj}}\cdot\sqrt{p_{vj}}\,|\lambda_j|\Big)^2 \le \Big(\sum_{j\ge2} p_{vj}\Big)\Big(\sum_{j\ge2} p_{vj}\lambda_j^2\Big) = \rho_v\sigma_v,$$

which is $\mathcal{E}(v) \le U_v$. Equality holds if and only if the vectors $(\sqrt{p_{vj}})_{j\ge2}$ and $(\sqrt{p_{vj}}|\lambda_j|)_{j\ge2}$ are proportional, i.e. if and only if $|\lambda_j|$ takes a single value θ on $\{j \ge 2 : p_{vj} > 0\}$ (if $\rho_v = 0$ the statement is void; note, however, that $\rho_v > 0$ whenever $n \ge 2$, because $x_v^2 < \sum_w x_w^2 = 1$). Then $E^\circ = \theta\rho_v$.

Lower bound and (a). If $\tau_v = 0$ then $\sigma_v = 0$ by Lemma 8 and there is nothing to prove. Otherwise, by Hölder's inequality with exponents 3/2

and 3,

$$\begin{aligned}\sigma_v &= \sum_{j\ge 2} \big(p_{vj}|\lambda_j|\big)^{2/3}\big(p_{vj}\lambda_j^4\big)^{1/3} \\ &\le \Big(\sum_{j\ge 2} p_{vj}|\lambda_j|\Big)^{2/3}\Big(\sum_{j\ge 2} p_{vj}\lambda_j^4\Big)^{1/3} = (E^\circ)^{2/3}\tau_v^{1/3},\end{aligned}$$

so $E^\circ \ge \sigma_v^{3/2}\tau_v^{-1/2}$, i.e. $\mathcal{E}(v) \ge L_v$. Equality in Hölder's inequality holds if and only if the vectors $(p_{vj}|\lambda_j|)_{j\ge 2}$ and $(p_{vj}\lambda_j^4)_{j\ge 2}$ are proportional; indices with $\lambda_j = 0$ contribute zero to both, and on the remaining indices with $p_{vj} > 0$ proportionality means that $|\lambda_j|^3$ is constant. This is (a).

Comparison with the walk bound and (c). Consider $\phi(a,b) = a^{3/2}b^{-1/2}$ for $a \ge 0$, $b > 0$ (extended by $\phi(0,0) = 0$). It is the perspective $b\,f(a/b)$ of the convex function $f(t) = t^{3/2}$, hence jointly convex and positively homogeneous of degree one, and therefore subadditive:

$$\phi(a_1+a_2, b_1+b_2) = 2\phi\Big(\tfrac{a_1+a_2}{2}, \tfrac{b_1+b_2}{2}\Big) \le \phi(a_1,b_1) + \phi(a_2,b_2).$$

Apply this with $(a_1,b_1) = (\lambda_1^2 x_v^2, \lambda_1^4 x_v^2)$ and $(a_2,b_2) = (\sigma_v, \tau_v)$. Since $a_1 + a_2 = d_v$, $b_1 + b_2 = W_4(v)$ and $\phi(a_1,b_1) = \lambda_1 x_v^2$, we get $d_v^{3/2} W_4(v)^{-1/2} \le L_v$. Because f is strictly convex, equality holds if and only if $(a_2,b_2) = (0,0)$ or $b_2/a_2 = b_1/a_1 = \lambda_1^2$. The first alternative means $\lambda_j = 0$ for all $j \ge 2$ with $p_{vj} > 0$. The second means $\sum_{j\ge 2} p_{vj}\lambda_j^2(\lambda_1^2 - \lambda_j^2) = 0$; all summands are nonnegative, so $\lambda_j \in \{0, \pm\lambda_1\}$ on the support, and $\lambda_j = \lambda_1$ is impossible for $j \ge 2$ since λ_1 is simple. This proves (c).

The last inequality and (d). For vectors $a, b \in \mathbb{R}^2$, Lagrange's identity reads $|a|^2|b|^2 - \langle a,b\rangle^2 = (a_1 b_2 - a_2 b_1)^2$. With $a = (x_v, \sqrt{\rho_v})$ and $b = (\lambda_1 x_v, \sqrt{\sigma_v})$ we have $|a|^2 = 1$, $|b|^2 = \lambda_1^2 x_v^2 + \sigma_v = d_v$ and $\langle a,b\rangle = U_v$, which gives (15). Since $x_v > 0$, equality $U_v = \sqrt{d_v}$ holds if and only if $\sigma_v = \lambda_1^2 \rho_v$, that is $d_v - \lambda_1^2 x_v^2 = \lambda_1^2 - \lambda_1^2 x_v^2$, that is $d_v = \lambda_1^2$. As $d_v \le \Delta \le \lambda_1^2$ with $\lambda_1^2 = \Delta$ only for the star $K_{1,\Delta}$ (Lemma 4), this happens exactly when G is a star and $d_v = \Delta$. ∎

Remark. Theorem 13 simultaneously improves Theorem 2 (lower bound) and the bound $\mathcal{E}(v) \le \sqrt{d_v}$ of [4] (upper bound), and by (d) the improve-

ment of the upper bound is strict at every vertex other than the centre of a star. Its equality conditions are different: for $K_{a,b}$ with $a, b \geq 2$, every vertex satisfies $\mathcal{E}(v) = L_v$ (the support of μ_v° is contained in $\{0, -\sqrt{ab}\}$), but $\mathcal{E}(v) < U_v$ because the zero eigenvalue is charged. For K_n both bounds are attained, with $\theta = 1$.

Corollary 9. For every connected graph G with $n \geq 2$ vertices,

$$\begin{aligned} \sum_v \frac{d_v^{3/2}}{\sqrt{W_4(v)}} \leq \lambda_1 + \sum_v \frac{\sigma_v^{3/2}}{\sqrt{\tau_v}} \;&\leq\; \mathcal{E}(G) \\ &\leq\; \lambda_1 + \sum_v \sqrt{\rho_v \sigma_v} \;\leq\; \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)}. \end{aligned} \tag{16}$$

Moreover

$$\mathrm{EM}_1(G) \leq \sum_v U_v^2 = 2m - \sum_v x_v^2 \bigl(\sqrt{\sigma_v} - \lambda_1 \sqrt{\rho_v}\bigr)^2. \tag{17}$$

Proof. Sum (14) over v and use $\sum_v \lambda_1 x_v^2 = \lambda_1$. The last inequality in (16) is the Cauchy–Schwarz inequality together with Lemma 8: $\sum_v \sqrt{\rho_v \sigma_v} \leq \sqrt{\sum_v \rho_v}\sqrt{\sum_v \sigma_v} = \sqrt{(n-1)(2m - \lambda_1^2)}$. For (17) square $\mathcal{E}(v) \leq U_v$, sum, and use (15) with $\sum_v d_v = 2m$. ∎

The right-most expression in (16) is the intermediate inequality from which Koolen and Moulton [35] derive their bound $\mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\bigl(2m - (\frac{2m}{n})^2\bigr)}$. Thus Corollary 9 shows that the Koolen–Moulton argument can be carried out vertex by vertex, and that the vertex-wise version is never weaker. Table 1 illustrates (16).

12 Regular graphs and their complements

For regular graphs the Perron vector is constant, and the all-ones vector is a common eigenvector of $A(G)$ and $A(\overline{G})$. This makes it possible to compare the vertex energies of a regular graph and of its complement, and to prove Nordhaus–Gaddum-type inequalities at the level of single vertices. We do not assume connectivity in this section. Vertex energies of regular graphs were recently studied from a different, distributional viewpoint in [42].

G	$\sum_v d_v^{3/2} W_4(v)^{-1/2}$	$\lambda_1 + \sum_v \sigma_v^{3/2}\tau_v^{-1/2}$	$\mathcal{E}(G)$	$\lambda_1 + \sum_v \sqrt{\rho_v \sigma_v}$	$\lambda_1 + \sqrt{(n-1)(2m-\lambda_1^2)}$
P_5	5.0987	5.1568	5.4641	6.1434	6.2042
$K_{1,4}$	4.0000	4.0000	4.0000	5.6458	6.0000
$K_{2,3}$	4.8990	4.8990	4.8990	7.3094	7.3485
C_5	5.7735	5.9279	6.4721	6.8990	6.8990
$K_4 - e$	4.4721	5.0111	5.1231	5.7573	5.7733
W_5	7.0840	8.8254	9.3711	9.8036	9.8139
F_3	7.6343	9.2218	10.0000	10.1699	10.3485
Q_3	9.0711	9.2284	12.0000	13.2470	13.2470
Petersen	13.4164	14.5852	16.0000	16.7477	16.7477
K_5	5.5470	8.0000	8.0000	8.0000	8.0000

Table 1. The chain (16) for some graphs; W_5 is the wheel with five spokes and F_3 the friendship graph with three triangles (see Section 14). For vertex-transitive graphs the last two columns coincide.

Let G be r-regular of order n and $\bar{r} = n - 1 - r$. Since $A\mathbf{1} = r\mathbf{1}$ and A is symmetric, we can choose an orthonormal eigenbasis $u_1 = \mathbf{1}/\sqrt{n}, u_2, \dots, u_n$ of A with $u_j \perp \mathbf{1}$ for $j \geq 2$. In this section $p_{vj} = u_{vj}^2$ refers to this basis, so $p_{v1} = 1/n$.

Theorem 14. *Let G be an r-regular graph of order n with $1 \leq r \leq n-1$, and let $v \in V(G)$ lie in q_v quadrangles. Then*

$$\frac{r}{n} + \frac{\big(r(n-r)/n\big)^{3/2}}{\sqrt{2r^2 - r + 2q_v - r^4/n}} \;\leq\; \mathcal{E}(v) \;\leq\; \frac{r + \sqrt{(n-1)\,r\,(n-r)}}{n}. \tag{18}$$

The upper bound is attained if and only if $|\lambda_j|$ is constant on $\{j \geq 2 : p_{vj} > 0\}$, and the lower bound if and only if the nonzero values of $|\lambda_j|$ on this set coincide. Consequently, for every VE_f with f nondecreasing in each variable,

$$\mathrm{VE}_f(G) \leq \frac{nr}{2}\, f(\omega, \omega), \qquad \omega = \frac{r + \sqrt{(n-1)r(n-r)}}{n}; \tag{19}$$

in particular $\mathrm{ESO}(G) \leq \frac{nr}{\sqrt{2}}\,\omega$ and $\mathrm{EM}_2(G) \leq \frac{nr}{2}\,\omega^2$.

Proof. The argument of Theorem 13 only used that u_1 is a unit eigenvector for λ_1 with $p_{v1} = x_v^2$; here $u_1 = \mathbf{1}/\sqrt{n}$ and $\lambda_1 = r$, even if G is disconnected (in which case some λ_j, $j \geq 2$, also equal r, which does not affect the Cauchy–Schwarz and Hölder steps). Thus the upper and lower bounds

of (14) hold with $x_v^2 = 1/n$:

$$\rho_v = 1 - \frac{1}{n}, \qquad \sigma_v = r - \frac{r^2}{n} = \frac{r(n-r)}{n}, \qquad \tau_v = W_4(v) - \frac{r^4}{n}.$$

By (1), $W_4(v) = r^2 + r(r-1) + 2q_v = 2r^2 - r + 2q_v$. Now $\lambda_1 x_v^2 + \sqrt{\rho_v \sigma_v} = \frac{r}{n} + \sqrt{\frac{n-1}{n} \cdot \frac{r(n-r)}{n}}$, which is the right-hand side of (18), and the lower bound is L_v. Since $1 \le r \le n-1$ we have $\sigma_v > 0$ and hence $\tau_v \ge \sigma_v^2/\rho_v > 0$. The equality conditions are those of Theorem 13(a),(b). Finally (19) follows by applying the monotone function f to the pointwise bound on every one of the $nr/2$ edges. ∎

Example 7. For the Petersen graph ($n = 10$, $r = 3$, $q_v = 0$) (18) gives $1.4585 \le \mathcal{E}(v) \le 1.6748$, while $\mathcal{E}(v) = 1.6$; the nonprincipal eigenvalues are 1 and -2, so neither bound is attained. For K_n both bounds equal $2(n-1)/n$. For the cocktail-party graph $K_{2,2,\dots,2}$ (and more generally for regular complete multipartite graphs) the lower bound is attained, since its nonprincipal eigenvalues are 0 and -2. For C_n with $n \ge 5$ the bounds read $\frac{2}{n} + \frac{(2(n-2)/n)^{3/2}}{\sqrt{6-16/n}} \le \frac{\mathcal{E}(C_n)}{n} \le \frac{2+\sqrt{2(n-1)(n-2)}}{n}$.

Theorem 15. *Let G be an r-regular graph of order $n \ge 2$, $\bar{r} = n - 1 - r$, and $v \in V(G)$. Then:*

(a) $\mathcal{E}_G(v) = \dfrac{r}{n} + \displaystyle\sum_{j \ge 2} p_{vj} |\lambda_j|$ *and* $\mathcal{E}_{\overline{G}}(v) = \dfrac{\bar{r}}{n} + \displaystyle\sum_{j \ge 2} p_{vj} |1 + \lambda_j|$;

(b) $\mathcal{E}_G(v) - \dfrac{2r}{n} \le \mathcal{E}_{\overline{G}}(v) \le \mathcal{E}_G(v) + \dfrac{2\bar{r}}{n}$, *with equality on the right if and only if $\lambda_j \ge 0$, and on the left if and only if $\lambda_j \le -1$, for every $j \ge 2$ with $p_{vj} > 0$;*

(c) *(Nordhaus–Gaddum)*

$$\begin{aligned} \frac{2(n-1)}{n} &\le \mathcal{E}_G(v) + \mathcal{E}_{\overline{G}}(v) \\ &\le \frac{n - 1 + \sqrt{(n-1)r(n-r)} + \sqrt{(n-1)\bar{r}(n-\bar{r})}}{n}; \end{aligned}$$

(d) *equality holds on the left of* (c) *for every vertex v if and only if $G \cong K_n$ or $G \cong \overline{K_n}$.*

Proof. (a) Since $A(\overline{G}) = J - I - A$ and $Ju_j = 0$ for $j \geq 2$, the basis (u_j) is also an eigenbasis of $A(\overline{G})$, with eigenvalue $n-1-r = \bar{r}$ on u_1 and $-1-\lambda_j$ on u_j, $j \geq 2$. Apply Lemma 1 to both matrices.

(b) For real t we have $|t|-1 \leq |1+t| \leq |t|+1$, with equality on the right iff $t \geq 0$ and on the left iff $t \leq -1$. Multiply by p_{vj} and sum over $j \geq 2$; since $\sum_{j\geq 2} p_{vj} = 1 - \frac{1}{n}$, (a) gives

$$\mathcal{E}_{\overline{G}}(v) \leq \frac{\bar{r}}{n} + \left(\mathcal{E}_G(v) - \frac{r}{n}\right) + \frac{n-1}{n} = \mathcal{E}_G(v) + \frac{2\bar{r}}{n},$$

and similarly $\mathcal{E}_{\overline{G}}(v) \geq \frac{\bar{r}}{n} + \mathcal{E}_G(v) - \frac{r}{n} - \frac{n-1}{n} = \mathcal{E}_G(v) - \frac{2r}{n}$.

(c) For every real t, $|t| + |1+t| \geq 1$, with equality iff $-1 \leq t \leq 0$. Hence, by (a),

$$\mathcal{E}_G(v) + \mathcal{E}_{\overline{G}}(v) \geq \frac{r+\bar{r}}{n} + \frac{n-1}{n} = \frac{2(n-1)}{n}.$$

For the upper bound apply the upper bound of Theorem 14 to G and to the $\bar{r}$-regular graph $\overline{G}$ (if $r = 0$ or $\bar{r} = 0$ the corresponding term is $\frac{r}{n} = 0$, resp. $\frac{\bar{r}}{n} = 0$, since then all λ_j vanish, resp. equal -1 for $j \geq 2$) and add.

(d) By the proof of (c), equality for every v holds iff $-1 \leq \lambda_j \leq 0$ for every $j \geq 2$ (each j has $p_{vj} > 0$ for some v). If $r = 0$, $G = \overline{K_n}$. If $r \geq 1$, then G has exactly one positive eigenvalue, so G is connected (a second component would contribute a second eigenvalue $r > 0$) and, by Smith's theorem (Lemma 6), complete multipartite; being regular, $G \cong K_{a,\dots,a}$ with k parts, whose spectrum is $\{a(k-1), 0^{(k(a-1))}, (-a)^{(k-1)}\}$. The condition $-a \geq -1$ forces $a = 1$, i.e. $G \cong K_n$. Conversely, K_n has nonprincipal eigenvalues -1 and $\overline{K_n}$ has nonprincipal eigenvalues 0. ■

Corollary 10. For every r-regular graph G of order n,

$$2(n-1) \;\leq\; \mathcal{E}(G)+\mathcal{E}(\overline{G}) \;\leq\; n-1+\sqrt{(n-1)r(n-r)}+\sqrt{(n-1)\bar{r}(n-\bar{r})},$$

with equality on the left if and only if $G \in \{K_n, \overline{K_n}\}$, and

$$\mathrm{ED}(G)+\mathrm{ED}(\overline{G}) = r\,\mathcal{E}(G)+\bar{r}\,\mathcal{E}(\overline{G}), \qquad \mathrm{EM}_1(G)+\mathrm{EM}_1(\overline{G}) \;\geq\; \frac{2(n-1)^2}{n}.$$

Proof. Sum Theorem 15(c),(d) over v. The formula for ED is $\mathrm{ED}(G) = \sum_v d_v \mathcal{E}(v)$ for regular graphs. For EM_1 use $a^2+b^2 \geq \frac{1}{2}(a+b)^2$ and (c): $\mathrm{EM}_1(G) + \mathrm{EM}_1(\overline{G}) \geq \frac{1}{2}\sum_v \left(\mathcal{E}_G(v) + \mathcal{E}_{\overline{G}}(v)\right)^2 \geq \frac{n}{2} \cdot \frac{4(n-1)^2}{n^2}$. ∎

13 Cartesian products

In contrast to the tensor product (Theorem 11), vertex energy is not multiplicative, and not even additive, under the Cartesian product $G \square H$, whose adjacency matrix is $A(G) \otimes I + I \otimes A(H)$ [30]. Nevertheless it can be squeezed between the vertex energies of the factors, and it can be computed exactly when one factor is K_2.

Let G and H have orthonormal eigenbases (u_j) and (w_k) with eigenvalues (λ_j) and (μ_k), and write $p_{gj} = u_{gj}^2$, $q_{hk} = w_{hk}^2$.

Theorem 16. *Let $g \in V(G)$ and $h \in V(H)$. Then*

(a) $\mathcal{E}_{G\square H}(g,h) = \displaystyle\sum_{j,k} p_{gj}\, q_{hk}\, |\lambda_j + \mu_k|$;

(b) $\max\{\mathcal{E}_G(g), \mathcal{E}_H(h)\} \;\leq\; \mathcal{E}_{G\square H}(g,h) \;\leq\; \mathcal{E}_G(g) + \mathcal{E}_H(h)$;

(c) $\mathcal{E}_{G\square H}(g,h) = \mathcal{E}_G(g)$ *if and only if, for every j with $p_{gj} > 0$, the numbers $\lambda_j + \mu_k$ with $q_{hk} > 0$ are all ≥ 0 or all ≤ 0;*

(d) *if g and h are both non-isolated, the right inequality in* (b) *is strict; if h is isolated, then $\mathcal{E}_{G\square H}(g,h) = \mathcal{E}_G(g)$.*

Proof. (a) The vectors $u_j \otimes w_k$ form an orthonormal eigenbasis of $A(G) \otimes I + I \otimes A(H)$ with eigenvalues $\lambda_j + \mu_k$, and $(u_j \otimes w_k)_{(g,h)}^2 = p_{gj} q_{hk}$; apply Lemma 1.

(b), (c) Fix j. Since $(q_{hk})_k$ is a probability vector with mean $\sum_k q_{hk}\mu_k = A(H)_{hh} = 0$, the triangle inequality gives

$$\sum_k q_{hk} |\lambda_j + \mu_k| \;\geq\; \Big| \sum_k q_{hk} (\lambda_j + \mu_k) \Big| = |\lambda_j|, \tag{20}$$

with equality iff all $\lambda_j + \mu_k$ ($q_{hk} > 0$) have the same sign. Multiplying by p_{gj} and summing over j yields $\mathcal{E}_{G\square H}(g,h) \geq \mathcal{E}_G(g)$ together with the

equality condition (c); by symmetry also $\mathcal{E}_{G\square H}(g,h) \geq \mathcal{E}_H(h)$. The upper bound follows from $|\lambda_j + \mu_k| \leq |\lambda_j| + |\mu_k|$ and $\sum_{j,k} p_{gj} q_{hk}(|\lambda_j| + |\mu_k|) = \mathcal{E}_G(g) + \mathcal{E}_H(h)$.

(d) If g is non-isolated, the spectral measure of g has mean 0 and variance $d_g > 0$, so there are j, j' with $p_{gj}, p_{gj'} > 0$ and $\lambda_j > 0 > \lambda_{j'}$; similarly for h. Choosing $\lambda_j > 0$ and $\mu_k < 0$ in the supports, $|\lambda_j + \mu_k| < |\lambda_j| + |\mu_k|$ with $p_{gj} q_{hk} > 0$, so the upper bound is strict. If h is isolated, $q_{hk} > 0$ only for $\mu_k = 0$ (see the proof of Lemma 3(c)), and (a) reduces to $\mathcal{E}_G(g)$. ∎

Corollary 11. For every graph G, every $g \in V(G)$ and $i \in V(K_2)$,

$$\mathcal{E}_{G\square K_2}(g,i) = \sum_j p_{gj} \max\{|\lambda_j|, 1\} = \mathcal{E}_G(g) + \sum_{|\lambda_j|<1} p_{gj}\big(1 - |\lambda_j|\big).$$

Hence $\max\{\mathcal{E}_G(g), 1\} \leq \mathcal{E}_{G\square K_2}(g,i) \leq \mathcal{E}_G(g) + 1$, and $\mathcal{E}_{G\square K_2}(g,i) = \mathcal{E}_G(g)$ if and only if the spectral measure of g has no mass in the open interval $(-1,1)$. In particular every vertex of a prism $G\square K_2$ has energy at least 1, and $\mathcal{E}_{K_n\square K_2}(v) = \mathcal{E}_{K_n}(v) = 2(n-1)/n$.

Proof. K_2 has eigenvalues ± 1 with $q_{i,1} = q_{i,2} = \frac{1}{2}$, so by Theorem 16(a) the vertex energy equals $\sum_j p_{gj} \frac{|\lambda_j+1|+|\lambda_j-1|}{2} = \sum_j p_{gj} \max\{|\lambda_j|, 1\}$. The remaining statements are immediate, using $\sum_j p_{gj} = 1$; for K_n note that its eigenvalues $n-1$ and -1 lie outside $(-1,1)$. ∎

Proposition 17. *For every $d \geq 1$ and every vertex v of the hypercube $Q_d = K_2^{\square d}$,*

$$\mathcal{E}_{Q_d}(v) = \frac{d}{2^{d-1}} \binom{d-1}{\lfloor d/2 \rfloor}, \qquad \mathcal{E}_{Q_{2k}}(v) = \mathcal{E}_{Q_{2k-1}}(v) \ (k \geq 1),$$

$$\mathcal{E}_{Q_d}(v) \sim \sqrt{\frac{2d}{\pi}} \quad (d \to \infty).$$

Proof. Q_d is vertex-transitive with spectrum $\{(d-2i)^{\binom{d}{i}} : 0 \leq i \leq d\}$, so $\mathcal{E}_{Q_d}(v) = 2^{-d} \sum_i \binom{d}{i} |d-2i|$. From $(d-i)\binom{d}{i} = d\binom{d-1}{i}$ and $i\binom{d}{i} = d\binom{d-1}{i-1}$

we get $(d-2i)\binom{d}{i} = d\big(\binom{d-1}{i} - \binom{d-1}{i-1}\big)$, which telescopes:

$$\sum_{i=0}^{\lfloor d/2 \rfloor} (d-2i)\binom{d}{i} = d\binom{d-1}{\lfloor d/2 \rfloor}.$$

By the symmetry $i \mapsto d-i$ the terms with $i > d/2$ contribute the same amount, and the term $i = d/2$ (if present) vanishes; this gives the formula. The equality $\mathcal{E}_{Q_{2k}} = \mathcal{E}_{Q_{2k-1}}$ also follows from Corollary 11, since $Q_{2k} = Q_{2k-1}\square K_2$ and all eigenvalues of Q_{2k-1} are odd integers. Finally, $\binom{d-1}{\lfloor d/2 \rfloor} \sim 2^{d-1}\sqrt{2/(\pi d)}$ by Stirling's formula. ∎

Remark. For Q_d we have $W_4(v) = 3d^2 - 2d$, so Theorem 2 gives $\mathcal{E}(v) \geq d^{3/2}/\sqrt{3d^2-2d} \sim \sqrt{d/3}$, and the upper bound is $\sqrt{d}$. By Proposition 17 both bounds have the correct order of magnitude $\sqrt{d}$; the true constant $\sqrt{2/\pi} \approx 0.798$ lies between $1/\sqrt{3} \approx 0.577$ and 1.

Corollary 12. Let G and H have n_G, n_H vertices and m_G, m_H edges. Then

$$\max\{n_H\mathcal{E}(G),\, n_G\mathcal{E}(H)\} \leq \mathcal{E}(G\square H) \leq n_H\mathcal{E}(G) + n_G\mathcal{E}(H),$$
$$n_H\mathrm{ED}(G) + n_G\mathrm{ED}(H) \leq \mathrm{ED}(G\square H),$$
$$\mathrm{ED}(G\square H) \leq n_H\mathrm{ED}(G) + n_G\mathrm{ED}(H) + 2m_H\mathcal{E}(G) + 2m_G\mathcal{E}(H),$$
$$\max\{n_H\mathrm{EM}_1(G),\, n_G\mathrm{EM}_1(H)\} \leq \mathrm{EM}_1(G\square H),$$
$$\mathrm{EM}_1(G\square H) \leq n_H\mathrm{EM}_1(G) + n_G\mathrm{EM}_1(H) + 2\mathcal{E}(G)\mathcal{E}(H).$$

If G and H have no isolated vertices, all upper bounds are strict.

Proof. Sum Theorem 16(b) over (g,h), respectively multiply it by $d_{(g,h)} = d_g + d_h$ or square it before summing, and use $\sum_{g,h} d_g\mathcal{E}_G(g) = n_H\mathrm{ED}(G)$, $\sum_{g,h} d_h\mathcal{E}_G(g) = 2m_H\mathcal{E}(G)$ and $\sum_{g,h} \mathcal{E}_G(g)\mathcal{E}_H(h) = \mathcal{E}(G)\mathcal{E}(H)$. For the lower bound for ED use $d_g\mathcal{E}_{G\square H}(g,h) \geq d_g\mathcal{E}_G(g)$ and $d_h\mathcal{E}_{G\square H}(g,h) \geq d_h\mathcal{E}_H(h)$ separately. Strictness follows from Theorem 16(d). ∎

14 Joins with regular graphs

The join $G \vee H$ is obtained from the disjoint union of G and H by adding all edges between $V(G)$ and $V(H)$. Arizmendi and Sigarreta [7] showed that coalescing a tree with a bipartite graph changes the vertex energies in an alternating pattern. For joins of regular graphs the change is instead uniform and positive, and it can be computed in closed form.

Theorem 18. *Let G be r-regular of order n and H be s-regular of order m (connectivity is not assumed), and put $D = \sqrt{(r-s)^2 + 4nm}$. Then for $g \in V(G)$ and $h \in V(H)$,*

$$\mathcal{E}_{G\vee H}(g) = \mathcal{E}_G(g) + \alpha, \qquad \mathcal{E}_{G\vee H}(h) = \mathcal{E}_H(h) + \beta,$$

where

$$\alpha = \frac{r(r-s) + 2nm}{nD} - \frac{r}{n}, \qquad \beta = \frac{s(s-r) + 2nm}{mD} - \frac{s}{m}.$$

Moreover

(a) $0 < \alpha \le \dfrac{\sqrt{r^2+nm} - r}{n}$ *and* $0 < \beta \le \dfrac{\sqrt{s^2+nm} - s}{m}$, *with equality in either upper bound if and only if $r = s = 0$;*

(b) $n\alpha + m\beta = D - r - s$, *and hence $\mathcal{E}(G \vee H) = \mathcal{E}(G) + \mathcal{E}(H) + D - r - s$.*

In particular, joining two regular graphs strictly increases the energy of every vertex.

Proof. Order the vertices so that $A(G \vee H) = \left(\begin{smallmatrix} A_G & J \\ J & A_H \end{smallmatrix}\right)$, where J denotes all-ones matrices of the appropriate sizes. Choose orthonormal eigenbases $u_1 = \mathbf{1}_n/\sqrt{n}, u_2, \dots, u_n$ of A_G and $w_1 = \mathbf{1}_m/\sqrt{m}, w_2, \dots, w_m$ of A_H with $u_j \perp \mathbf{1}$ and $w_k \perp \mathbf{1}$ for $j, k \ge 2$, as in Section 12. Since $Ju_j = 0$ and $Jw_k = 0$, the vectors $(u_j, 0)$ $(j \ge 2)$ and $(0, w_k)$ $(k \ge 2)$ are eigenvectors of $A(G \vee H)$ with eigenvalues λ_j and μ_k. Their orthogonal complement is spanned by the orthonormal vectors $e = (\mathbf{1}_n/\sqrt{n}, 0)$ and $f = (0, \mathbf{1}_m/\sqrt{m})$, and in the basis (e, f) the matrix $A(G \vee H)$ acts on this invariant plane by

$$B = \begin{pmatrix} r & \sqrt{nm} \\ \sqrt{nm} & s \end{pmatrix}.$$

Hence $|A(G \vee H)|$ is the sum of the operator $|B|$ on $\operatorname{span}\{e, f\}$ and

$$\sum_{j\geq 2} |\lambda_j|(u_j, 0)(u_j, 0)^{\mathsf{T}} + \sum_{k\geq 2} |\mu_k|(0, w_k)(0, w_k)^{\mathsf{T}}.$$

Taking the diagonal entry at g and using $e_g^2 = 1/n$, $f_g = 0$,

$$\mathcal{E}_{G\vee H}(g) = \sum_{j\geq 2} p_{gj}|\lambda_j| + \frac{|B|_{11}}{n} = \mathcal{E}_G(g) - \frac{r}{n} + \frac{|B|_{11}}{n}.$$

The eigenvalues of B are $\nu_\pm = \frac{1}{2}(r + s \pm D)$; since $\det B = rs - nm < 0$ (because $r < n$ and $s < m$), $\nu_+ > 0 > \nu_-$. The polynomial $\psi(t) = (2t^2 - (r+s)t)/D$ satisfies $\psi(\nu_\pm) = \nu_\pm(2\nu_\pm - \nu_+ - \nu_-)/D = \pm\nu_\pm = |\nu_\pm|$, so $|B| = \psi(B) = (2B^2 - (r+s)B)/D$. As $(B^2)_{11} = r^2 + nm$,

$$|B|_{11} = \frac{2(r^2 + nm) - (r+s)r}{D} = \frac{r(r-s) + 2nm}{D},$$

which gives the formula for α; β is obtained by symmetry.

(a) We have $r(r-s) + 2nm \geq 2nm - rs > 0$ and

$$\begin{aligned}\big(r(r-s) + 2nm\big)^2 - r^2D^2 &= 4nm\, r(r-s) + 4n^2m^2 - 4nm\, r^2 \\ &= 4nm(nm - rs) > 0,\end{aligned}$$

so $|B|_{11} > r$, i.e. $\alpha > 0$. For the upper bound, $|B|$ is positive semidefinite with $|B|^2 = B^2$, hence $|B|_{11}^2 \leq |B|_{11}^2 + |B|_{12}^2 = (B^2)_{11} = r^2 + nm$, with equality iff $|B|_{12} = 0$. Since $|B|_{12} = (2(B^2)_{12} - (r+s)\sqrt{nm})/D = (r+s)\sqrt{nm}/D$, equality holds iff $r = s = 0$. The bounds for β are symmetric.

(b) $n\alpha + m\beta = |B|_{11} + |B|_{22} - r - s = \operatorname{tr}|B| - r - s = \nu_+ - \nu_- - r - s = D - r - s$. Summing the vertex energies gives the formula for $\mathcal{E}(G\vee H)$. ■

The formula in (b) for the total energy of a join of two regular graphs is classical (cf. [36]); Theorem 18 shows how the excess $D-r-s$ is distributed among the vertices. The case $r = s = 0$ recovers the vertex energies $\sqrt{m/n}$ and $\sqrt{n/m}$ of $K_{n,m}$ (Example 2).

Corollary 13. (a) If H is s-regular of order m, the apex a of the cone

$K_1 \vee H$ and the vertices $h \in V(H)$ satisfy

$$\mathcal{E}(a) = \frac{2m}{\sqrt{s^2+4m}}, \qquad \mathcal{E}(h) = \mathcal{E}_H(h) - \frac{s}{m} + \frac{s^2+2m}{m\sqrt{s^2+4m}}.$$

(b) For the wheel $W_n = K_1 \vee C_n$ ($n \geq 3$): $\mathcal{E}(\text{hub}) = \dfrac{n}{\sqrt{n+1}}$ and $\mathcal{E}(\text{rim}) = \dfrac{\mathcal{E}(C_n)-2}{n} + \dfrac{n+2}{n\sqrt{n+1}}$.

(c) For the friendship graph $F_k = K_1 \vee kK_2$: $\mathcal{E}(\text{centre}) = \dfrac{4k}{\sqrt{8k+1}}$ and every other vertex has energy $1 - \dfrac{1}{2k} + \dfrac{4k+1}{2k\sqrt{8k+1}}$, in agreement with [4, Sec. 5].

(d) For the complete split graph $\mathrm{CS}(k,t) = K_k \vee \overline{K_t}$, with $D = \sqrt{(k-1)^2+4kt}$, the clique vertices have energy $1 - \frac{1}{k} + \frac{(k-1)^2+2kt}{kD}$ and the independent vertices have energy $\frac{2k}{D}$.

Proof. (a) is Theorem 18 with $n=1$, $r=0$ and $\mathcal{E}_{K_1}=0$. (b) and (c) follow from (a) with $(s,m)=(2,n)$, $\mathcal{E}_{C_n}(h) = \mathcal{E}(C_n)/n$, and $(s,m)=(1,2k)$, $\mathcal{E}_{kK_2}(h)=1$, respectively. (d) is Theorem 18 with $(n,r)=(k,k-1)$, $(m,s)=(t,0)$, $\mathcal{E}_{K_k}(g) = 2(k-1)/k$ (Example 1) and $\mathcal{E}_{\overline{K_t}} = 0$. ∎

Corollary 14. With the notation of Theorem 18,

$$\begin{aligned}
\mathrm{EM}_1(G\vee H) &= \mathrm{EM}_1(G) + 2\alpha\mathcal{E}(G) + n\alpha^2 + \mathrm{EM}_1(H) + 2\beta\mathcal{E}(H) + m\beta^2,\\
\mathrm{ED}(G\vee H) &= (r+m)\big(\mathcal{E}(G)+n\alpha\big) + (s+n)\big(\mathcal{E}(H)+m\beta\big),\\
\mathrm{EM}_2(G\vee H) &= \mathrm{EM}_2(G) + r\alpha\mathcal{E}(G) + \tfrac{nr}{2}\alpha^2 + \mathrm{EM}_2(H) + s\beta\mathcal{E}(H) + \tfrac{ms}{2}\beta^2\\
&\quad + \big(\mathcal{E}(G)+n\alpha\big)\big(\mathcal{E}(H)+m\beta\big).
\end{aligned}$$

Moreover, for every VE_f with f increasing in each variable, $\mathrm{VE}_f(G\vee H) > \mathrm{VE}_f(G) + \mathrm{VE}_f(H) + \sum_{g\in V(G),h\in V(H)} f\big(\mathcal{E}_G(g),\mathcal{E}_H(h)\big)$ whenever the last sum is defined.

Proof. All formulas follow by inserting Theorem 18 into the definitions. For EM_2, the edges inside G contribute $\sum_{gg'}(\mathcal{E}_G(g)+\alpha)(\mathcal{E}_G(g')+\alpha) = \mathrm{EM}_2(G) + \alpha\mathrm{ED}(G) + \alpha^2|E(G)|$ with $\mathrm{ED}(G) = r\mathcal{E}(G)$ and

$|E(G)| = nr/2$; the nm edges between $V(G)$ and $V(H)$ contribute $\sum_{g,h}(\mathcal{E}_G(g)+\alpha)(\mathcal{E}_H(h)+\beta) = (\mathcal{E}(G)+n\alpha)(\mathcal{E}(H)+m\beta)$. The last statement follows from $\alpha,\beta>0$. ∎

Example 8. By Corollary 13(b), W_5 has hub energy $5/\sqrt{6}\approx 2.0412$ and rim energy ≈ 1.4660, and W_6 has hub energy $6/\sqrt{7}\approx 2.2678$ and rim energy ≈ 1.5040. Note that $W_4 = K_1 \vee C_4 \cong K_{1,2,2}$, and Corollary 13(b) and Proposition 7 give the same values $4/\sqrt{5}\approx 1.7889$ and 1.1708. As $n\to\infty$ the hub energy $n/\sqrt{n+1}$ is asymptotic to $\sqrt{d_{\text{hub}}}=\sqrt{n}$, so the upper bound $\mathcal{E}(v)\le\sqrt{d_v}$ is asymptotically attained by non-star graphs, while the rim energies converge to $4/\pi$, the limiting vertex energy of long cycles (Example 3). Similarly, for friendship graphs the centre energy $4k/\sqrt{8k+1}$ is asymptotic to $\sqrt{2k}=\sqrt{d_{\text{centre}}}$, and the blade energies decrease to 1.

15 Neighbourhood sums and vertex-energy irregularity

The edge inequality of Theorem 5 has a useful vertex form.

Proposition 19. *For every non-isolated vertex v put $N_{\mathcal{E}}(v) = \sum_{u\in N(v)}\mathcal{E}(u)$. Then*

$$N_{\mathcal{E}}(v) \;\ge\; \frac{1}{\mathcal{E}(v)}\sum_{u\in N(v)}\bigl(1+||A|_{uv}|\bigr)^2 \;\ge\; \frac{d_v}{\mathcal{E}(v)} \;\ge\; \sqrt{d_v},$$

and $N_{\mathcal{E}}(v)=d_v/\mathcal{E}(v)$ if and only if $\mathcal{E}(u)\mathcal{E}(v)=1$ for every $u\in N(v)$. Consequently

$$\mathrm{ED}(G)=\sum_v N_{\mathcal{E}}(v) \;\ge\; \sum_v \frac{d_v}{\mathcal{E}(v)} \;\ge\; \sum_v \sqrt{d_v}, \tag{21}$$

the sums running over non-isolated vertices, and equality holds in the first inequality of (21) *if and only if every non-trivial component of G is complete bipartite.*

Proof. By Theorem 5, $\mathcal{E}(u) \geq (1 + ||A|_{uv}|)^2/\mathcal{E}(v) \geq 1/\mathcal{E}(v)$ for every $u \in N(v)$; summing over $N(v)$ gives the first two inequalities, and $d_v/\mathcal{E}(v) \geq \sqrt{d_v}$ because $\mathcal{E}(v) \leq \sqrt{d_v}$. The identity $\mathrm{ED}(G) = \sum_v d_v \mathcal{E}(v) = \sum_v \sum_{u \in N(v)} \mathcal{E}(u)$ is double counting. Equality in the first inequality of (21) means $\mathcal{E}(u)\mathcal{E}(v) = 1$ on every edge, which by Theorem 5 characterizes disjoint unions of complete bipartite graphs (and isolated vertices). ∎

For the star $K_{1,k}$ both sides of the first inequality in (21) equal $\sqrt{k}(k+1)$.

Definition 3. The *vertex-energy irregularity* and the *vertex-energy forgotten index* of G are

$$\mathrm{EIrr}(G) = \sum_{uv \in E(G)} \big|\mathcal{E}(u) - \mathcal{E}(v)\big|,$$
$$\mathrm{EF}(G) = \sum_{uv \in E(G)} \big(\mathcal{E}(u)^2 + \mathcal{E}(v)^2\big) = \sum_v d_v \mathcal{E}(v)^2.$$

These are the vertex-energy analogues of the Albertson irregularity and of the forgotten index $F = \sum_v d_v^3$. A graph is *energy-uniform* if all its non-isolated vertices in each component have the same energy; walk-regular graphs are energy-uniform (Proposition 1).

Proposition 20. *For every graph G with $m \geq 1$ edges:*

(a) $\mathrm{EIrr}(G) = 0$ *if and only if G is energy-uniform;*

(b) $\mathrm{EF}(G) - 2\mathrm{EM}_2(G) = \sum_{uv} (\mathcal{E}(u) - \mathcal{E}(v))^2$ *and* $\mathrm{EIrr}(G)^2 \leq m\big(\mathrm{EF}(G) - 2\mathrm{EM}_2(G)\big)$*;*

(c) $\mathrm{ESO}(G)^2 \leq m\,\mathrm{EF}(G)$*, with equality iff $\mathcal{E}(u)^2 + \mathcal{E}(v)^2$ is the same for all edges;*

(d) $\dfrac{\mathrm{ED}(G)}{\sqrt{2}} \leq \mathrm{ESO}(G) \leq \dfrac{\mathrm{ED}(G)}{\sqrt{2}} + \Big(1 - \dfrac{1}{\sqrt{2}}\Big)\mathrm{EIrr}(G)$*, and each inequality is an equality if and only if G is energy-uniform.*

Proof. (a) is clear for each component, since a connected graph is energy-uniform iff $\mathcal{E}$ is constant along every edge. (b) and (c) are the expansion $(a-b)^2 = a^2 + b^2 - 2ab$ and the Cauchy–Schwarz inequality.

(d) For $a, b > 0$ we claim $\frac{a+b}{\sqrt{2}} \le \sqrt{a^2+b^2} \le \frac{a+b}{\sqrt{2}} + \bigl(1 - \frac{1}{\sqrt{2}}\bigr)|a-b|$. The left inequality is $(a-b)^2 \ge 0$. For the right one we may assume $a \ge b$; the function $\Phi(a,b) = \sqrt{a^2+b^2}$ is convex and positively homogeneous, and on the cone $\{a \ge b \ge 0\}$ the right-hand side is the linear function $\Lambda(a,b) = a + (\sqrt{2}-1)b$, which agrees with Φ on the two boundary rays $b = 0$ and $a = b$. Every point of the cone is a nonnegative combination $a = \xi + \eta$, $b = \eta$ of $(1,0)$ and $(1,1)$, so by sublinearity $\Phi(a,b) \le \xi\Phi(1,0) + \eta\Phi(1,1) = \Lambda(a,b)$, with equality iff $\xi\eta = 0$ (strict convexity of Φ off rays), i.e. iff $b = 0$ or $a = b$. Apply the claim to $a = \mathcal{E}(u)$, $b = \mathcal{E}(v) > 0$ and sum over the edges, recalling $\mathrm{ED} = \sum_{uv}(\mathcal{E}(u) + \mathcal{E}(v))$. Equality in either inequality forces $\mathcal{E}(u) = \mathcal{E}(v)$ on every edge. ∎

Example 9. For the star, $\mathrm{EIrr}(K_{1,k}) = k(\sqrt{k} - 1/\sqrt{k}) = \sqrt{k}\,(k-1)$ and $\mathrm{EF}(K_{1,k}) = k^2 + 1$. For the friendship graph F_3 one finds $\mathrm{EIrr} = 6.8$, and for the wheels $\mathrm{EIrr}(W_5) = 2.8763$, $\mathrm{EIrr}(W_6) = 4.5830$ (Table 2); vertex-transitive graphs such as Q_4 and $K_3 \square K_3$ have $\mathrm{EIrr} = 0$.

16 Further examples

Table 2 collects the vertex energies and indices of the families treated in Sections 13 and 14. All entries agree (to the printed precision) with direct numerical diagonalization, and the vertex energies of the joins agree with the closed forms of Corollary 13.

G	vertex energies	$\mathcal{E}(G)$	EM_1	EM_2	ER	ESO	ED	EIrr
W_5	2.0412; 1.4660	9.3711	14.9121	25.7075	6.3011	22.9316	32.1958	2.8763
W_6	2.2678; 1.5040	11.2915	18.7141	34.0351	7.2384	29.0884	40.6779	4.5830
F_3	2.4000; 1.2667	10.0000	15.3867	23.0533	5.8097	21.6565	29.6000	6.8000
F_4	2.7852; 1.2449	12.7446	20.1561	33.9384	7.5093	31.4487	42.2006	12.3226
$\mathrm{CS}(3,3)$	1.8262; 0.9487	8.3246	12.7047	25.5968	8.4805	26.2687	35.9307	7.8974
Q_4	1.5000	24.0000	36.0000	72.0000	21.3333	67.8823	96.0000	0
$K_3 \square K_3$	1.7778	16.0000	28.4444	56.8889	10.1250	45.2548	64.0000	0
$P_4 \square K_2$	1.1708; 1.4472	10.4721	13.8610	17.8971	7.5450	18.9443	26.7331	1.1056

Table 2. Vertex-energy indices of wheels, friendship graphs, a complete split graph and some Cartesian products. For joins the first listed energy is that of the hub, centre or clique vertices.

Example 10. The eigenvalues of P_4 are $\pm\varphi$ and $\pm\varphi^{-1}$, where $\varphi = (1 + \sqrt{5})/2$. The spectral measure of an end vertex puts mass $\frac{5+\sqrt{5}}{10}$ on $\{\pm\varphi^{-1}\}$

and that of an inner vertex puts mass $\frac{5-\sqrt{5}}{10}$ there, and $\mathcal{E}_{P_4}(\text{end}) = 2/\sqrt{5} \approx 0.8944$, $\mathcal{E}_{P_4}(\text{inner}) = 3/\sqrt{5} \approx 1.3416$. By Corollary 11, in $P_4 \square K_2$ each vertex gains $(1-\varphi^{-1})$ times this mass:

$$\mathcal{E}(\text{end}) = \frac{2}{\sqrt{5}} + \frac{5+\sqrt{5}}{10}\Big(1 - \frac{\sqrt{5}-1}{2}\Big) \approx 1.1708,$$
$$\mathcal{E}(\text{inner}) = \frac{3}{\sqrt{5}} + \frac{5-\sqrt{5}}{10}\Big(1 - \frac{\sqrt{5}-1}{2}\Big) \approx 1.4472,$$

in accordance with Table 2. The gap between the two energies shrinks from 0.4472 to 0.2764: the prism operation tends to equalize vertex energies, because it raises precisely the small eigenvalues.

Example 11. Let $X_d = d - 2\,\mathrm{Bin}(d, \frac{1}{2})$, a symmetric random variable whose law is the spectral measure of every vertex of Q_d, and put $\kappa_d(t) = \mathbb{E}|t + X_d|$. By Theorem 16(a), $\mathcal{E}_{G\square Q_d}(g,y) = \sum_j p_{gj}\kappa_d(\lambda_j)$ for every $y \in V(Q_d)$, and $\kappa_d(0) = \mathcal{E}_{Q_d}(y)$. For fixed t we have $|t+x| - |x| = t\,\mathrm{sgn}(x)$ whenever $|x| \geq |t|$, and $\mathbb{E}[t\,\mathrm{sgn}(X_d)\mathbf{1}_{|X_d|\geq|t|}] = 0$ by symmetry; hence

$$\begin{aligned} 0 \leq \kappa_d(t) - \kappa_d(0) &= \mathbb{E}\big[(|t+X_d| - |X_d|)\mathbf{1}_{|X_d|<|t|}\big] \\ &\leq 2|t|\,(|t|+1)\max_i 2^{-d}\binom{d}{i} \longrightarrow 0, \end{aligned}$$

where nonnegativity is (20). Consequently $\mathcal{E}_{G\square Q_d}(g,y) - \mathcal{E}_{Q_d}(y) \to 0$ as $d \to \infty$ for every graph G and vertex g: in high-dimensional iterated prisms all vertex energies become asymptotically equal to $\sqrt{2d/\pi}$ (Proposition 17), and the local structure of G is forgotten.

17 Explicit values and computational evidence

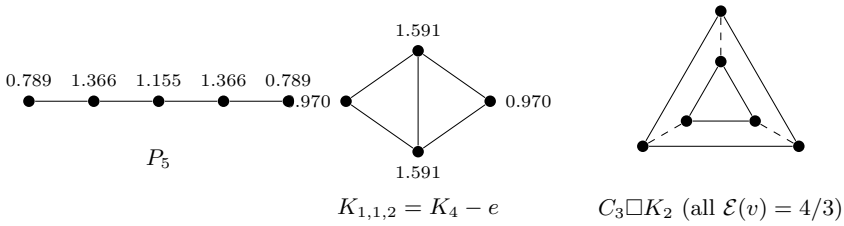

Figure 1. Vertex energies of P_5 and $K_{1,1,2}$ (rounded), and the prism. In the prism $|A|_{uv} = 1/3$ on the six triangle edges and $|A|_{uv} = -1/3$ on the three dashed edges.

Example 12. For P_5 the vertex energies are, from the end towards the centre, $\frac{3+\sqrt{3}}{6}$, $\frac{1+\sqrt{3}}{2}$ and $\frac{2}{\sqrt{3}}$ (computed from [4, (5.11)]). The centre c satisfies $\mathcal{E}(c) = d_c/\lambda_1 = 2/\sqrt{3}$: its spectral measure is supported on $\{0, \pm\sqrt{3}\}$ because the eigenvectors of P_5 for the eigenvalues ± 1 vanish at c. Thus the pointwise equality in Theorem 2 can occur at single vertices of graphs that are not complete bipartite; only the simultaneous equality at all vertices forces $K_{a,b}$.

Table 3 lists the indices of Definition 2 for several small graphs, and Table 4 compares the lower bounds for the energy obtained in this paper with the classical ones. All values were computed in double precision from the spectral decomposition. Here F_2 is the friendship graph (two triangles sharing a vertex); for the friendship graph F_k one has $\mathcal{E}(\text{centre}) = 4k/\sqrt{8k+1}$ [4].

Table 4 illustrates that neither of the two new lower bounds dominates the other: the refined Randić bound (11) is exact for K_4, the prism and $K_{1,4}$, while the walk bound $\sum_v h_v$ is better for P_5, C_5 and the Petersen graph.

We now report on a computational experiment. We computed all vertex energies and all indices of Definition 2 for: (i) all 995 connected graphs with $2 \le n \le 7$ vertices; (ii) all 205002 trees with $3 \le n \le 18$ vertices; (iii) several thousand random graphs $G(n,p)$ with $8 \le n \le 30$ and p uniformly

G	$\mathcal{E}(G)$	EM_1	EM_2	ER	ESO	$\chi_{1/2}$	SO
P_4	4.4721	5.2000	4.2000	2.5711	5.1223	5.4641	7.3006
P_5	5.4641	6.3094	5.3094	3.5193	6.7321	7.4641	10.1290
$K_{1,4}$	4.0000	5.0000	4.0000	4.0000	8.2462	8.9443	16.4924
C_5	6.4721	8.3777	8.3777	3.8627	9.1530	10.0000	14.1421
C_6	8.0000	10.6667	10.6667	4.5000	11.3137	12.0000	16.9706
K_4	6.0000	9.0000	13.5000	4.0000	12.7279	14.6969	25.4558
$K_4 - e$	5.1231	6.9475	8.7082	3.8476	9.7058	11.3938	18.6648
$K_{2,3}$	4.8990	5.0000	6.0000	6.0000	8.8318	13.4164	21.6333
$K_{1,2,2}$	6.4721	8.6833	13.8610	6.1803	15.1750	20.3810	36.9706
F_2	7.1231	10.4801	13.4139	4.0663	12.9974	13.7980	23.5454
Prism	8.0000	10.6667	16.0000	6.7500	16.9706	22.0454	38.1838
Q_3	12.0000	18.0000	27.0000	8.0000	25.4558	29.3939	50.9117
Petersen	16.0000	25.6000	38.4000	9.3750	33.9411	36.7423	63.6396

Table 3. Energy and vertex-energy indices of some small graphs, together with $\chi_{1/2}$ and SO (cf. Theorem 10(b)).

distributed. Every inequality proved in this paper was confirmed on all of these graphs. In addition, the following observations were made.

(O1) For every connected graph with $n \geq 3$ vertices in the sample, $\mathcal{E}(G) < \mathrm{ESO}(G)$. The smallest value of $\mathrm{ESO}(G)/\mathcal{E}(G)$ is $\sqrt{5}/2 \approx 1.1180$, attained only by P_3. For each fixed order $3 \leq n \leq 7$ (all connected graphs) and $3 \leq n \leq 18$ (all trees), the minimum of $\mathrm{ESO}(G)/\mathcal{E}(G)$ is attained uniquely by the path P_n, and these minima increase with n: 1.1180, 1.1454, 1.2321, 1.2487, 1.2841, ..., 1.3639 (for $n = 18$).

(O2) Among trees of order $5 \leq n \leq 14$, the star uniquely minimizes EM_1 (with value $\mathrm{EM}_1(K_{1,n-1}) = n$) and EM_2 (as proved in Corollary 8) and maximizes ER (as proved) and ESO, while the path uniquely minimizes ESO.

(O3) Among connected graphs with $n \leq 7$ vertices, the equality $\mathcal{E}(u)\mathcal{E}(v) = (1 + ||A|_{uv}|)^2$ holds on every edge precisely for the complete multipartite graphs and the prism $C_3 \square K_2$.

Observation (O1) should be contrasted with the inequality $\mathcal{E}(G) < \mathrm{SO}(G)$ of [51, Thm. 3.1]: since $\mathrm{ESO}(G) \leq \chi_{1/2}(G) < \mathrm{SO}(G)$ for $G \ncong K_2$, a proof of the inequality $\mathrm{ESO}(G) \geq \frac{\sqrt{5}}{2}\mathcal{E}(G)$ for all connected graphs with

G	$\frac{2m}{\lambda_1}$	$2R$	(11)	$\sum_v h_v$	$\mathcal{E}(G)$	$\sqrt{n\mathrm{EM}_1}$	Cor. 5	$\sqrt{2mn}$
P_5	4.6188	4.8284	4.8284	5.0987	5.4641	5.6167	6.0802	6.3246
$K_{1,4}$	4.0000	4.0000	4.0000	4.0000	4.0000	5.0000	6.0208	6.3246
C_5	5.0000	5.0000	5.2361	5.7735	6.4721	6.4721	6.7610	7.0711
K_4	4.0000	4.0000	6.0000	4.5356	6.0000	6.0000	6.2790	6.9282
$K_4 - e$	3.9039	3.9327	5.1190	4.4721	5.1231	5.2716	5.8985	6.3246
$K_{1,2,2}$	4.9443	4.9761	6.4644	5.6569	6.4721	6.5891	8.1326	8.9443
F_2	4.6847	4.8284	6.1058	5.7889	7.1231	7.2388	7.4293	7.7460
Prism	6.0000	6.0000	8.0000	7.1525	8.0000	8.0000	9.5877	10.3923
Petersen	10.0000	10.0000	10.6667	13.4164	16.0000	16.0000	16.5289	17.3205

Table 4. Lower bounds (left of $\mathcal{E}(G)$) and upper bounds (right of $\mathcal{E}(G)$) for the energy: $2m/\lambda_1$ (Corollary 1), $2R$ [1], the refined bound (11), the walk bound $\sum_v h_v = \sum_v d_v^{3/2} W_4(v)^{-1/2}$ (Corollary 1), and the bounds of Corollary 5 compared with McClelland's $\sqrt{2mn}$.

$n \geq 3$ vertices, suggested by (O1), would be a considerable strengthening. Note that, by Theorem 10(c), $\mathrm{ESO}(G) \geq \sqrt{2}\,\mathcal{E}(G)$ holds for every connected graph with $\delta \geq 2$.

18 Concluding remarks

We have introduced topological indices in which vertex degrees are replaced by vertex energies, and developed a local spectral theory that allows one to prove sharp inequalities for them. The main tools are the Hölder-type lower bound and the common-neighbour upper bound for $\mathcal{E}(v)$ (Theorems 2 and 3), the 2×2-minor identities for the positive and negative parts of A (Lemma 3 and Theorem 5), and the multiplicativity of $|A|$ under Kronecker products (Theorem 11). Along the way we obtained several results of independent interest for graph energy itself: the lower bounds $\mathcal{E}(G) \geq \sum_v d_v^{3/2} W_4(v)^{-1/2} \geq 2m/\lambda_1$, a refinement of McClelland's inequality involving the number of quadrangles, a refinement of the energy–Randić inequality which is exact for complete graphs, a characterization of complete multipartite graphs by an edge condition on vertex energies, and improvements of recent energy–Sombor inequalities.

Beyond these edge-level tools, the Perron-refined bounds of Section 11 show that the classical Koolen–Moulton argument works vertex by vertex, and the product and join theorems of Sections 9, 13 and 14 show that

vertex energies behave multiplicatively under tensor products, are sandwiched under Cartesian products and shift by explicit constants under joins of regular graphs. These results make it possible to compute the new indices exactly for many infinite families.

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