International Journal of Computer Applications (0975 - 8887)
Volume 187 - No.135, July 2026

The Minimum Hop Hub Distance Energy of a Graph

Abdulkafi Sanad
School of Mathematics and Statistics
Yunnan University, Kunming 650500, China

Abaid Ullah
School of Mathematics and Statistics
Yunnan University, Kunming 650500, China

Abdulqawe Kaed
Department of Mathematics, Faculty of Applied Science
Thamar University, Dhamar, Yemen

ABSTRACT

This paper introduces the minimum hop hub distance matrix of a connected graph and the associated graph energy, denoted $E_{hd}(G)$. The matrix is obtained from the distance matrix by placing the value 1 in every diagonal position indexed by a vertex of a prescribed minimum hop hub set, so that the new invariant couples the metric structure of the graph with the hop hub number $h_h(G)$. Exact closed forms of the characteristic polynomial, the spectrum and the energy are established for complete graphs, complete bipartite graphs $K_{p,p}$ and double stars $S_{p,p}$, each derived by an explicit eigenvector decomposition rather than by inspection. Two coefficient identities that had been stated in terms of the size q are shown to depend instead on the second distance moment $W_2(G) = \sum_{i<j} d(v_i, v_j)^2$, equivalently on the Wiener and hyper-Wiener indices; corrected statements and proofs are supplied. A structural decomposition $\mathcal{A}^H_{hd}(G) = D(G) + \mathrm{diag}(\chi_H)$ is exploited to obtain Weyl-type eigenvalue interlacing with the distance matrix, the perturbation bound $|E_{hd}(G) - E_D(G)| \leq h_h(G)$, bounds of McClelland and Koolen–Moulton type, and the sharp lower bound $E_{hd}(G) \geq p$ for every connected graph of order p, with equality precisely for the complete graph. Since the energy depends on the choice of minimum hop hub set, the genuine invariants $E^-_{hd}(G)$, $E^+_{hd}(G)$ and the spread $\sigma(G) = E^+_{hd}(G) - E^-_{hd}(G)$ are introduced and bounded by $2h_h(G)$. All theoretical claims are supported by an exhaustive computational evaluation over 45 named graphs, 448 minimum hop hub sets and 2074 random connected graphs, reported through six tables and four figures.

General Terms

Graph Theory, Spectral Graph Theory, Algorithms

Keywords

Minimum hop hub set, minimum hop hub distance matrix, minimum hop hub distance energy, distance energy, Wiener index, hyper-Wiener index, graph energy

1. INTRODUCTION

Throughout this paper $G = (V, E)$ denotes a simple, finite, undirected and *connected* graph without loops or multiple edges. The order and the size of G are written $p = |V|$ and $q = |E|$, and $\Delta(G)$, $\delta(G)$ denote the maximum and the minimum degree. The distance $d(u, v)$ is the length of a shortest (u, v)-path, and $\mathrm{diam}(G) = \max_{u,v} d(u, v)$. Connectivity is assumed throughout because every matrix considered below has the distances of G as its off-diagonal entries, and these are finite only when G is connected. For graph theoretic terminology not defined here the reader is referred to Harary [18].

1.1 Hub sets, hop domination and hop hub sets

Walsh [33] introduced hub sets in 2006. For $H \subseteq V$ and $x, y \in V$, an *H-path* between x and y is a path all of whose internal vertices belong to H; the degenerate cases in which the path is the single edge xy, or a single vertex when $x = y$, are admitted and are called trivial. A set $H \subseteq V$ is a *hub set* of G if for every $x, y \in V - H$ there exists an H-path in G between x and y. The minimum cardinality of a hub set is the *hub number* $h(G)$. Structural and algorithmic properties of $h(G)$ were developed by Grauman et al. [12]. A set $S \subseteq V$ is *dominating* if every vertex of $V - S$ has a neighbour in S, and the corresponding minimum cardinality is the domination number $\gamma(G)$ [19].
Ayyaswamy and Natarajan [3] introduced hop domination in 2015: a set $S \subseteq V$ is *hop dominating* if every $v \in V - S$ satisfies $d(u, v) = 2$ for some $u \in S$, and $\gamma_h(G)$ denotes the minimum cardinality of such a set. Further properties of hop domination were obtained by Chen and Wang [9]. Combining the two notions, Sahal et al. [30] introduced the *hop hub number* $h_h(G)$ in 2023; related parameters were studied in [24, 31], and domination-type parameters in hypergraphs in [32].

1.2 Graph energy

The energy of a graph was introduced by Gutman [14] in 1978 as the sum of the absolute values of the eigenvalues of the adjacency matrix $A(G)$, where $A_{ij} = 1$ if $v_iv_j \in E$ and $A_{ij} = 0$ otherwise. Writing the eigenvalues of $A(G)$ in non-increasing order as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$ and listing the distinct eigenvalues $\lambda_1, \ldots, \lambda_s$ with multiplicities $m_1, \ldots, m_s$, the multiset

$$\mathrm{Spec}(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_s \\ m_1 & m_2 & \cdots & m_s \end{pmatrix}$$

is the adjacency spectrum of G. The concept originates in the work of Coulson [10] on the total π-electron energy within the Hückel molecular orbital model, and it retains chemical significance in the molecular orbital theory of conjugated molecules [2, 11, 13, 16]. General mathematical properties, bounds and extremal results are surveyed in [1, 4, 5, 7, 8, 15, 17, 20, 22, 23, 26, 28].
Replacing the adjacency matrix by the distance matrix $D(G) = (d(v_i, v_j))$ yields the *distance energy* $E_D(G)$ of Indulal, Gutman and Vijayakumar [20], whose bounds and extremal properties were studied in [7, 8, 17, 28]. A parallel line of research seeds the diagonal of a matrix with the indicator vector of a distinguished minimum vertex set: Adiga et al. [1] did so with a minimum covering set, Mathad and Mahde [25] with a minimum hub set, giving the minimum hub energy $\mathcal{E}_H(G)$, and Palani and Lalitha [27] with a minimum hop dominating set, giving the minimum hop dominating energy $\mathcal{E}_h(G)$.

1.3 Research gap and contribution

Two observations motivate the present work. First, all of the seeded energies mentioned above perturb the *adjacency* matrix and therefore see only the first neighbourhood of each vertex; none of them records the global metric structure of the graph. Second, the distance energy $E_D(G)$ records the metric structure but is blind to the connectivity role played by individual vertices. The hop hub number is precisely a parameter that measures how few vertices suffice to route all remaining pairs while simultaneously hop dominating the graph, so seeding the *distance* matrix with a minimum hop hub set produces an invariant that reflects both aspects at once. To the best of the authors' knowledge no such matrix has been studied.
The contributions of this paper are the following.

—The minimum hop hub distance matrix $\mathcal{A}^H_{hd}(G)$ and its energy $E_{hd}(G)$ are defined for connected graphs (Section 3), and the decomposition $\mathcal{A}^H_{hd}(G) = D(G) + \mathrm{diag}(\chi_H)$ is isolated as the structural tool used throughout.

—Because $E_{hd}(G)$ depends on the chosen minimum hop hub set, the quantities $E^-_{hd}(G)$, $E^+_{hd}(G)$ and the spread $\sigma(G)$ are introduced; these *are* graph invariants, and $\sigma(G) \le 2h_h(G)$ is proved (Theorem 8).

—Two coefficient identities announced in terms of the size q are shown to be false in general and are replaced by correct statements involving the second distance moment $W_2(G)$, equivalently the Wiener and hyper-Wiener indices (Theorems 10 and 12, Remark 11).

—Weyl-type interlacing with the distance matrix, the perturbation bound $|E_{hd}(G) - E_D(G)| \le h_h(G)$, bounds of McClelland and Koolen–Moulton type, a Wiener-index lower bound on the spectral radius, and the sharp bound $E_{hd}(G) \ge p$ with equality only for K_p are established (Section 5).

—Exact spectra and energies of K_p, $K_{p,p}$ and $S_{p,p}$ are derived by explicit eigenvector decomposition (Section 6); the double star formula is shown to require a case distinction that had been overlooked (Theorem 27).

—A structural analysis (Section 7) and an exhaustive computational evaluation (Section 8) are provided, the latter covering 45 named graphs, 448 minimum hop hub sets and 2074 random connected graphs, and reported in six tables and four figures.

2. PRELIMINARIES

This section collects the notions used later. Beyond the distance $d(u, v)$, the following distance-based topological indices are required.

DEFINITION 1. *Let G be a connected graph of order p. The* Wiener index *[34] and the* second distance moment *of G are*

$$W(G) = \sum_{1 \le i < j \le p} d(v_i, v_j), \quad W_2(G) = \sum_{1 \le i < j \le p} d(v_i, v_j)^2,$$

and the hyper-Wiener index *[29, 21] is $WW(G) = \frac{1}{2}\big(W(G) + W_2(G)\big)$. Consequently $W_2(G) = 2WW(G) - W(G)$.*

Since $d(v_i, v_j) \ge 1$ for $i \ne j$, one has $W_2(G) \ge W(G) \ge \binom{p}{2}$, with either equality holding if and only if $\mathrm{diam}(G) = 1$, that is, if and only if $G \cong K_p$. Moreover $W_2(G) = q$ holds only when $G \cong K_p$, a fact that will explain the corrections made in Section 4.

DEFINITION 2. *[30] A hub set H of G is a* hop hub set *if for every $v \in V - H$ there exists $u \in H$ with $d(u, v) = 2$. The minimum cardinality of a hop hub set of G is the* hop hub number, *denoted $h_h(G)$. A hop hub set of cardinality $h_h(G)$ is called a* minimum hop hub set, *and $\mathcal{H}(G)$ denotes the family of all minimum hop hub sets of G.*

THEOREM 3. *[30] The hop hub numbers of some specific classes of graphs are as follows.*

(*1*) *For the complete graph K_n, $h_h(K_n) = n$.*
(*2*) *For the complete bipartite graph $K_{n,m}$ with $n + m \ge 3$, $h_h(K_{n,m}) = 2$.*
(*3*) *For the double star $S_{n,m}$, $h_h(S_{n,m}) = 2$.*

The complete graph, the complete bipartite graph and the double star are recalled in Definitions 21, 24 and 26 respectively.
Two classical facts from matrix analysis are used repeatedly and are recorded here for completeness. For real symmetric $p \times p$ matrices X and Y with eigenvalues arranged in non-increasing order, Weyl's inequality gives

$$\lambda_i(X) + \lambda_p(Y) \;\le\; \lambda_i(X + Y) \;\le\; \lambda_i(X) + \lambda_1(Y) \qquad (1)$$

and the trace norm $\|X\|_* = \sum_{i=1}^{p} |\lambda_i(X)|$ is a norm on the space of real symmetric matrices, so that

$$\big|\, \|X + Y\|_* - \|X\|_* \,\big| \;\le\; \|Y\|_*. \qquad (2)$$

Both statements may be found in Bhatia [6].

3. THE MINIMUM HOP HUB DISTANCE MATRIX AND ENERGY

DEFINITION 4. *Let G be a connected graph of order p with $V = \{v_1, v_2, \ldots, v_p\}$, and let H be a minimum hop hub set of G. The* minimum hop hub distance matrix *of G with respect to H is the $p \times p$ matrix $\mathcal{A}^H_{hd}(G) = (a_{ij})$ defined by*

$$a_{ij} = \begin{cases} 1, & \text{if } i = j \text{ and } v_i \in H, \\ d(v_i, v_j), & \text{otherwise.} \end{cases}$$

Its characteristic polynomial is $f_p(G, \lambda) = \det\big(\lambda I - \mathcal{A}^H_{hd}(G)\big)$, and its eigenvalues, which are real because $\mathcal{A}^H_{hd}(G)$ is real and *symmetric, are written* $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$ *and are called the* minimum hop hub distance eigenvalues *of* G. *The* minimum hop hub distance energy *of G is*

$$E^H_{hd}(G) = \sum_{i=1}^{p} |\lambda_i|.$$

When the choice of H *is clear from the context the superscript is suppressed and one writes* $\mathcal{A}_{hd}(G)$ *and* $E_{hd}(G)$.

Note that $a_{ii} = d(v_i, v_i) = 0$ whenever $v_i \notin H$, so the diagonal of $\mathcal{A}^H_{hd}(G)$ is exactly the indicator vector of H. This yields the decomposition on which the entire paper rests.

OBSERVATION 5. *Let* $D(G)$ *be the distance matrix of* G *and let* $\chi_H \in \{0,1\}^p$ *be the indicator vector of* H. *Then*

$$\mathcal{A}^H_{hd}(G) = D(G) + \operatorname{diag}(\chi_H), \tag{3}$$

where $\operatorname{diag}(\chi_H)$ *is positive semidefinite with eigenvalues* 1 *(multiplicity* $h_h(G)$*) and* 0 *(multiplicity* $p - h_h(G)$*); in particular* $\|\operatorname{diag}(\chi_H)\|_* = \operatorname{tr}\operatorname{diag}(\chi_H) = h_h(G)$.

Equation (3) states that $\mathcal{A}^H_{hd}(G)$ is a rank-$h_h(G)$, norm-one, positive semidefinite perturbation of the distance matrix. Every spectral result of Section 5 is a consequence of this single observation, and it also explains why $E_{hd}(G)$ and $E_D(G)$ are numerically so close in the computations of Section 8.

3.1 Dependence on the chosen minimum hop hub set

A graph may possess many minimum hop hub sets, and different choices may produce different spectra. The cycle C_6 illustrates this phenomenon completely.

EXAMPLE 6. *Let* $G = C_6$ *with* $V = \{v_1, \ldots, v_6\}$ *and edges* $v_i v_{i+1}$ *(indices modulo* 6*). Exhaustive enumeration shows* $h_h(C_6) = 3$ *and* $|\mathcal{H}(C_6)| = 18$.
For $H_1 = \{v_1, v_2, v_3\}$,

$$\mathcal{A}^{H_1}_{hd}(G) = \begin{pmatrix} 1 & 1 & 2 & 3 & 2 & 1 \\ 1 & 1 & 1 & 2 & 3 & 2 \\ 2 & 1 & 1 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{pmatrix},$$

whose characteristic polynomial factors over $\mathbb{Z}$ *as*

$$f_6(G,\lambda) = \big(\lambda^2 + 3\lambda - 2\big)\big(\lambda^4 - 6\lambda^3 - 34\lambda^2 + 3\lambda + 16\big)$$

$$= \lambda^6 - 3\lambda^5 - 54\lambda^4 - 87\lambda^3 + 93\lambda^2 + 42\lambda - 32.$$

Two eigenvalues are therefore $(-3 \pm \sqrt{17})/2$, *and the full spectrum is listed in Table 2, giving* $E^{H_1}_{hd}(G) = 18.5482$.
For $H_2 = \{v_1, v_3, v_4\}$ *the matrix differs from* $\mathcal{A}^{H_1}_{hd}(G)$ *only in the diagonal, and*

$$f_6(G,\lambda) = \lambda^6 - 3\lambda^5 - 54\lambda^4 - 87\lambda^3 + 85\lambda^2 + 34\lambda - 12,$$

which is irreducible over $\mathbb{Q}$*; here* $E^{H_2}_{hd}(G) = 18.1800$.
Hence $E_{hd}(C_6)$ *is not determined by* C_6 *alone: the minimum hop hub distance energy is not a graph invariant in general.*

Exhaustive computation over all 18 minimum hop hub sets of C_6 shows that only two distinct energies occur, 18.5482 realised by 6 sets and 18.1800 realised by the remaining 12; the two classes are exactly the orbits of $\mathcal{H}(C_6)$ under $\operatorname{Aut}(C_6)$, the first consisting of the sets of three consecutive vertices. Full data appear in Table 2. The following definition converts the failure of invariance into three genuine invariants, so that the theory can proceed unambiguously.

DEFINITION 7. *For a connected graph G put*

$$E^-_{hd}(G) = \min_{H \in \mathcal{H}(G)} E^H_{hd}(G),$$

$$E^+_{hd}(G) = \max_{H \in \mathcal{H}(G)} E^H_{hd}(G),$$

and call $\sigma(G) = E^+_{hd}(G) - E^-_{hd}(G)$ *the* minimum hop hub distance energy spread *of* G. *The graph* G *is* hop hub energetic *if* $\sigma(G) = 0$, *that is, if* $E_{hd}(G)$ *is well defined.*

Since $\mathcal{H}(G)$ is determined by G, the three quantities of Definition 7 are graph invariants. The spread admits a sharp and elementary bound.

THEOREM 8. *Let G be a connected graph. For all* $H_1, H_2 \in \mathcal{H}(G)$,

$$\big|E^{H_1}_{hd}(G) - E^{H_2}_{hd}(G)\big| \;\leq\; |H_1 \triangle H_2|$$

$$=\; 2\big(h_h(G) - |H_1 \cap H_2|\big),$$

and consequently $\sigma(G) \leq 2h_h(G)$.

PROOF. By Observation 5, $\mathcal{A}^{H_1}_{hd}(G) - \mathcal{A}^{H_2}_{hd}(G) = \operatorname{diag}(\chi_{H_1} - \chi_{H_2})$, a diagonal matrix whose entries are $+1$ on $H_1 - H_2$, -1 on $H_2 - H_1$ and 0 elsewhere. Its trace norm is therefore $|H_1 \triangle H_2|$. Applying (2) with $X = \mathcal{A}^{H_2}_{hd}(G)$ and $Y = \operatorname{diag}(\chi_{H_1} - \chi_{H_2})$ gives the first inequality. Since $|H_1| = |H_2| = h_h(G)$, one has $|H_1 \triangle H_2| = 2(h_h(G) - |H_1 \cap H_2|) \leq 2h_h(G)$. ■

PROPOSITION 9. *If* $\operatorname{Aut}(G)$ *acts transitively on* $\mathcal{H}(G)$, *then G is hop hub energetic.*

PROOF. Let $H_1, H_2 \in \mathcal{H}(G)$ and let $\varphi \in \operatorname{Aut}(G)$ satisfy $\varphi(H_1) = H_2$. Let P be the permutation matrix of φ. Automorphisms preserve distances, so $P^{\mathsf{T}} D(G) P = D(G)$, and $P^{\mathsf{T}} \operatorname{diag}(\chi_{H_2}) P = \operatorname{diag}(\chi_{H_1})$. Hence $P^{\mathsf{T}} \mathcal{A}^{H_2}_{hd}(G) P = \mathcal{A}^{H_1}_{hd}(G)$, so the two matrices are similar and share a spectrum, whence $E^{H_1}_{hd}(G) = E^{H_2}_{hd}(G)$. ■
Proposition 9 accounts for every hop hub energetic graph detected in Section 8; it also shows that Example 6 is sharp in the sense that $\mathcal{H}(C_6)$ splits into exactly two automorphism orbits and exactly two energies occur.

4. SPECTRAL PROPERTIES

THEOREM 10. *Let G be a connected graph of order p, let* $H \in \mathcal{H}(G)$, *and let*

$$f_p(G,\lambda) = c_0\lambda^p + c_1\lambda^{p-1} + c_2\lambda^{p-2} + \cdots + c_p$$

be the characteristic polynomial of $\mathcal{A}^H_{hd}(G)$. *Then*

$$c_0 = 1, \quad c_1 = -h_h(G), \quad c_2 = \binom{h_h(G)}{2} - W_2(G),$$

where $W_2(G)$ *is the second distance moment of Definition 1.*

PROOF. That $c_0 = 1$ is immediate from $f_p(G,\lambda) = \det(\lambda I - \mathcal{A}^H_{hd}(G))$.
For $k \geq 1$, $(-1)^k c_k$ equals the sum of the determinants of all $k \times k$ principal submatrices of $\mathcal{A}^H_{hd}(G)$. For $k = 1$ this sum is the trace,

and by Definition 4 the diagonal entries are 1 on H and 0 off H, so $(-1)^1 c_1 = \operatorname{tr}\mathcal{A}_{hd}^H(G) = |H| = h_h(G)$, that is $c_1 = -h_h(G)$. For $k = 2$, using $a_{ij} = a_{ji}$,

$$\begin{aligned} c_2 &= \sum_{1\le i<j\le p} \begin{vmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{vmatrix} \\ &= \sum_{1\le i<j\le p} \left(a_{ii}a_{jj} - a_{ij}^2\right) \\ &= \sum_{1\le i<j\le p} a_{ii}a_{jj} - \sum_{1\le i<j\le p} a_{ij}^2. \end{aligned}$$

In the first sum the product $a_{ii}a_{jj}$ equals 1 exactly when both v_i and v_j lie in H, and 0 otherwise; the number of such pairs is $\binom{|H|}{2} = \binom{h_h(G)}{2}$. In the second sum $a_{ij} = d(v_i, v_j)$ for $i \neq j$, so $\sum_{i<j} a_{ij}^2 = \sum_{i<j} d(v_i, v_j)^2 = W_2(G)$. Combining the two evaluations gives the stated formula. ■

REMARK 11. *The second sum above must not be read as the size q of G. That reading is valid for a $\{0,1\}$ matrix, where $a_{ij}^2 = a_{ij}$ and each edge contributes 1, but here the off-diagonal entries are distances and $\sum_{i<j} a_{ij}^2 = W_2(G)$. Since $W_2(G) \ge W(G) \ge \binom{p}{2} \ge q$, with $W_2(G) = q$ only for $G \cong K_p$, replacing $W_2(G)$ by q underestimates $|c_2|$ for every non-complete graph. Example 6 confirms the corrected statement: for C_6 one has $h_h = 3$, $q = 6$ and $W_2(C_6) = 57$, and the computed coefficient is $c_2 = -54 = \binom{3}{2} - 57$, whereas $\binom{3}{2} - q = -3$. The same correction applies to Theorem 12(ii) below.*

THEOREM 12. *Let G be a connected graph of order p, let $H \in \mathcal{H}(G)$ and let $\lambda_1, \ldots, \lambda_p$ be the eigenvalues of $\mathcal{A}_{hd}^H(G)$. Then*

(i) $\displaystyle\sum_{i=1}^{p} \lambda_i = h_h(G)$;

(ii) $\displaystyle\sum_{i=1}^{p} \lambda_i^2 = h_h(G) + 2W_2(G) = h_h(G) + 4WW(G) - 2W(G)$;

(iii) $\displaystyle\sum_{1\le i<j\le p} \lambda_i\lambda_j = \binom{h_h(G)}{2} - W_2(G)$.

PROOF. (i) The sum of the eigenvalues equals the trace, and as in the proof of Theorem 10 the trace is $|H| = h_h(G)$.
(ii) The sum of the squares of the eigenvalues equals $\operatorname{tr}\left(\mathcal{A}_{hd}^H(G)\right)^2$. Hence

$$\begin{aligned} \sum_{i=1}^{p} \lambda_i^2 &= \sum_{i=1}^{p}\sum_{j=1}^{p} a_{ij}a_{ji} = \sum_{i=1}^{p} a_{ii}^2 + \sum_{i\neq j} a_{ij}^2 \\ &= \sum_{i=1}^{p} a_{ii}^2 + 2\sum_{1\le i<j\le p} a_{ij}^2. \end{aligned}$$

Since $a_{ii} \in \{0,1\}$, the first sum equals $|H| = h_h(G)$, and by Definition 4 the second equals $2\sum_{i<j} d(v_i, v_j)^2 = 2W_2(G)$. The alternative form follows from $W_2(G) = 2WW(G) - W(G)$ recorded in Definition 1.
(iii) This is Newton's identity $\sum_{i<j} \lambda_i\lambda_j = c_2$ together with Theorem 10, or equivalently $\sum_{i<j} \lambda_i\lambda_j = \frac{1}{2}\left[\left(\sum_i \lambda_i\right)^2 - \sum_i \lambda_i^2\right] = \frac{1}{2}\left[h_h(G)^2 - h_h(G) - 2W_2(G)\right] = \binom{h_h(G)}{2} - W_2(G)$. ■

Throughout the remainder of the paper the abbreviation

$$Q(G) \;=\; h_h(G) + 2W_2(G) \;=\; \sum_{i=1}^{p} \lambda_i^2 \tag{4}$$

is used for the second spectral moment.

THEOREM 13. *Let G be a connected graph with minimum hop hub set H. If $E_{hd}^H(G)$ is a rational number, then*

$$E_{hd}^H(G) \equiv |H| \pmod 2.$$

PROOF. Let $\lambda_1, \ldots, \lambda_p$ be the eigenvalues of $\mathcal{A}_{hd}^H(G)$, indexed so that $\lambda_1, \ldots, \lambda_r$ are positive and $\lambda_{r+1}, \ldots, \lambda_p$ are non-positive, and set $s = \lambda_1 + \cdots + \lambda_r$. Then

$$\begin{aligned} E_{hd}^H(G) &= (\lambda_1 + \cdots + \lambda_r) \\ &\quad -(\lambda_{r+1} + \cdots + \lambda_p) \\ &= 2(\lambda_1 + \cdots + \lambda_r) - \sum_{i=1}^{p} \lambda_i \\ &= 2s - |H|, \end{aligned}$$

the last step by Theorem 12(i). It remains to prove $s \in \mathbb{Z}$. The matrix $\mathcal{A}_{hd}^H(G)$ has integer entries, so its characteristic polynomial is monic with integer coefficients and each λ_i is an algebraic integer. Algebraic integers form a ring, hence s, being a sum of some of the λ_i, is an algebraic integer. By hypothesis $E_{hd}^H(G) \in \mathbb{Q}$, so $s = \frac{1}{2}\left(E_{hd}^H(G) + |H|\right) \in \mathbb{Q}$. A rational algebraic integer is a rational integer, so $s \in \mathbb{Z}$ and $E_{hd}^H(G) = 2s - |H| \equiv |H| \pmod 2$. ■

REMARK 14. *The argument that s is an algebraic integer cannot be omitted: without it the identity $E_{hd}^H(G) = 2s - |H|$ carries no arithmetic information, since s is a priori only a real number. The same device underlies the classical result of Bapat and Pati [5] that the ordinary graph energy is never an odd integer.*

5. BOUNDS AND COMPARISON WITH THE DISTANCE ENERGY

This section exploits the decomposition (3) systematically. Write $\mu_1 \ge \cdots \ge \mu_p$ for the eigenvalues of the distance matrix $D(G)$ and $E_D(G) = \sum_i |\mu_i|$ for the distance energy [20].

THEOREM 15 INTERLACING WITH THE DISTANCE MATRIX. *Let G be connected of order p and let $H \in \mathcal{H}(G)$. Then*

$$\mu_i \;\le\; \lambda_i \;\le\; \mu_i + 1, \qquad 1 \le i \le p.$$

PROOF. Apply (1) to $X = D(G)$ and $Y = \operatorname{diag}(\chi_H)$. By Observation 5 the eigenvalues of Y lie in $\{0,1\}$, so $\lambda_p(Y) = 0$ when $H \neq V$ and $\lambda_p(Y) = 1$ when $H = V$; in either case $\lambda_p(Y) \ge 0$ and $\lambda_1(Y) \le 1$. Hence $\mu_i + 0 \le \lambda_i \le \mu_i + 1$. ■

THEOREM 16 PERTURBATION BOUND. *Let G be connected and let $H \in \mathcal{H}(G)$. Then*

$$\left|E_{hd}^H(G) - E_D(G)\right| \;\le\; h_h(G).$$

Consequently $E_D(G) - h_h(G) \le E_{hd}^-(G) \le E_{hd}^+(G) \le E_D(G) + h_h(G)$.

PROOF. By Observation 5 and (2) with $X = D(G)$ and $Y = \operatorname{diag}(\chi_H)$,

$$\big|\, \|D(G) + \operatorname{diag}(\chi_H)\|_* - \|D(G)\|_* \,\big|$$

$$\le \|\mathrm{diag}(\chi_H)\|_* = h_h(G),$$

which is the assertion since $\|\mathcal{A}_{hd}^H(G)\|_* = E_{hd}^H(G)$ and $\|D(G)\|_* = E_D(G)$. ■

Theorem 16 explains the empirical closeness of E_{hd} and E_D observed in Table 5 and Figure 3: the new energy never departs from the distance energy by more than the hop hub number, which for many families is a small constant. It also re-derives $\sigma(G) \le 2h_h(G)$ independently of Theorem 8.

THEOREM 17 SPECTRAL RADIUS AND THE WIENER INDEX. *Let G be connected of order p and let $H \in \mathcal{H}(G)$. Then*

$$\lambda_1 \ \ge \ \frac{h_h(G) + 2W(G)}{p},$$

with equality if and only if the all-ones vector is an eigenvector of $\mathcal{A}_{hd}^H(G)$. Moreover

$$E_{hd}^H(G) \ \ge \ 2\lambda_1 - h_h(G)$$

$$\ge \ \frac{2\big(h_h(G) + 2W(G)\big)}{p} - h_h(G).$$

PROOF. Let $\mathbf{1}$ be the all-ones vector. The Rayleigh quotient gives

$$\lambda_1 \ \ge \ \frac{\mathbf{1}^\mathsf{T}\mathcal{A}_{hd}^H(G)\mathbf{1}}{\mathbf{1}^\mathsf{T}\mathbf{1}} = \frac{1}{p}\Big(\sum_i a_{ii} + \sum_{i\ne j} a_{ij}\Big)$$

$$= \frac{h_h(G) + 2W(G)}{p},$$

because $\sum_i a_{ii} = h_h(G)$ and $\sum_{i\ne j} a_{ij} = 2\sum_{i<j} d(v_i, v_j) = 2W(G)$. Equality in the Rayleigh quotient holds precisely when $\mathbf{1}$ is an eigenvector for λ_1.

For the second chain, let s be the sum of the positive eigenvalues. As in the proof of Theorem 13, $E_{hd}^H(G) = 2s - h_h(G)$. Since $\mathrm{tr}\,\mathcal{A}_{hd}^H(G) = h_h(G) > 0$ the matrix has at least one positive eigenvalue, so $s \ge \lambda_1$ and $E_{hd}^H(G) \ge 2\lambda_1 - h_h(G)$; the last inequality then follows from the first part. ■

The next result is the sharpest general lower bound obtained here. It shows that among all connected graphs of a given order the complete graph uniquely minimises the minimum hop hub distance energy, and that the minimum equals the order.

THEOREM 18. *Let G be a connected graph of order $p \ge 2$ and let $H \in \mathcal{H}(G)$. Then*

$$E_{hd}^H(G) \ \ge \ \Big(\frac{2}{p} - 1\Big)h_h(G) + \frac{4W(G)}{p} \ \ge \ p,$$

and $E_{hd}^H(G) = p$ holds if and only if $G \cong K_p$.

PROOF. The first inequality is Theorem 17 rearranged. For the second, note that $2/p - 1 \le 0$ for $p \ge 2$ and that $h_h(G) \le p$ always, whence

$$\Big(\frac{2}{p} - 1\Big)h_h(G) \ \ge \ \Big(\frac{2}{p} - 1\Big)p \ = \ 2 - p.$$

Moreover $d(v_i, v_j) \ge 1$ for $i \ne j$ gives $W(G) \ge \binom{p}{2}$ and therefore $4W(G)/p \ge 2(p-1)$. Adding the two estimates yields $E_{hd}^H(G) \ge (2-p) + 2(p-1) = p$.

Suppose now $E_{hd}^H(G) = p$. Every inequality used must then be an equality. The inequality $4W(G)/p \ge 2(p-1)$ enters with the strictly positive coefficient $4/p$, so $W(G) = \binom{p}{2}$, which forces $d(v_i, v_j) = 1$ for all $i \ne j$, that is $\mathrm{diam}(G) = 1$ and $G \cong K_p$. Conversely, if $G \cong K_p$ then $h_h(K_p) = p$ by Theorem 3, so $H = V$ and $\mathcal{A}_{hd}^H(K_p) = J_p$, the all-ones matrix, whose spectrum is $\{p, 0^{p-1}\}$; hence $E_{hd}(K_p) = p$. ■

THEOREM 19 MCCLELLAND-TYPE BOUNDS. *Let G be connected of order p, let $H \in \mathcal{H}(G)$, let $Q = Q(G)$ be as in* (4) *and let $\Delta_H = \big|\det \mathcal{A}_{hd}^H(G)\big|$. Then*

$$\sqrt{Q + p(p-1)\Delta_H^{2/p}} \ \le \ E_{hd}^H(G) \ \le \ \sqrt{pQ}.$$

In particular $E_{hd}^H(G) \ge \sqrt{Q}$, with equality if and only if $G \cong K_p$.

PROOF. For the upper bound, the Cauchy–Schwarz inequality gives

$$\Big(\sum_{i=1}^{p} |\lambda_i|\Big)^2 \le p\sum_{i=1}^{p} \lambda_i^2 = pQ.$$

For the lower bound, expand

$$E_{hd}^H(G)^2 = \sum_{i=1}^{p} \lambda_i^2 + \sum_{i\ne j} |\lambda_i||\lambda_j| = Q + \sum_{i\ne j} |\lambda_i||\lambda_j|.$$

The $p(p-1)$ summands are non-negative, so the arithmetic–geometric mean inequality yields

$$\sum_{i\ne j} |\lambda_i||\lambda_j| \ \ge \ p(p-1)\Big(\prod_{i\ne j} |\lambda_i||\lambda_j|\Big)^{1/(p(p-1))}$$

$$= p(p-1)\Delta_H^{2/p},$$

since $\prod_{i\ne j} |\lambda_i||\lambda_j| = \big(\prod_i |\lambda_i|\big)^{2(p-1)} = \Delta_H^{2(p-1)}$.

Finally $E_{hd}^H(G) \ge \sqrt{Q}$ is immediate from $E_{hd}^H(G)^2 = Q + \sum_{i\ne j} |\lambda_i||\lambda_j| \ge Q$, with equality if and only if $\lambda_i\lambda_j = 0$ for all $i \ne j$, that is, if and only if $\mathcal{A}_{hd}^H(G)$ has rank at most 1. A rank-one real symmetric matrix has the form $\varepsilon ww^\mathsf{T}$ with $\varepsilon \in \{\pm 1\}$; since the trace $h_h(G)$ is positive, $\varepsilon = +1$. If some $v_i \notin H$ then $a_{ii} = 0$ forces $w_i = 0$ and hence $a_{ij} = w_iw_j = 0$ for all j, contradicting $a_{ij} = d(v_i, v_j) \ge 1$. Therefore $H = V$, so $a_{ii} = w_i^2 = 1$ for every i and $a_{ij} = w_iw_j \in \{\pm 1\}$; as $a_{ij} = d(v_i, v_j) \ge 1$ this gives $d(v_i, v_j) = 1$ for all $i \ne j$, that is $G \cong K_p$. Conversely $\mathcal{A}_{hd}(K_p) = J_p$ has rank one and $\sqrt{Q} = \sqrt{p + 2\binom{p}{2}} = p = E_{hd}(K_p)$. ■

THEOREM 20 KOOLEN–MOULTON-TYPE BOUND. *Let G be connected of order $p \ge 2$ and let $H \in \mathcal{H}(G)$. Then*

$$E_{hd}^H(G) \ \le \ \lambda_1 + \sqrt{(p-1)\big(Q - \lambda_1^2\big)}.$$

PROOF. Since $\mathrm{tr}\,\mathcal{A}_{hd}^H(G) = h_h(G) > 0$, one has $\lambda_1 > 0$ and $E_{hd}^H(G) = \lambda_1 + \sum_{i=2}^{p} |\lambda_i|$. Cauchy–Schwarz applied to the last sum gives $\sum_{i=2}^{p} |\lambda_i| \le \sqrt{(p-1)\sum_{i=2}^{p} \lambda_i^2} = \sqrt{(p-1)(Q - \lambda_1^2)}$. ■

Theorem 20 is sharper than the McClelland upper bound of Theorem 19 whenever λ_1 is large relative to $\sqrt{Q/p}$, which is the typical situation here because $\mathcal{A}_{hd}^H(G)$ is a non-negative matrix with a dominant Perron-type eigenvalue. Numerical evidence is given in Table 4.

6. ENERGY OF SOME STANDARD FAMILIES

Exact spectra are now derived for three families. In each case the derivation proceeds by exhibiting an explicit invariant subspace decomposition, so that the characteristic polynomial is obtained constructively rather than asserted. Below J_n and I_n denote the all-ones and the identity matrix of order n, $\mathbf{1}_n$ the all-ones vector, and e_1 the first standard basis vector.

6.1 Complete graphs

DEFINITION 21. *[18] A graph G is a* complete graph *if every pair of its vertices is adjacent; the complete graph on p vertices is denoted K_p.*

THEOREM 22. *For every $p \geq 2$, $\mathcal{A}_{hd}(K_p) = J_p$,*

$$f_p(K_p, \lambda) = \lambda^{p-1}(\lambda - p),$$

$$\operatorname{Spec}\big(\mathcal{A}_{hd}(K_p)\big) = \begin{pmatrix} p & 0 \\ 1 & p-1 \end{pmatrix},$$

and $E_{hd}(K_p) = p$. Moreover K_p is hop hub energetic.

PROOF. By Theorem 3, $h_h(K_p) = p$, so the unique minimum hop hub set is $H = V$ and $\mathcal{H}(K_p) = \{V\}$; in particular $\sigma(K_p) = 0$. Every diagonal entry of $\mathcal{A}_{hd}(K_p)$ therefore equals 1, and every off-diagonal entry equals $d(v_i, v_j) = 1$, so $\mathcal{A}_{hd}(K_p) = J_p$. The matrix J_p has rank one with $J_p\mathbf{1}_p = p\mathbf{1}_p$ and $J_p x = 0$ for every $x \perp \mathbf{1}_p$, giving the stated spectrum and $f_p(K_p, \lambda) = \lambda^{p-1}(\lambda - p)$. Hence $E_{hd}(K_p) = |p| + (p-1)\cdot|0| = p$. ■

REMARK 23. *The complete graph is the extremal configuration for three of the results of Section 5 simultaneously. Since $D(K_p) = J_p - I_p$ has spectrum $\{p-1, (-1)^{p-1}\}$ and $\mathcal{A}_{hd}(K_p) = D(K_p) + I_p$, every distance eigenvalue is shifted by exactly $+1$, so Theorem 15 is attained at the upper end for all p indices at once. The $p-1$ eigenvalues equal to -1 are annihilated, which is why $E_{hd}(K_p) = p$ while $E_D(K_p) = 2(p-1)$; the discrepancy $E_D(K_p) - E_{hd}(K_p) = p - 2$ is within the bound $h_h(K_p) = p$ of Theorem 16. Finally K_p is the unique graph attaining both $E_{hd} = p$ in Theorem 18 and $E_{hd} = \sqrt{Q}$ in Theorem 19. Thus, although K_p has the largest possible hop hub number, it has the smallest possible minimum hop hub distance energy.*

6.2 Complete bipartite graphs

DEFINITION 24. *[18] A graph G is* bipartite *if V admits a partition into sets V_1 and V_2 such that every edge joins a vertex of V_1 to a vertex of V_2. If in addition every vertex of V_1 is joined to every vertex of V_2, then G is* complete bipartite *and is denoted $K_{m,n}$ where $|V_1| = m$ and $|V_2| = n$. The graph $K_{1,n}$ is a star.*

THEOREM 25. *Let $p \geq 2$. Then*

$$f_{2p}(K_{p,p}, \lambda) = (\lambda+2)^{2p-4}\big[\lambda^2 - (p-3)\lambda - (p-1)\big]$$

$$\times \big[\lambda^2 - (3p-3)\lambda - (3p+1)\big],$$

and

$$E_{hd}(K_{p,p}) = (4p-8) + \sqrt{p^2 - 2p + 5}$$

$$+ \sqrt{9p^2 - 6p + 13}.$$

Moreover $K_{p,p}$ is hop hub energetic.

PROOF. Write $V = U \cup V'$ with $U = \{u_1, \ldots, u_p\}$ and $V' = \{v_1, \ldots, v_p\}$. In $K_{p,p}$ two vertices in the same part are at distance 2 and two vertices in different parts at distance 1. By Theorem 3, $h_h(K_{p,p}) = 2$, and a set $\{u_i, v_j\}$ with one vertex in each part is a minimum hop hub set: any two vertices of the same part are joined by a path through the chosen vertex of the other part, any two vertices of different parts are adjacent, and every vertex outside the set is at distance 2 from the chosen vertex of its own part. Conversely a 2-set inside one part fails the hop condition, since every vertex of the opposite part is at distance 1 from both of its elements. Hence $\mathcal{H}(K_{p,p})$ consists exactly of the p^2 transversal pairs, on which $\operatorname{Aut}(K_{p,p})$ acts transitively, so $K_{p,p}$ is hop hub energetic by Proposition 9 and one may take $H = \{u_1, v_1\}$.
Ordering the vertices as $u_1, \ldots, u_p, v_1, \ldots, v_p$ gives the block form

$$\mathcal{A}^H_{hd}(K_{p,p}) = \begin{pmatrix} B & J_p \\ J_p & B \end{pmatrix}, \qquad B = 2(J_p - I_p) + e_1e_1^{\mathsf{T}}.$$

For a vector $x \in \mathbb{R}^p$ the block structure maps $(x, x)^{\mathsf{T}}$ to $((B + J_p)x, (B + J_p)x)^{\mathsf{T}}$ and $(x, -x)^{\mathsf{T}}$ to $((B - J_p)x, -(B - J_p)x)^{\mathsf{T}}$. Therefore

$$\operatorname{Spec}\big(\mathcal{A}^H_{hd}(K_{p,p})\big) = \operatorname{Spec}(B + J_p) \uplus \operatorname{Spec}(B - J_p),$$

and it suffices to analyse $C_a = aJ_p - 2I_p + e_1e_1^{\mathsf{T}}$ for $a = 3$ (giving $B + J_p$) and $a = 1$ (giving $B - J_p$).
Let $\mathcal{U} = \{x \in \mathbb{R}^p : x_1 = 0,\ \mathbf{1}_p^{\mathsf{T}}x = 0\}$, a subspace of dimension $p-2$. For $x \in \mathcal{U}$ one has $J_p x = 0$ and $e_1e_1^{\mathsf{T}}x = 0$, so $C_a x = -2x$. This produces the eigenvalue -2 with multiplicity $p-2$ in each of the two blocks, hence multiplicity $2p-4$ in total.
The orthogonal complement of $\mathcal{U}$ inside $\mathbb{R}^p$ is spanned by e_1 and $s = \sum_{i\geq 2} e_i$, and this pair spans a C_a-invariant subspace:

$$C_a e_1 = (a-1)e_1 + as,$$

$$C_a s = a(p-1)e_1 + \big(a(p-1) - 2\big)s.$$

The matrix of C_a restricted to $\operatorname{span}\{e_1, s\}$ in this basis is $\begin{pmatrix} a-1 & a(p-1) \\ a & a(p-1)-2 \end{pmatrix}$, with trace $ap - 3$ and determinant $(a-1)(a(p-1)-2) - a^2(p-1) = 2 - a(p+1)$. The corresponding characteristic polynomial is $\lambda^2 - (ap-3)\lambda + 2 - a(p+1)$. Substituting $a = 1$ gives $\lambda^2 - (p-3)\lambda - (p-1)$ and $a = 3$ gives $\lambda^2 - (3p-3)\lambda - (3p+1)$, which establishes the stated factorisation.
Each of the two quadratics has negative constant term for $p \geq 2$, namely $-(p-1)$ and $-(3p+1)$, so each has one positive and one negative root, and the sum of the absolute values of its roots equals the square root of its discriminant. These discriminants are $(p-3)^2 + 4(p-1) = p^2 - 2p + 5$ and $(3p-3)^2 + 4(3p+1) = 9p^2 - 6p + 13$. Adding the contribution $2(2p-4) = 4p - 8$ of the eigenvalue -2 gives the energy formula. For $p = 2$ the exponent $2p - 4$ vanishes and the formula remains valid. ■

6.3 Double stars

DEFINITION 26. *[13] The* double star $S_{n,m}$ *is obtained from $K_{1,n-1}$ and $K_{1,m-1}$ by joining their centres v_0 and u_0, so that $V(S_{n,m}) = V(K_{1,n-1}) \cup V(K_{1,m-1})$ and $E(S_{n,m}) = \{v_0u_0,\ v_0v_i,\ u_0u_j : 1 \leq i \leq n-1,\ 1 \leq j \leq m-1\}$.*

Every double star is a tree and hence bipartite. The next theorem corrects the range of validity of the energy formula: the closed form $(9p - 13) + \sqrt{p^2 + 6p - 3}$ is valid only for $p \geq 5$, because for $p \in \{3, 4\}$ one of the two quadratic factors acquires a negative root and its contribution to the energy changes.

THEOREM 27. *Let $p \geq 3$. Then*

$$f_{2p}(S_{p,p}, \lambda) = (\lambda+2)^{2p-4}\big[\lambda^2 + (p+1)\lambda - (p-1)\big]$$

$$\times \big[\lambda^2 - (5p-5)\lambda + (p-5)\big],$$

and

$$E_{hd}(S_{p,p}) = \begin{cases} (4p-8) + \sqrt{p^2+6p-3} \\ \quad +\sqrt{25p^2-54p+45}, & p \in \{3,4\}, \\ (9p-13) + \sqrt{p^2+6p-3}, & p \geq 5. \end{cases}$$

Moreover $S_{p,p}$ is hop hub energetic, $\mathcal{H}(S_{p,p}) = \{\{v_0, u_0\}\}$.

PROOF. Put $n = p-1$ and order the vertices as $v_0, v_1, \ldots, v_n, u_0, u_1, \ldots, u_n$. The distances in $S_{p,p}$ are $d(v_0,u_0) = 1$, $d(v_0,v_i) = d(u_0,u_j) = 1$, $d(v_0,u_j) = d(u_0,v_i) = 2$, $d(v_i,v_j) = d(u_i,u_j) = 2$ for $i \neq j$, and $d(v_i,u_j) = 3$, for $1 \leq i,j \leq n$.
The set $H = \{v_0, u_0\}$ is a hop hub set: any two leaves are joined by a path whose internal vertices are centres, and every leaf is at distance 2 from the opposite centre. It is minimum since $h_h(S_{p,p}) = 2$ by Theorem 3. It is also the only one: a 2-set containing a leaf v_i and any other vertex fails the hub condition, because the leaves u_j and u_k with $j \neq k$ then possess no H-path unless $u_0 \in H$, and symmetrically for v_0. Hence $\mathcal{H}(S_{p,p}) = \{\{v_0,u_0\}\}$ and $\sigma(S_{p,p}) = 0$.
With the above ordering,

$$\mathcal{A}^H_{hd}(S_{p,p}) = \begin{pmatrix} X & Y \\ Y & X \end{pmatrix},$$

$$X = \begin{pmatrix} 1 & \mathbf{1}_n^\mathsf{T} \\ \mathbf{1}_n & 2(J_n - I_n) \end{pmatrix}, \quad Y = \begin{pmatrix} 1 & 2\mathbf{1}_n^\mathsf{T} \\ 2\mathbf{1}_n & 3J_n \end{pmatrix}.$$

Both X and Y are symmetric, so exactly as in Theorem 25 the spectrum splits as $\operatorname{Spec}(X+Y) \uplus \operatorname{Spec}(X-Y)$, where

$$X + Y = \begin{pmatrix} 2 & 3\mathbf{1}_n^\mathsf{T} \\ 3\mathbf{1}_n & 5J_n - 2I_n \end{pmatrix},$$

$$X - Y = \begin{pmatrix} 0 & -\mathbf{1}_n^\mathsf{T} \\ -\mathbf{1}_n & -J_n - 2I_n \end{pmatrix}.$$

Let $\mathcal{U} = \{(0,x)^\mathsf{T} : \mathbf{1}_n^\mathsf{T} x = 0\}$ with $x \in \mathbb{R}^n$, of dimension $n-1 = p-2$. For such vectors $J_n x = 0$ and the coupling terms vanish, so $(X+Y)(0,x)^\mathsf{T} = -2(0,x)^\mathsf{T}$ and likewise $(X-Y)(0,x)^\mathsf{T} = -2(0,x)^\mathsf{T}$. This yields the eigenvalue -2 with total multiplicity $2(p-2) = 2p-4$.
On the complementary invariant subspace spanned by e_0 and $s = \sum_{i=1}^n e_i$ one computes

$$(X+Y)e_0 = 2e_0 + 3s, \qquad (X+Y)s = 3n\, e_0 + (5n-2)s,$$

$$(X-Y)e_0 = -s, \qquad (X-Y)s = -n\, e_0 - (n+2)s.$$

The associated 2×2 matrices are $\left(\begin{smallmatrix} 2 & 3n \\ 3 & 5n-2 \end{smallmatrix}\right)$ and $\left(\begin{smallmatrix} 0 & -n \\ -1 & -n-2 \end{smallmatrix}\right)$, with traces $5n = 5p-5$ and $-(n+2) = -(p+1)$, and determinants $2(5n-2) - 9n = n-4 = p-5$ and $-n = -(p-1)$ respectively. Hence the two quadratic factors are $\lambda^2 - (5p-5)\lambda + (p-5)$ and $\lambda^2 + (p+1)\lambda - (p-1)$, as claimed.
For the energy, the factor $\lambda^2 + (p+1)\lambda - (p-1)$ has constant term $-(p-1) < 0$ for $p \geq 3$, so its roots have opposite signs and the sum of their absolute values is $\sqrt{(p+1)^2 + 4(p-1)} = \sqrt{p^2+6p-3}$. The factor $\lambda^2 - (5p-5)\lambda + (p-5)$ has root sum $5p-5 > 0$ and root product $p-5$, and its discriminant $25p^2 - 54p + 45$ is positive for all real p, since the discriminant of $25p^2 - 54p + 45$ regarded as a quadratic in p equals $54^2 - 4 \cdot 25 \cdot 45 = -1584 < 0$. Two cases arise.

—If $p \geq 5$ then $p-5 \geq 0$ and the root sum is positive, so both roots are non-negative and the sum of their absolute values equals $5p-5$. Adding $2(2p-4) = 4p-8$ gives $E_{hd}(S_{p,p}) = (9p-13) + \sqrt{p^2+6p-3}$.

—If $p \in \{3,4\}$ then $p-5 < 0$, so the roots have opposite signs and the sum of their absolute values equals $\sqrt{25p^2-54p+45}$ rather than $5p-5$. This yields the first branch of the formula.

■

REMARK 28. *The two branches differ genuinely: for $p = 3$ the correct value is $4 + 2\sqrt{6} + 6\sqrt{3} = 19.2913$ whereas $(9p-13) + \sqrt{p^2+6p-3} = 18.8990$, and for $p = 4$ the correct value is $8 + \sqrt{37} + \sqrt{229} = 29.2155$ whereas the single formula gives 29.0828. The two branches agree at $p = 5$, where $p - 5 = 0$ makes one root vanish. Consequently $\det \mathcal{A}_{hd}(S_{p,p}) = 0$ if and only if $p = 5$, so $S_{5,5}$ is the unique member of the family whose minimum hop hub distance matrix is singular, and it is therefore also the member for which the McClelland lower bound of Theorem 19 degenerates to $\sqrt{Q}$. This is visible in Table 4, where the two lower bounds for $S_{5,5}$, namely 21.6333 and 21.6400, agree to within 0.007.*

7. STRUCTURAL ANALYSIS AND INTERPRETATION

This section interprets the results obtained above. All numerical values quoted here are produced by the computational procedure described in Section 8.

7.1 Energy density and asymptotic behaviour

Expanding the closed forms of Theorems 22, 25 and 27 for large p gives

$$E_{hd}(K_p) = p, \qquad E_{hd}(K_{p,p}) = 8p - 10 + O(p^{-1}),$$

$$E_{hd}(S_{p,p}) = 10p - 10 + O(p^{-1}).$$

Since $K_{p,p}$ and $S_{p,p}$ have order $n = 2p$ while K_p has order $n = p$, the *energy density* E_{hd}/n converges to 1, 4 and 5 respectively; this is the content of Figure 1(b). The ordering is the reverse of the edge density ordering: K_p is the densest and has the smallest density, the double star is the sparsest, being a tree, and has the largest. The explanation is metric rather than combinatorial. By Theorem 12(ii) the second spectral moment is $h_h(G) + 2W_2(G)$, and W_2 grows with the distances, so graphs of large diameter carry large spectral mass. Complete graphs have $\operatorname{diam} = 1$ and therefore minimal W_2, whereas $\operatorname{diam}(S_{p,p}) = 3$ and $\operatorname{diam}(K_{p,p}) = 2$. Thus E_{hd} behaves as a measure of metric spread, tempered by the hop hub number through the diagonal seeding.

7.2 The role of the diagonal seeding

Theorems 15 and 16 bound the effect of replacing $D(G)$ by $\mathcal{A}^H_{hd}(G)$: each eigenvalue moves right by at most one, and the energy moves by at most $h_h(G)$. Two regimes are visible in Table 5.
For families with $h_h(G) = 2$, such as $K_{p,p}$, $S_{p,p}$ and stars, the seeding is a rank-two perturbation and E_{hd} and E_D differ by well

under 1; for instance $E_D(S_{5,5}) = 39.8087$ against $E_{hd}(S_{5,5}) = 39.2111$. Here E_{hd} is essentially a corrected distance energy.
For K_p, where $h_h(K_p) = p$ is as large as possible, the seeding is a full-rank perturbation and its effect is dramatic: as noted in Remark 23 it shifts the entire spectrum by $+1$ and annihilates the $p-1$ eigenvalues equal to -1, halving the energy from $2(p-1)$ to p. The complete graph is thus the unique case in which the hop hub structure dominates the metric structure, which is exactly the content of the extremal characterisations in Theorems 18 and 19.
Table 5 also positions E_{hd} among the four earlier energies. The adjacency-seeded energies $\mathcal{E}_H(G)$ of [25] and $\mathcal{E}_h(G)$ of [27] remain within roughly one unit of the ordinary energy $\mathcal{E}(G)$ for every graph tested, because they perturb only the diagonal of $A(G)$; they consequently carry little information beyond $\mathcal{E}(G)$ itself. By contrast $E_{hd}(G)$ is of the order of $E_D(G)$, which for graphs of diameter at least 2 is between 1.4 and 3.5 times larger, and it separates graphs that the adjacency-based energies do not. For example $\mathcal{E}_h(C_6) = 8.25$ and $\mathcal{E}_h(K_{3,3}) = 7.46$ differ by less than 0.8, whereas E_{hd} separates the two graphs as 18.55 and 15.55; likewise $\mathcal{E}_H^-(P_6) = 7.46$ and $\mathcal{E}_H^-(S_{3,3}) = 6.29$, while $E_{hd}^+(P_6) = 22.62$ and $E_{hd}(S_{3,3}) = 19.29$.

7.3 Eigenvalue structure

Three structural features recur across all computed spectra.
First, the matrix $\mathcal{A}_{hd}^H(G)$ is entrywise non-negative and irreducible, so by the Perron–Frobenius theorem λ_1 is simple, positive, and strictly dominant. Numerically λ_1 absorbs the overwhelming majority of the spectral mass: for C_6 with H_1 one has $\lambda_1 = 9.5198$ against $Q = 117$, so $\lambda_1^2/Q = 0.774$. This is the reason Theorem 20 outperforms the McClelland upper bound of Theorem 19, as Table 4 confirms.
Second, the trace is small and positive, equal to $h_h(G)$, while the second moment Q is large. Since $\sum_i \lambda_i = h_h(G)$ and λ_1 is already of order $\sqrt{Q}$, the remaining eigenvalues must be predominantly negative and of small modulus. This explains the pattern seen in Theorems 25 and 27, where a single large positive eigenvalue is balanced by a long run of eigenvalues equal to -2.
Third, the eigenvalue -2 of multiplicity $2p-4$ occurring in both $K_{p,p}$ and $S_{p,p}$ is not a coincidence. In both proofs it arises from vectors supported on a part and orthogonal to the all-ones vector of that part; on such vectors every distance block acts as a multiple of J plus $-2I$, and the J terms vanish. The common value -2 therefore reflects the fact that in both families all within-part distances equal 2.

7.4 Quantifying the failure of invariance

The dependence of E_{hd} on the chosen minimum hop hub set is mild in practice. Over the 448 minimum hop hub sets examined in Section 8 the largest spread recorded is $\sigma(C_9) = 1.0379$, that is 2.73% of $E_{hd}^-(C_9)$, and the largest relative spread of any graph tested is likewise 2.73%; the bound $\sigma \le 2h_h$ of Theorem 8 is therefore correct but far from tight. Table 6 and Figure 4 record the details.
Two further patterns emerge. The number $|\mathcal{H}(G)|$ of minimum hop hub sets grows rapidly, reaching 110 for C_{10}, while the number of distinct energies grows much more slowly, reaching only 7; by Proposition 9 the distinct values are indexed by automorphism orbits, and highly symmetric graphs collapse many sets to one value. Indeed every vertex-transitive graph tested with $h_h(G) \le 2$, namely C_4, C_5, $K_{p,p}$ and K_p, is hop hub energetic, whereas C_6, C_9 and the Petersen graph are not. Vertex transitivity alone is therefore insufficient; what matters is transitivity on $\mathcal{H}(G)$, in agreement with Proposition 9.

Input: a connected graph $G = (V, E)$ with $|V| = p$.
Output: $h_h(G)$, $\mathcal{H}(G)$, $E_{hd}^-(G)$, $E_{hd}^+(G)$, $\sigma(G)$.

1. Compute the distance matrix $D(G)$ by breadth-first search from every vertex.
2. For $k = 0, 1, 2, \ldots, p$ and for each $S \subseteq V$ with $|S| = k$:
   (a) test the hop condition: every $v \notin S$ has some $u \in S$ with $D_{uv} = 2$;
   (b) test the hub condition: for every $x, y \notin S$, either $xy \in E$, or x and y have neighbours in a common connected component of $G[S]$;
   (c) if both hold, append S to $\mathcal{H}(G)$.
   Stop at the first k for which $\mathcal{H}(G) \neq \emptyset$ and set $h_h(G) = k$.
3. For each $H \in \mathcal{H}(G)$ form $\mathcal{A}_{hd}^H(G) = D(G) + \mathrm{diag}(\chi_H)$, compute its eigenvalues and set $E_{hd}^H(G) = \sum_i |\lambda_i|$.
4. Return $\min_H E_{hd}^H$, $\max_H E_{hd}^H$ and their difference.

Algorithm 1: Computation of the minimum hop hub distance energy spectrum of a connected graph.

7.5 Tightness of the bounds

Table 4 and Figure 2 evaluate all bounds of Section 5 on twelve graphs. Three observations follow. The McClelland upper bound $\sqrt{pQ}$ is weak, exceeding E_{hd} by a factor between 1.30 and 2.24, and it degrades as p grows since it discards the dominance of λ_1. The McClelland lower bound $\sqrt{Q + p(p-1)\Delta_H^{2/p}}$ is considerably stronger than $\sqrt{Q}$ whenever Δ_H is large, for instance 20.25 against 11.40 for $K_{4,4}$, but collapses to $\sqrt{Q}$ when the matrix is near-singular, as for $S_{5,5}$ and Q_3. The Wiener-based bound $2\lambda_1 - h_h$ of Theorem 17 is the most accurate lower bound in the sample, attaining 38.00 against the true value 39.21 for $S_{5,5}$, a relative error of 3.09%, and it is exact for K_p.

8. COMPUTATIONAL EVALUATION

8.1 Algorithm and complexity

Algorithm 1 computes $E_{hd}^-(G)$, $E_{hd}^+(G)$ and $\sigma(G)$ exactly.
Step 1 costs $O(pq)$ time. The hub test in Step 2(b) is a reformulation of the definition: an S-path between $x, y \notin S$ exists exactly when xy is an edge or when x and y each have a neighbour in one and the same component of the subgraph induced by S. Computing the components of $G[S]$ costs $O(p+q)$ and the pairwise test costs $O(p^2)$, so a single candidate is processed in $O(p^2+q)$ time, against $O(p^2(p+q))$ for a literal implementation of the definition. Step 2 therefore runs in $O\big(2^p(p^2+q)\big)$ in the worst case, and Step 3 in $O(|\mathcal{H}(G)|\, p^3)$. The exponential factor reflects the exhaustive search over subsets; no polynomial algorithm for $h_h(G)$ is known to the authors, which is consistent with the difficulty of the related hub number studied in [12, 33]. For the orders considered here, $p \le 10$, the procedure terminates in seconds.

8.2 Experimental setup

All computations were carried out in Python 3 using NumPy for eigenvalue decomposition in IEEE double precision, NetworkX for graph construction and breadth-first search, and SymPy together with exact integer arithmetic for the characteristic polynomials. Characteristic polynomial coefficients were obtained in exact integer form and cross-checked against the floating-point spectra;

Table 1. Exhaustive verification over 45 named graphs (448 minimum hop hub sets). A violation is a minimum hop hub set on which the stated relation fails beyond a tolerance of 10^{-7}

Relation tested	Source	Violations
$c_1 = -h_h(G)$	Thm. 10	0
$c_2 = \binom{h_h}{2} - q$	superseded	440
$c_2 = \binom{h_h}{2} - W_2(G)$	Thm. 10	**0**
$\sum_i \lambda_i = h_h(G)$	Thm. 12	0
$\sum_i \lambda_i^2 = h_h(G) + 2q$	superseded	440
$\sum_i \lambda_i^2 = h_h(G) + 2W_2(G)$	Thm. 12	**0**
$\mu_i \le \lambda_i \le \mu_i + 1$	Thm. 15	0
$\lvert E_{hd} - E_D\rvert \le h_h(G)$	Thm. 16	0
$\lambda_1 \ge (h_h + 2W)/p$	Thm. 17	0
$E_{hd} \ge 2\lambda_1 - h_h$	Thm. 17	0
$E_{hd} \ge p$, equality iff K_p	Thm. 18	0
$\sqrt{Q} \le E_{hd} \le \sqrt{pQ}$	Thm. 19	0
$E_{hd} \ge \sqrt{Q + p(p-1)\Delta_H^{2/p}}$	Thm. 19	0
$E_{hd} \le \lambda_1 + \sqrt{(p-1)(Q-\lambda_1^2)}$	Thm. 20	0
$\sigma(G) \le \lvert H_1 \triangle H_2\rvert \le 2h_h(G)$	Thm. 8	0

eigenvalues were additionally recomputed at 25 significant digits with multiprecision root finding for Example 6. The hub test of Algorithm 1, Step 2(b), was validated against a literal implementation of the definition on 26,904 vertex subsets of random connected graphs, with complete agreement. All values reported below are rounded to four decimal places.

8.3 Verification of the spectral identities

Table 1 reports an exhaustive test of Theorems 10–20 over 45 named graphs comprising 448 minimum hop hub sets, together with 2,074 random connected graphs of order at most 9 generated from the Erdős–Rényi model. Each identity or inequality was evaluated on every minimum hop hub set of every graph.

The two superseded rows are decisive. The identity $c_2 = \binom{h_h}{2} - q$ fails on 440 of the 448 instances; the eight instances on which it happens to hold are exactly the complete graphs contained in the sample, namely $K_2, \ldots, K_7$ together with $C_3 \cong K_3$ and $W_4 \cong K_4$, each of which has a unique minimum hop hub set and satisfies $W_2(G) = q$ because its diameter is 1. The same is true of $\sum_i \lambda_i^2 = h_h + 2q$. The corrected forms of Theorems 10 and 12 hold without exception. All bounds of Section 5 likewise hold without exception, on the named graphs and on the 2,074 random graphs alike.

8.4 The cycle C_6 in full

Table 2 lists the complete spectral data for the two energy classes of C_6 identified in Example 6.

Both classes satisfy $\sum_i \lambda_i = h_h(C_6) = 3$ and $\sum_i \lambda_i^2 = h_h + 2W_2 = 3 + 114 = 117$, in agreement with Theorem 12, and both have $c_2 = \binom{3}{2} - 57 = -54$, in agreement with Theorem 10. Had $c_2 = \binom{3}{2} - q$ been correct, the value would have been -3. The two classes are distinguished only from the third significant digit onwards, which is why the failure of invariance is easy to overlook and why the invariants of Definition 7 are needed. Note also that $\sigma(C_6) = 0.3681$, comfortably inside the bound $2h_h(C_6) = 6$ of Theorem 8.

Table 2. The two spectral classes of C_6. Here $h_h(C_6) = 3$, $\lvert\mathcal{H}(C_6)\rvert = 18$, $W = 27$, $W_2 = 57$ and $Q = 117$.

	class I	class II
representative H	$\{v_1, v_2, v_3\}$	$\{v_1, v_3, v_4\}$
number of such sets	6	12
λ_1	9.5198	9.5255
λ_2	0.6927	0.8187
λ_3	0.5616	0.2458
λ_4	-0.6885	-0.5016
λ_5	-3.5240	-3.2620
λ_6	-3.5616	-3.8264
$\sum_i \lambda_i$	3	3
$\sum_i \lambda_i^2$	117	117
c_2	-54	-54
$E_{hd}^H(C_6)$	**18.5482**	**18.1800**

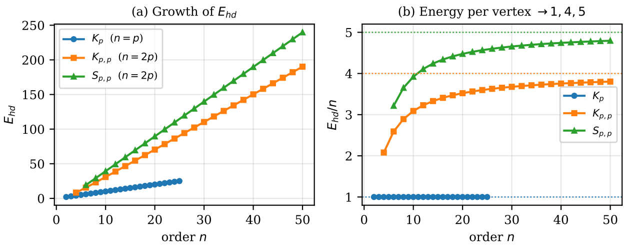

Fig. 1. (a) Growth of E_{hd} for K_p, $K_{p,p}$ and $S_{p,p}$ plotted against the order n of the graph. (b) The energy density E_{hd}/n converges to 1, 4 and 5 respectively (dotted lines).

8.5 Closed-form families

Table 3 lists exact surd values of the three closed forms and confirms them against independently computed spectra.

Every exact value in Table 3 agrees with the numerically computed energy to within 10^{-9}. The last two columns isolate the correction established in Theorem 27: the single formula $(9p - 13) + \sqrt{p^2 + 6p - 3}$ understates the energy by 0.3923 at $p = 3$ and by 0.1327 at $p = 4$, and is exact from $p = 5$ onwards. Figure 1 plots the three families against the order n and displays the convergence of the energy density to 1, 4 and 5.

8.6 Tightness of the bounds

Table 4 shows that the Koolen–Moulton bound of Theorem 20 is sharper than the McClelland upper bound of Theorem 19 for every graph tested, the ratio $\sqrt{pQ}$ to the Koolen–Moulton value ranging from 1.21 for P_5 to 2.24 for K_5, and that both are exact for K_5, where all bounds collapse to the common value 5 in accordance with Theorems 18 and 19. Among the lower bounds, $2\lambda_1 - h_h$ is best for 10 of the 12 graphs, the exceptions being $K_{3,3}$ and $K_{4,4}$, where the determinant is large and the McClelland lower bound takes over. Figure 2 displays the same comparison for paths and cycles of orders 3 to 10 and shows the admissible band closing around E_{hd}.

Table 3. Exact and numerical minimum hop hub distance energies of the three closed-form families. The column "single formula" evaluates $(9p-13)+\sqrt{p^2+6p-3}$ for $S_{p,p}$ irrespective of p; it disagrees with the true value for $p=3$ and $p=4$.

p	$E_{hd}(K_p)$	$E_{hd}(K_{p,p})$ exact	numerical	$E_{hd}(S_{p,p})$ exact	numerical	single formula	agreement
3	3	$4+\sqrt{8}+\sqrt{76}$	15.5462	$4+\sqrt{24}+\sqrt{108}$	19.2913	18.8990	no
4	4	$8+\sqrt{13}+\sqrt{133}$	23.1381	$8+\sqrt{37}+\sqrt{229}$	29.2155	29.0828	no
5	5	$12+\sqrt{20}+\sqrt{208}$	30.8943	$32+\sqrt{52}$	39.2111	39.2111	yes
6	6	$16+\sqrt{29}+\sqrt{301}$	38.7345	$41+\sqrt{69}$	49.3066	49.3066	yes
7	7	$20+\sqrt{40}+\sqrt{412}$	46.6223	$50+\sqrt{88}$	59.3808	59.3808	yes
8	8	$24+\sqrt{53}+\sqrt{541}$	54.5395	$59+\sqrt{109}$	69.4403	69.4403	yes
9	9	$28+\sqrt{68}+\sqrt{688}$	62.4760	$68+\sqrt{132}$	79.4891	79.4891	yes
10	10	$32+\sqrt{85}+\sqrt{853}$	70.4257	$77+\sqrt{157}$	89.5300	89.5300	yes

Table 4. Numerical evaluation of the bounds of Section 5. Here $Q=h_h+2W_2$ and $\Delta_H=|\det \mathcal{A}^H_{hd}|$; the value of E_{hd} is E^+_{hd}. All lower bounds are at most E_{hd} and all upper bounds at least E_{hd}, as required.

				lower bounds				upper bounds	
G	p	h_h	W	$\sqrt{Q}$	McClelland	$2\lambda_1-h_h$	E_{hd}	Koolen–Moulton	$\sqrt{pQ}$
P_5	5	3	20	10.1489	11.8774	14.7380	15.4768	18.7363	22.6936
P_7	7	5	56	19.9249	21.6849	29.8932	31.0460	41.0198	52.7162
C_6	6	3	27	10.8167	14.5686	16.0397	18.5482	21.0030	26.4953
C_8	8	5	64	18.8944	23.1846	28.2722	32.6567	40.3360	53.4416
K_5	5	5	10	5.0000	5.0000	5.0000	5.0000	5.0000	11.1803
$K_{3,3}$	6	2	21	8.2462	14.0451	12.7178	15.5462	15.6795	20.1990
$K_{4,4}$	8	2	40	11.4018	20.2457	18.5326	23.1381	23.3897	32.2490
$S_{4,4}$	8	2	58	16.5529	20.5280	28.1327	29.2155	33.2056	46.8188
$S_{5,5}$	10	2	97	21.6333	21.6400	38.0000	39.2111	44.7386	68.4105
W_7	7	3	30	9.9499	12.8655	15.1900	16.7904	18.9786	26.3249
Petersen	10	4	75	16.5529	22.1527	26.8324	30.4853	33.5012	52.3450
Q_3	8	3	48	13.9642	13.9648	21.7878	24.9155	29.4156	39.4968

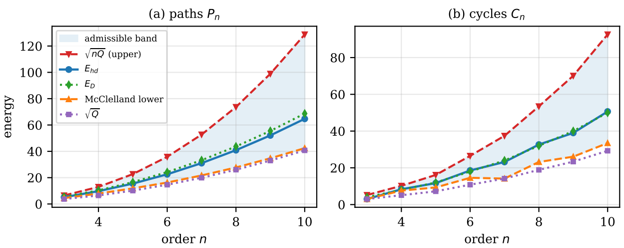

Fig. 2. Bounds of Section 5 evaluated on (a) paths and (b) cycles. The shaded band is the region admitted by the McClelland lower bound and the upper bound $\sqrt{nQ}$. The distance energy E_D is included to illustrate Theorem 16.

8.7 Comparison with related energies

Table 5 and Figure 3 confirm the two regimes described in Section 7. For all eight graphs $|E_{hd}-E_D|\le h_h$, as Theorem 16 requires; the extreme case is K_6, where $h_h=6$ and $E_D-E_{hd}=4$. The adjacency-seeded energies $\mathcal{E}_H$ and $\mathcal{E}_h$ never differ from $\mathcal{E}$ by more than 1.47 except for K_6, whereas E_{hd} ranges from 0.60 to 3.24 times $\mathcal{E}$, showing that the new invariant carries information that the earlier seeded energies do not.

Table 5. Comparison of five graph energies. Here $\mathcal{E}$ is the ordinary energy [14], $\mathcal{E}_H$ the minimum hub energy [25], $\mathcal{E}_h$ the minimum hop dominating energy [27], E_D the distance energy [20], and $E^{\pm}_{hd}$ the extreme minimum hop hub distance energies. Like E_{hd}, the energies $\mathcal{E}_H$ and $\mathcal{E}_h$ depend on the chosen minimum set, so the minimum over all minimum hub, respectively hop dominating, sets is reported. Values are rounded to two decimal places for readability.

G	p	h_h	$\mathcal{E}$	$\mathcal{E}^-_H$	$\mathcal{E}^-_h$	E_D	E^-_{hd}	E^+_{hd}
P_6	6	4	6.99	7.46	7.17	24.22	22.27	22.62
C_6	6	3	8.00	8.28	8.25	18.00	18.18	18.55
K_6	6	6	10.00	10.00	6.00	10.00	6.00	6.00
$K_{3,3}$	6	2	6.00	7.44	7.46	16.00	15.55	15.55
$S_{3,3}$	6	2	6.00	6.29	6.29	20.00	19.29	19.29
W_6	6	3	9.37	9.05	9.49	13.48	12.72	12.72
Q_3	8	3	12.00	12.32	12.19	24.00	24.92	24.92
Petersen	10	4	16.00	17.10	16.62	30.00	30.36	30.49

8.8 The energy spread

Table 6 and Figure 4 quantify the failure of invariance. The relative spread never exceeds 2.73% over the entire sample, so although E_{hd} is not a graph invariant, it is nearly one; reporting E^-_{hd} and E^+_{hd} therefore loses very little. The number of minimum hop hub

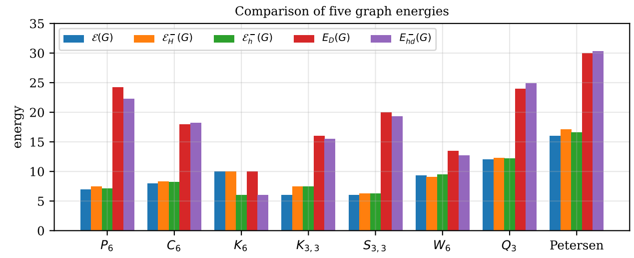

Fig. 3. Comparison of the ordinary energy $\mathcal{E}(G)$, the minimum hub energy $\mathcal{E}_H^-(G)$, the minimum hop dominating energy $\mathcal{E}_h^-(G)$, the distance energy $E_D(G)$ and the minimum hop hub distance energy $E_{hd}^-(G)$ on eight graphs; for the three set-dependent energies the minimum over all minimum sets is plotted. The complete graph K_6 is the only case in which E_{hd} falls below $\mathcal{E}$.

Table 6. Failure of invariance on paths and cycles: number of minimum hop hub sets, number of distinct energies, spread σ, relative spread, and the bound $2h_h$ of Theorem 8.

G	h_h	$\lvert\mathcal{H}(G)\rvert$	distinct	$\sigma(G)$	rel. (%)	$2h_h$
P_4	2	4	3	0.0781	0.81	4
P_6	4	11	7	0.3513	1.58	8
P_8	6	24	14	0.4591	1.13	12
P_{10}	8	41	23	0.5139	0.80	16
C_4	2	4	1	0	0	4
C_6	3	18	2	0.3681	2.02	6
C_8	5	48	4	0.4669	1.45	10
C_9	6	75	6	1.0379	2.73	12
C_{10}	7	110	7	0.4565	0.91	14

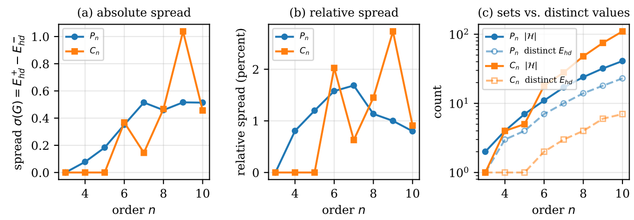

Fig. 4. Failure of invariance for paths and cycles: (a) absolute spread $\sigma(G)$, (b) relative spread as a percentage of $E_{hd}^-(G)$, (c) number of minimum hop hub sets against the number of distinct energies, on a logarithmic scale.

sets grows roughly geometrically, from 4 to 110 for cycles of order 4 to 10, while the number of distinct energies grows only linearly, from 1 to 7, confirming the orbit interpretation of Proposition 9. Cycles have markedly fewer distinct values than paths of the same order, which is consistent with their larger automorphism groups.

9. CONCLUSION AND OPEN PROBLEMS

This paper has introduced the minimum hop hub distance matrix and the associated energy $E_{hd}(G)$ of a connected graph, and has developed the invariant from first principles. The decomposition $\mathcal{A}_{hd}^H(G) = D(G) + \mathrm{diag}(\chi_H)$ was shown to govern the entire theory: it yields Weyl-type interlacing with the distance matrix, the perturbation bound $|E_{hd}(G) - E_D(G)| \le h_h(G)$, and the bound $\sigma(G) \le 2h_h(G)$ on the energy spread. Two coefficient identities were corrected, the correct forms being expressed through the second distance moment $W_2(G)$ and hence through the Wiener and hyper-Wiener indices. Exact spectra and energies were derived for K_p, $K_{p,p}$ and $S_{p,p}$ by explicit eigenvector decomposition, and the double star formula was shown to require a case distinction at $p \in \{3, 4\}$. The sharp lower bound $E_{hd}(G) \ge p$ was established, with equality exactly for the complete graph, and bounds of McClelland and Koolen–Moulton type were obtained and compared numerically. Since $E_{hd}(G)$ depends on the chosen minimum hop hub set, the invariants $E_{hd}^-(G)$, $E_{hd}^+(G)$ and $\sigma(G)$ were introduced; computations over 448 minimum hop hub sets show that the relative spread never exceeds 2.73%, so the failure of invariance, though real, is numerically mild.
The following problems remain open.

(1) Determine $E_{hd}(G)$ in closed form for further families, in particular for paths P_p, cycles C_p, wheels W_p and complete multipartite graphs. Table 6 shows that for paths and cycles the hop hub number and the number of minimum hop hub sets both vary with the residue of p modulo small integers, so a single uniform closed form is unlikely.

(2) Characterise the hop hub energetic graphs, that is, those with $\sigma(G) = 0$. Proposition 9 gives a sufficient condition; whether transitivity of $\mathrm{Aut}(G)$ on $\mathcal{H}(G)$ is also necessary is unresolved.

(3) Improve the bound $\sigma(G) \le 2h_h(G)$ of Theorem 8. The computations of Table 6 suggest that $\sigma(G)$ may be bounded by an absolute constant, or at least by a function growing far more slowly than $h_h(G)$.

(4) Determine the graphs of order p maximising $E_{hd}(G)$. The lower extremal problem is settled by Theorem 18; the upper one is open, and the data of Section 8 suggest that trees of large diameter are the natural candidates.

(5) Establish the computational complexity of $h_h(G)$ and hence of Algorithm 1.

10. REFERENCES

[1] C. Adiga, A. Bayad, I. Gutman, S. A. Srinivas, The minimum covering energy of a graph, Kragujevac Journal of Science. **34**, 39–56, 2012.

[2] U. Alper, G. Arif, K. Necla, I. Gutman, Relating graph energy and Sombor index, Discrete Mathematics Letters. **8**, 6–9, 2021.

[3] S. K. Ayyaswamy, C. Natarajan, Hop domination in graphs, Analele Ştiinţifice ale Universităţii Ovidius Constanţa, Seria Matematică. **23**, 187–199, 2015.

[4] R. B. Bapat, Graphs and Matrices, Hindustan Book Agency, New Delhi, 2011.

[5] R. B. Bapat, S. Pati, Energy of a graph is never an odd integer, Bulletin of the Kerala Mathematics Association. **1**, 129–132, 2004.

[6] R. Bhatia, Matrix Analysis, Graduate Texts in Mathematics **169**, Springer, New York, 1997.

[7] S. B. Bozkurt, A. D. Güngör, B. Zhou, Note on the distance energy of graphs, MATCH Communications in Mathematical and in Computer Chemistry. **64**, 129–134, 2010.

[8] G. Caporossi, E. Chasset, B. Furtula, Some conjectures and properties on distance energy, Les Cahiers du GERAD. **64**, 1–7, 2009.

[9] X. G. Chen, Y. F. Wang, On total domination and hop domination in diamond-free graphs, Bulletin of the Malaysian Mathematical Sciences Society. **43**, 1885–1891, 2020.

[10] C. A. Coulson, On the calculation of the energy in unsaturated hydrocarbon molecules, Proceedings of the Cambridge Philosophical Society. **36**, 201–203, 1940.

[11] A. Graovac, I. Gutman, N. Trinajstić, Topological Approach to the Chemistry of Conjugated Molecules, Springer, Berlin, 1977.

[12] T. Grauman, S. Hartke, A. Jobson, B. Kinnersley, D. West, L. Wiglesworth, P. Worah, H. Wu, The hub number of a graph, Information Processing Letters. **108**, 226–228, 2008.

[13] J. W. Grossman, F. Harary, M. Klawe, Generalized Ramsey theory for graphs, X: Double stars, Discrete Mathematics. **28**, 247–254, 1979.

[14] I. Gutman, The energy of a graph, Berichte der Mathematisch-Statistischen Sektion im Forschungszentrum Graz. **103**, 1–22, 1978.

[15] I. Gutman, X. Li, J. Zhang, Graph energy, in: Analysis of Complex Networks: From Biology to Linguistics, Wiley-VCH, Weinheim, 145–174, 2009.

[16] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.

[17] A. D. Güngör, S. B. Bozkurt, On the distance spectral radius and distance energy of graphs, Linear and Multilinear Algebra. **59**, 365–370, 2011.

[18] F. Harary, Graph Theory, Addison-Wesley, Massachusetts, 1969.

[19] T. W. Haynes, S. T. Hedetniemi, P. J. Slater, Fundamentals of Domination in Graphs, Marcel Dekker, New York, 1998.

[20] G. Indulal, I. Gutman, A. Vijayakumar, On distance energy of graphs, MATCH Communications in Mathematical and in Computer Chemistry. **60**, 461–472, 2008.

[21] D. J. Klein, I. Lukovits, I. Gutman, On the definition of the hyper-Wiener index for cycle-containing structures, Journal of Chemical Information and Computer Sciences. **35**, 50–52, 1995.

[22] J. H. Koolen, V. Moulton, Maximal energy graphs, Advances in Applied Mathematics. **26**, 47–52, 2001.

[23] X. Li, Y. Shi, I. Gutman, Graph Energy, Springer, New York, 2012.

[24] S. S. Mahde, A. S. Sand, Hop hub-integrity of graphs, International Journal of Mathematics and its Applications. **4**, 91–100, 2021.

[25] V. Mathad, S. S. Mahde, The minimum hub energy of a graph, Palestine Journal of Mathematics. **6**, 247–256, 2017.

[26] B. J. McClelland, Properties of the latent roots of a matrix: the estimation of π-electron energies, The Journal of Chemical Physics. **54**, 640–643, 1971.

[27] K. Palani, M. Lalitha Kumari, Minimum hop dominating energy of a graph, Advances and Applications in Mathematical Sciences. **21**, 3–12, 2022.

[28] H. S. Ramane, D. S. Revankar, I. Gutman, S. B. Rao, B. D. Acharya, H. B. Walikar, Bounds for the distance energy of a graph, Kragujevac Journal of Mathematics. **31**, 59–68, 2008.

[29] M. Randić, Novel molecular descriptor for structure-property studies, Chemical Physics Letters. **211**, 478–483, 1993.

[30] A. M. Sahal, A. S. Sand, S. S. Mahde, Hop hub number in graphs, Bulletin of the Korean Mathematical Society. **33**, 319–329, 2023.

[31] A. S. Sanad, S. S. Mahde, Hop hubtic number and hop hub polynomial of graphs, International Journal of Computer Applications. **183**, 1–5, 2022.

[32] A. Sanad, C. Li, Partial total domination in hypergraphs, Mathematics. **13**(6), 910, 2025.

[33] M. Walsh, The hub number of graphs, International Journal of Mathematics and Computer Science. **1**, 117–124, 2006.

[34] H. Wiener, Structural determination of paraffin boiling points, Journal of the American Chemical Society. **69**, 17–20, 1947.