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Coulson–type Integral Formulae for the Energy Changes of Graph Perturbations

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Abstract

The energy of a graph G on n vertices is the sum of the absolute values of the eigenvalues of G. For many molecular graphs, this sum is equivalent to an integral formula used by Coulson to obtain the total π–electron energy of a molecule. Using the resolvent of the adjacency matrix of G, we present integral formulae, of a form similar to that of Coulson, that determine the difference between the energy of G and that of some slight modification applied to G. The graph perturbations considered include the addition of a vertex or edge to G, as well as the removal of a vertex or edge from G. We also provide a decomposition of the energy of G into the sum of n values, where each value is associated with a vertex of G.

1 Introduction

Only simple graphs will be considered in this paper, that is, undirected, unweighted graphs with no loops or multiple edges. The vertex and edge sets of the graph G are $\mathcal{V}(G)$ and $\mathcal{E}(G)$ respectively. The symmetric adjacency matrix $\mathbf{A}$ of G is the $n \times n$ matrix where, for all p, q, the entry $\mathbf{A}_{pq}$ in the p^{th} row and q^{th} column of $\mathbf{A}$ is 1 if $\{p, q\} \in \mathcal{E}(G)$ and is 0 otherwise. The transpose of matrix $\mathbf{M}$ is denoted by $\mathbf{M}^{\mathsf{T}}$. For all k, the k^{th} column of the identity matrix $\mathbf{I}$ is $\mathbf{e}_k$. The *characteristic polynomial* of G, denoted by $\phi(G, x)$, is $|x\mathbf{I} - \mathbf{A}|$, the characteristic polynomial of the adjacency matrix associated with G. The n roots of $\phi(G, x)$ are the *eigenvalues* $\lambda_1, \lambda_2, \ldots, \lambda_n$ of G, with possible repetitions. The eigenvalue λ has *multiplicity* q if it is a root of multiplicity q of $\phi(G, x)$. Since $\mathbf{A}$ is symmetric and has real entries, its eigenvalues are real numbers; moreover, since the entries of $\mathbf{A}$ are integers, its characteristic polynomial has integer coefficients.

In [3], Coulson calculated the energy $E(G)$ in an unsaturated hydrocarbon molecule by the Cauchy principal value[1] of the following integral:

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left[n - \frac{\mathrm{i}x\, \phi'(G, \mathrm{i}x)}{\phi(G, \mathrm{i}x)} \right] dx \tag{1}$$

where i is the imaginary unit and G is the graph whose n vertices are the atoms in the molecule and whose edges represent the chemical bonds between the atoms. For any graph G on n vertices, the integral (1) can be shown to be equal to

$$E(G) = \sum_{j=1}^{n} |\lambda_j|. \tag{2}$$

Proofs of this assertion may be found in [13, 16, 20]. In view of the equivalence of statements (1) and (2), Gutman, in his seminal paper [9], defined the energy $E(G)$ of a graph G to be the right hand side of (2). A vast amount of research on $E(G)$ has been conducted since then. See [16, 10] for a survey of the main results on graph energies and [12] for variants of $E(G)$ that obtain 'energy–like' parameters of G by using different matrices and polynomials associated with G.

However, (1) and (2) are equivalent statements whether G represents an actual molecule or not. As a consequence, the graph theory community saw no reason why the study of graph energies should be limited solely to graphs representing molecules. Indeed, in [12, 18], Nikiforov remarks that the energy of a graph is the *trace norm* of its adjacency matrix, which, he argues, is a fundamentally important graph parameter to study without the need of any external applicative motivation.

In [8], Gutman obtained the following variant of (1) as well.

Theorem 1.1 [8] *If G is a graph on n vertices, then*

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dx}{x^2} \ln \left| (-\mathrm{i}x)^n \phi(G, \mathrm{i}/x) \right|.$$

A *bipartite graph* is a graph having no circuits of odd order. Using Theorem 1.1 and taking advantage of the fact that the characteristic polynomial of bipartite graphs is of

[1]The Cauchy principal value of the integral $\int_{-\infty}^{\infty} f(x)\, dx$ is defined as $\lim_{t\to\infty} \int_{-t}^{t} f(x)\, dx$. In this paper, it is assumed that all such integrals are determined by calculating their Cauchy principal value.

the form

$$\phi(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \, b(G,k) \, x^{n-2k}, \quad b(G,k) \geq 0 \text{ for all } k = 0,1,\ldots,\lfloor \tfrac{n}{2} \rfloor$$

it was deduced that $E(G)$ is a monotonically increasing function of $b(G,k)$. This enabled countless applications of the Coulson formula for finding graphs with extremal (maximal or minimal) energy value; for details see [16].

Coulson and Jacobs [4] have the following formula for the difference between the energies of two graphs G_1 and G_2 having the same number of vertices.

Theorem 1.2 [4] *If G_1 and G_2 are two graphs having the same number of vertices, then*

$$E(G_1) - E(G_2) = \frac{1}{\pi} \int_{-\infty}^{\infty} \ln \left(\frac{\phi(G_1, \mathrm{i}x)}{\phi(G_2, \mathrm{i}x)} \right) dx.$$

In this paper, we shall use (1) to deduce new expressions, similar in vein to Theorem 1.2, for the change in the energy of a graph G after being modified by the addition or removal of an edge or vertex. Such a slight change in G will be called a *perturbation* of G. Our approach uses the *resolvent matrix* of the adjacency matrix $\mathbf{A}$ of G. The resolvent matrix of $\mathbf{A}$ is $\mathcal{R}_{\mathbf{A}}(z) = (z\mathbf{I} - \mathbf{A})^{-1}$, where z is a complex variable [17, 21]. A graph energy variant that utilizes $\mathcal{R}_{\mathbf{A}}(z)$, called the *resolvent energy*, was recently introduced in [11] (see also [12]). We shall use the following form of $\mathcal{R}_{\mathbf{A}}(z)$ with z replaced by $\mathrm{i}x$:

$$\mathbf{R}(x) = \mathcal{R}_{\mathbf{A}}(\mathrm{i}x) = (\mathrm{i}x\mathbf{I} - \mathbf{A})^{-1}. \tag{3}$$

We write $\mathbf{R}_G(x)$ instead of $\mathbf{R}(x)$ if the graph G associated with our resolvent needs to be clarified or emphasized. Note that each entry of $\mathbf{R}(x)$ is a rational function whose numerator and denominator are polynomials having coefficients in $\mathbb{Z} \cup \{N\mathrm{i} \mid N \in \mathbb{Z}\}$. Moreover, since $\mathbf{R}(x) = \dfrac{\mathrm{adj}(\mathrm{i}x\mathbf{I} - \mathbf{A})}{|\mathrm{i}x\mathbf{I} - \mathbf{A}|}$, where $\mathrm{adj}(\mathbf{M})$ is the adjugate of matrix $\mathbf{M}$, each pole of any arbitrary entry of $\mathbf{R}(x)$ is situated at $x = -\mathrm{i}\lambda$ for some (real) eigenvalue λ of G. Thus, all of these poles lie on the imaginary axis of the complex plane.

2 Preliminary Results

We shall be using the following result from matrix theory regarding the trace of the product of matrices. We denote the trace of matrix $\mathbf{M}$ by $\mathrm{tr}(\mathbf{M})$.

Lemma 2.1 *If $q > 1$ and the matrix product $\mathbf{M}_1\mathbf{M}_2\cdots\mathbf{M}_q$ exists and is a square matrix, then* $\mathrm{tr}(\mathbf{M}_1\mathbf{M}_2\cdots\mathbf{M}_q) = \mathrm{tr}(\mathbf{M}_2\mathbf{M}_3\cdots\mathbf{M}_q\mathbf{M}_1) = \cdots = \mathrm{tr}(\mathbf{M}_q\mathbf{M}_1\mathbf{M}_2\cdots\mathbf{M}_{q-1})$.

Proof Let p be any number in the set $\{1, 2, \ldots, q-1\}$. Define $\mathbf{M}$ to be the $r \times s$ matrix $\mathbf{M}_1\mathbf{M}_2\cdots\mathbf{M}_p$ and $\mathbf{N}$ to be the $s \times r$ matrix $\mathbf{M}_{p+1}\mathbf{M}_{p+2}\cdots\mathbf{M}_q$. To prove the result, we show that $\mathrm{tr}(\mathbf{MN}) = \mathrm{tr}(\mathbf{NM})$. The k^{th} diagonal entry of the $r \times r$ matrix $\mathbf{MN}$ is $\sum_{j=1}^{s} \mathbf{M}_{jk}\mathbf{N}_{kj}$. Thus

$$\mathrm{tr}(\mathbf{MN}) = \sum_{k=1}^{r}\left(\sum_{j=1}^{s} \mathbf{M}_{jk}\mathbf{N}_{kj}\right). \tag{4}$$

On the other hand, the j^{th} diagonal entry of the $s \times s$ matrix $\mathbf{NM}$ is $\sum_{k=1}^{r} \mathbf{N}_{kj}\mathbf{M}_{jk}$. Thus

$$\mathrm{tr}(\mathbf{NM}) = \sum_{j=1}^{s}\left(\sum_{k=1}^{r} \mathbf{N}_{kj}\mathbf{M}_{jk}\right). \tag{5}$$

Comparing (4) and (5), the result follows. ■

From the proof of Lemma 2.1, we obtain the following corollary.

Corollary 2.2 *If $\mathbf{M}$ is an $r \times s$ matrix and $\mathbf{N}$ is an $s \times r$ matrix, then $\mathrm{tr}(\mathbf{MN})$ is the sum of all the entries of the Hadamard (entrywise) product of $\mathbf{M}^{\mathsf{T}}$ and $\mathbf{N}$.*

If we remove vertex v and all edges incident to v from a graph G, then we obtain the *vertex–deleted subgraph $G - v$*. We quote the following result relating the derivative of the characteristic polynomial of a graph to those of its n vertex–deleted subgraphs.

Theorem 2.3 [2, 6] *For any graph G, $\displaystyle\sum_{v=1}^{n} \phi(G - v, x) = \phi'(G, x)$.*

Note that $\phi(G-v, x)$ is one of the $(n-1)\times(n-1)$ principal submatrices of $\mathrm{adj}(x\mathbf{I}-\mathbf{A})$. Since $(x\mathbf{I}-\mathbf{A})^{-1}$ is equal to this adjugate divided by $|x\mathbf{I}-\mathbf{A}|$, we have $((x\mathbf{I}-\mathbf{A})^{-1})_{vv} = \dfrac{\phi(G-v, x)}{\phi(G, x)}$. This leads to the following result.

Theorem 2.4 *If G is a graph with adjacency matrix $\mathbf{A}$, then*

$$\mathrm{tr}\left((x\mathbf{I}-\mathbf{A})^{-1}\right) = \frac{\phi'(G, x)}{\phi(G, x)}.$$

Proof $\mathrm{tr}\left((x\mathbf{I}-\mathbf{A})^{-1}\right) = \sum_{v=1}^{n}\left((x\mathbf{I}-\mathbf{A})^{-1}\right)_{vv} = \dfrac{\sum_{v=1}^{n} \phi(G-v, x)}{\phi(G, x)}$. The result thus follows by Theorem 2.3. ■

Combining Theorem 2.4 with (1), Coulson's original integral formula for the energy of a graph, we obtain:

Theorem 2.5 *If G is a graph on n vertices and $\mathbf{R}(x)$ is as in* (3)*, then*

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \Big[n - \mathrm{i}x \, \mathrm{tr}(\mathbf{R}(x)) \Big] \, dx. \tag{6}$$

Theorem 2.5 is the starting point from which our main results on graph energies will emerge in Section 4. This result expresses the energy of a graph G in terms of the resolvent of its adjacency matrix.

Before we reveal our main results, we first express Theorem 2.5 as two different sums of simpler integrals using $\mathbf{R}(x)$, rediscovering an early result made by Coulson and Longuet–Higgins in the process. This illustrates the techniques that are going to be used to deduce our subsequent new results of Section 4.

3 Vertex and Edge Decomposition of Graph Energy Using R(x)

Combining our last three theorems together, we may rewrite (6) as

$$\begin{aligned} E(G) &= \frac{1}{\pi} \int_{-\infty}^{\infty} \left[n - \mathrm{i}x \left(\frac{\sum_{k=1}^{n} \phi(G-k, \mathrm{i}x)}{\phi(G, \mathrm{i}x)} \right) \right] dx \\ E(G) &= \frac{1}{\pi} \int_{-\infty}^{\infty} \sum_{k=1}^{n} \left[1 - \frac{\mathrm{i}x \, \phi(G-k, \mathrm{i}x)}{\phi(G, \mathrm{i}x)} \right] dx. \end{aligned} \tag{7}$$

The coefficient of x^{n-1} of $\phi(G, x)$ is zero, since it is equal to the negative of $\mathrm{tr}(\mathbf{A})$. Thus, $\phi(G, \mathrm{i}x) = (\mathrm{i}x)^n + \sum_{j=0}^{n-2} a_j (\mathrm{i}x)^j$ for some coefficients $a_0, \ldots, a_{n-2}$, and similarly $\phi(G-k, \mathrm{i}x) = (\mathrm{i}x)^{n-1} + \sum_{j=0}^{n-3} b_j (\mathrm{i}x)^j$ for some coefficients $b_0, \ldots, b_{n-3}$. Because of this, the expression $1 - \dfrac{\mathrm{i}x \, \phi(G-k, \mathrm{i}x)}{\phi(G, \mathrm{i}x)}$ in (7) can be rewritten as

$$\begin{aligned} 1 - \frac{\mathrm{i}x \, \phi(G-k, \mathrm{i}x)}{\phi(G, \mathrm{i}x)} &= \frac{\phi(G, \mathrm{i}x) - \mathrm{i}x \, \phi(G-k, \mathrm{i}x)}{\phi(G, \mathrm{i}x)} \\ &= \frac{\left((\mathrm{i}x)^n + \sum_{j=0}^{n-2} a_j (\mathrm{i}x)^j \right) - \mathrm{i}x \left((\mathrm{i}x)^{n-1} + \sum_{j=0}^{n-3} b_j (\mathrm{i}x)^j \right)}{\phi(G, \mathrm{i}x)} \\ 1 - \frac{\mathrm{i}x \, \phi(G-k, \mathrm{i}x)}{\phi(G, \mathrm{i}x)} &= \frac{\sum_{j=0}^{n-2} a_j (\mathrm{i}x)^j - \sum_{j=0}^{n-3} b_j (\mathrm{i}x)^{j+1}}{\phi(G, \mathrm{i}x)}. \end{aligned} \tag{8}$$

Note that, by Cauchy's Interlacing theorem [6, Corollary 1.3.12], the multiplicity of the eigenvalue λ of $G-k$ is at least one less than that of the eigenvalue λ of G. Thus, if 0 is an eigenvalue of G with multiplicity q, then none of the poles of the rational function $\dfrac{\mathrm{i}x\,\phi(G-k,\mathrm{i}x)}{\phi(G,\mathrm{i}x)}$ is equal to zero. Consequently, the integral $\displaystyle\int_{-\infty}^{\infty}\left[1-\frac{\mathrm{i}x\,\phi(G-k,\mathrm{i}x)}{\phi(G,\mathrm{i}x)}\right]dx$ has purely imaginary poles. Moreover, since the numerator of the right hand side of (8) is two less than that of the denominator, this integral converges. This allows us to split $E(G)$ in (7) into the sum of n converging integrals. Also, recall that the rational function $\dfrac{\phi(G-k,\mathrm{i}x)}{\phi(G,\mathrm{i}x)}$ is equal to the k^{th} diagonal entry of $\mathbf{R}(x)$. Hence the following result is deduced.

Theorem 3.1 [5] $E(G)=\displaystyle\sum_{k=1}^{n}\left[\frac{1}{\pi}\int_{-\infty}^{\infty}\Big(1-\mathrm{i}x\,[\mathbf{R}(x)]_{kk}\,dx\Big)\right].$

Thus, we have decomposed the energy of G into the sum of n values, where each of these values is associated with a vertex of G.

Another way of looking at Theorem 2.5 is from the following perspective. Since $\mathrm{tr}(\mathbf{I})=n$, the expression to be integrated in (6) becomes

$$n-\mathrm{i}x\,\mathrm{tr}\left((\mathrm{i}x\mathbf{I}-\mathbf{A})^{-1}\right)=\mathrm{tr}\left(\mathbf{I}-\mathrm{i}x(\mathrm{i}x\mathbf{I}-\mathbf{A})^{-1}\right).$$

However, note that

$$\begin{aligned}(\mathrm{i}x\mathbf{I}-\mathbf{A})(\mathrm{i}x\mathbf{I}-\mathbf{A})^{-1} &= \mathbf{I}\\ \mathrm{i}x(\mathrm{i}x\mathbf{I}-\mathbf{A})^{-1}-\mathbf{A}(\mathrm{i}x\mathbf{I}-\mathbf{A})^{-1} &= \mathbf{I}\\ -\mathbf{A}(\mathrm{i}x\mathbf{I}-\mathbf{A})^{-1} &= \mathbf{I}-\mathrm{i}x(\mathrm{i}x\mathbf{I}-\mathbf{A})^{-1}\end{aligned}$$

and hence

$$n-\mathrm{i}x\,\mathrm{tr}(\mathrm{i}x\mathbf{I}-\mathbf{A})^{-1}=-\mathrm{tr}\left(\mathbf{A}(\mathrm{i}x\mathbf{I}-\mathbf{A})^{-1}\right)=-\mathrm{tr}(\mathbf{A}\,\mathbf{R}(x)).$$

By Corollary 2.2, $\mathrm{tr}(\mathbf{A}\,\mathbf{R}(x))$ is the sum of the entries of $\mathbf{R}(x)$ that correspond to entries of $\mathbf{A}$ that are equal to 1. Hence, we obtain

$$n-\mathrm{i}x\,\mathrm{tr}(\mathrm{i}x\mathbf{I}-\mathbf{A})^{-1}=-2\sum_{\{u,v\}\in\mathcal{E}(G)}[\mathbf{R}(x)]_{uv}.$$

Now the adjugate $\mathrm{adj}(z\mathbf{I}-\mathbf{A})$ satisfies the relation $(z\mathbf{I}-\mathbf{A})\,\mathrm{adj}(z\mathbf{I}-\mathbf{A})=|z\mathbf{I}-\mathbf{A}|\,\mathbf{I}$. We can also write down $\mathrm{adj}(z\mathbf{I}-\mathbf{A})$ as a polynomial in z with matrix coefficients. Since the degree of this polynomial cannot exceed $(n-1)$, we have

$$\mathrm{adj}(z\mathbf{I}-\mathbf{A})=\mathbf{M}_{n-1}z^{n-1}+\mathbf{M}_{n-2}z^{n-2}+\cdots+\mathbf{M}_0$$

for appropriate matrices $\mathbf{M}_0, \ldots, \mathbf{M}_{n-1}$. Hence

$$(z\mathbf{I} - \mathbf{A})\left(\mathbf{M}_{n-1}z^{n-1} + \mathbf{M}_{n-2}z^{n-2} + \cdots + \mathbf{M}_0\right) = \phi(G,z)\,\mathbf{I}$$

$$\left(\mathbf{M}_{n-1}z^{n} + \mathbf{M}_{n-2}z^{n-1} + \cdots + \mathbf{M}_0 z\right) - \left(\mathbf{A}\mathbf{M}_{n-1}z^{n-1} + \mathbf{A}\mathbf{M}_{n-2}z^{n-2} + \cdots + \mathbf{A}\mathbf{M}_0\right)$$
$$= \mathbf{I}z^n + \sum_{k=0}^{n-2}(a_k\mathbf{I})z^k$$

for some appropriate coefficients $a_0, \ldots, a_{n-2}$ of $\phi(G,z)$. By comparing coefficients of z^n and of z^{n-1}, we discover that $\mathbf{M}_{n-1} = \mathbf{I}$ and $\mathbf{M}_{n-2} = \mathbf{A}$. Thus, $\operatorname{adj}(z\mathbf{I} - \mathbf{A})$ has polynomials of degree $(n-1)$ on its diagonal, polynomials of degree $(n-2)$ on entries corresponding to edges of G and polynomials of degree at most $(n-3)$ elsewhere. This means that the rational functions that are not on the diagonal of $\mathbf{R}(x)$ have numerators whose degree is at least two less than that of their denominator.

Moreover, the poles of any entry $[\mathbf{R}(x)]_{uv}$ of $\mathbf{R}(x)$ are all purely imaginary, except possibly if G has zero eigenvalues. However, since the Cauchy principal value of $\int_{-\infty}^{\infty} \frac{1}{x^k}\,dx$ converges for $k \in \{1,2,3,\ldots\}$, such poles are not problematic[2]. Consequently, for any edge $\{u,v\}$ in G, the integral $\int_{-\infty}^{\infty}[\mathbf{R}(x)]_{uv}\,dx$ converges, resulting in the following theorem.

Theorem 3.2 [5] $E(G) = \displaystyle\sum_{\{u,v\}\in\mathcal{E}(G)}\left(-\frac{2}{\pi}\int_{-\infty}^{\infty}[\mathbf{R}(x)]_{uv}\,dx\right).$

In the paper [5], the quantity $-\dfrac{1}{\pi}\displaystyle\int_{-\infty}^{\infty}[\mathbf{R}(x)]_{uv}\,dx$ corresponds to p_{uv}, the *bond order* between atoms u and v in the molecule represented by G. In Theorem 3.2, we multiply this quantity by two since clearly $p_{uv} = p_{vu}$ for undirected graphs.

Thus, the diagonal entries of $\mathbf{R}(x)$ are used to provide a vertex decomposition of $E(G)$, while the off–diagonal entries of $\mathbf{R}(x)$ that correspond to edges of G are used to provide an edge decomposition of G (Theorem 3.2), which is known to correspond to bond orders of G.

Remark 3.3 By the argument preceding the theorem statement of Theorem 3.2, the graph G can be deduced from $\mathbf{R}(x)$ in a straightforward manner. The number of vertices of G is clearly equal to the number of columns (or rows) of the matrix $\mathbf{R}(x)$. Moreover, for all

[2]This is not the case if, instead of the Cauchy principal value, the standard interpretation of $\int_{-\infty}^{\infty}\frac{1}{x^k}\,dx$ as being $\lim\limits_{\substack{s\to-\infty\\ t\to\infty}}\int_s^t \frac{1}{x^k}\,dx$ is used.

vertices u and v in $\mathcal{V}(G)$, $\{u,v\} \in \mathcal{E}(G)$ if and only if the degrees of the numerator and denominator of $[\mathbf{R}(x)]_{uv}$ differ by exactly 2.

4 Difference Between Energies of Graphs

We will now apply the techniques used in Section 3 in this section to provide exact formulae for the difference between the energies of graphs that differ by one vertex or edge.

To this end, we require the matrix $[\mathbf{R}(x)]^2$, that is, the square of the resolvent matrix of $\mathbf{A}$ with z replaced by $\mathrm{i}x$. To simplify our work, we denote this matrix by $\mathbf{S}(x)$ (or $\mathbf{S}_G(x)$ if the graph G is not clear from the context). Thus $\mathbf{S}(x) = (\mathrm{i}x\mathbf{I} - \mathbf{A})^{-2}$.

4.1 Difference Between the Energy of a Graph and that of an Overgraph

An *overgraph* G_S of G relative to a subset S of $\mathcal{V}(G)$ is the graph obtained by introducing a new vertex to G that is incident to the vertices in S [15]. The *indicator vector* $\mathbf{b}$ of S is the $n \times 1$ vector where, for all $k \in \{1, 2, \ldots, n\}$, the k^{th} entry of $\mathbf{b}$ is 1 if $k \in S$ and is 0 if $k \notin S$. Thus, the adjacency matrix of G_S is the block matrix $\mathbf{A}_S = \begin{pmatrix} \mathbf{A} & \mathbf{b} \\ \mathbf{b}^\mathsf{T} & 0 \end{pmatrix}$.

Theorem 4.1 below provides the increase in the energy of a graph G after being transformed to G_S, using $\mathbf{R}_G(x)$ and its square $\mathbf{S}_G(x)$.

Theorem 4.1 $E(G_S) - E(G) = \dfrac{1}{\pi}\displaystyle\int_{-\infty}^{\infty} \left[1 - \mathrm{i}x\left(\frac{1 + \mathbf{b}^\mathsf{T}[\mathbf{S}_G(x)]\mathbf{b}}{\mathrm{i}x - \mathbf{b}^\mathsf{T}[\mathbf{R}_G(x)]\mathbf{b}}\right)\right] dx.$

Proof The resolvent matrix $\mathbf{R}_{G_S}(x)$ is equal to $\begin{pmatrix} \mathrm{i}x\mathbf{I} - \mathbf{A} & -\mathbf{b} \\ -\mathbf{b}^\mathsf{T} & \mathrm{i}x \end{pmatrix}^{-1}$, or, equivalently, $\begin{pmatrix} (\mathbf{R}_G(x))^{-1} & -\mathbf{b} \\ -\mathbf{b}^\mathsf{T} & \mathrm{i}x \end{pmatrix}^{-1}$. By [14, p. 25], this matrix inverse can be expressed as the block matrix

$$\mathbf{R}_{G_S}(x) = \begin{pmatrix} \mathbf{R}_G(x) + c(x)[\mathbf{R}_G(x)]\mathbf{b}\mathbf{b}^\mathsf{T}[\mathbf{R}_G(x)] & c(x)[\mathbf{R}_G(x)]\mathbf{b} \\ c(x)\mathbf{b}^\mathsf{T}[\mathbf{R}_G(x)] & c(x) \end{pmatrix}$$

$$\text{where } c(x) = \frac{1}{\mathrm{i}x - \mathbf{b}^\mathsf{T}[\mathbf{R}_G(x)]\mathbf{b}}. \qquad (9)$$

Thus

$$\begin{aligned}
\operatorname{tr}(\mathbf{R}_{G_S}(x)) &= \operatorname{tr}(\mathbf{R}_G(x)) + c(x)\operatorname{tr}\left([\mathbf{R}_G(x)]\mathbf{b}\mathbf{b}^{\mathsf{T}}[\mathbf{R}_G(x)]\right) + c(x) \\
&= \operatorname{tr}(\mathbf{R}_G(x)) + c(x)\left(1 + \operatorname{tr}\left(\mathbf{b}^{\mathsf{T}}[\mathbf{R}_G(x)]^2\mathbf{b}\right)\right) \text{ by Lemma 2.1} \\
&= \operatorname{tr}(\mathbf{R}_G(x)) + c(x)\left(1 + \mathbf{b}^{\mathsf{T}}[\mathbf{S}_G(x)]\mathbf{b}\right) \\
\operatorname{tr}(\mathbf{R}_{G_S}(x)) &= \operatorname{tr}(\mathbf{R}_G(x)) + \frac{1 + \mathbf{b}^{\mathsf{T}}[\mathbf{S}_G(x)]\mathbf{b}}{\mathrm{i}x - \mathbf{b}^{\mathsf{T}}[\mathbf{R}_G(x)]\mathbf{b}}.
\end{aligned}$$

Hence, by Theorem 2.5, we have:

$$\begin{aligned}
E(G_S) &= \frac{1}{\pi}\int_{-\infty}^{\infty}\left[(n+1) - \mathrm{i}x\operatorname{tr}(\mathbf{R}_{G_S}(x))\right]dx \qquad (10) \\
&= \frac{1}{\pi}\int_{-\infty}^{\infty}\left[n + 1 - \mathrm{i}x\left(\operatorname{tr}(\mathbf{R}_G(x)) + \frac{1 + \mathbf{b}^{\mathsf{T}}[\mathbf{S}_G(x)]\mathbf{b}}{\mathrm{i}x - \mathbf{b}^{\mathsf{T}}[\mathbf{R}_G(x)]\mathbf{b}}\right)\right]dx \\
&= \frac{1}{\pi}\int_{-\infty}^{\infty}\left[\left(n - \mathrm{i}x\operatorname{tr}(\mathbf{R}_G(x))\right) + \left(1 - \mathrm{i}x\left(\frac{1 + \mathbf{b}^{\mathsf{T}}[\mathbf{S}_G(x)]\mathbf{b}}{\mathrm{i}x - \mathbf{b}^{\mathsf{T}}[\mathbf{R}_G(x)]\mathbf{b}}\right)\right)\right]dx \\
E(G_S) &= \frac{1}{\pi}\int_{-\infty}^{\infty}\left[n - \mathrm{i}x\operatorname{tr}(\mathbf{R}_G(x))\right]dx \\
&+ \frac{1}{\pi}\int_{-\infty}^{\infty}\left[1 - \mathrm{i}x\left(\frac{1 + \mathbf{b}^{\mathsf{T}}[\mathbf{S}_G(x)]\mathbf{b}}{\mathrm{i}x - \mathbf{b}^{\mathsf{T}}[\mathbf{R}_G(x)]\mathbf{b}}\right)\right]dx. \qquad (11)
\end{aligned}$$

Since the left hand side of (11) is a convergent integral (by (10)) and the first integral of the right hand side of (11) converges to $E(G)$ by Theorem 2.5, we are assured that the integral $\frac{1}{\pi}\int\limits_{-\infty}^{\infty}\left[1 - \mathrm{i}x\left(\frac{1 + \mathbf{b}^{\mathsf{T}}[\mathbf{S}_G(x)]\mathbf{b}}{\mathrm{i}x - \mathbf{b}^{\mathsf{T}}[\mathbf{R}_G(x)]\mathbf{b}}\right)\right]dx$ converges to $E(G_S) - E(G)$. This completes the proof. ■

4.2 Difference Between the Energy of a Graph and that of a Vertex–Deleted Subgraph

Let us, for a moment, keep our focus on the overgraph G_S whose resolvent matrix $\mathbf{R}_{G_S}(x)$ is given by (9). If $v = n + 1$, then clearly, from (9),

$$[\mathbf{R}_{G_S}(x)]_{vv} = c(x) = \frac{1}{\mathrm{i}x - \mathbf{b}^{\mathsf{T}}[\mathbf{R}_G(x)]\mathbf{b}}. \qquad (12)$$

Also, $[\mathbf{S}_{G_S}(x)]_{vv}$ is the last row of $\mathbf{R}_{G_S}(x)$ multiplied by its last column. Thus, from (9) again, we have

$$\begin{aligned} [\mathbf{S}_{G_S}(x)]_{vv} &= \begin{pmatrix} c(x)\mathbf{b}^\mathsf{T}[\mathbf{R}_G(x)] & c(x) \end{pmatrix} \begin{pmatrix} c(x)[\mathbf{R}_G(x)]\mathbf{b} \\ c(x) \end{pmatrix} \\ &= (c(x))^2\,\mathbf{b}^\mathsf{T}[\mathbf{R}_G(x)]^2\mathbf{b} + (c(x))^2 \\ &= (c(x))^2\left(1 + \mathbf{b}^\mathsf{T}[\mathbf{S}_G(x)]\mathbf{b}\right) \\ [\mathbf{S}_{G_S}(x)]_{vv} &= \frac{1 + \mathbf{b}^\mathsf{T}[\mathbf{S}_G(x)]\mathbf{b}}{\left(\mathrm{i}x - \mathbf{b}^\mathsf{T}[\mathbf{R}_G(x)]\mathbf{b}\right)^2}. \end{aligned} \tag{13}$$

By dividing (13) by (12), we obtain

$$\frac{[\mathbf{S}_{G_S}(x)]_{vv}}{[\mathbf{R}_{G_S}(x)]_{vv}} = \frac{1 + \mathbf{b}^\mathsf{T}[\mathbf{S}_G(x)]\mathbf{b}}{\mathrm{i}x - \mathbf{b}^\mathsf{T}[\mathbf{R}_G(x)]\mathbf{b}}. \tag{14}$$

Hence the expression in brackets of Theorem 4.1 containing resolvents of G can be transformed into another expression containing resolvents of G_S by using (14). Moreover, note that G can be considered as being $G_S - v$, one of the vertex–deleted subgraphs of G_S. After renaming the variables of Theorem 4.1 appropriately and rearranging the equation, we determine the following result.

Theorem 4.2 $E(G) - E(G - v) = \dfrac{1}{\pi}\displaystyle\int_{-\infty}^{\infty}\left[1 - \mathrm{i}x\left(\frac{[\mathbf{S}_G(x)]_{vv}}{[\mathbf{R}_G(x)]_{vv}}\right)\right]dx.$

4.3 Difference Between the Energies of Two Graphs That Vary by One Edge

We now discuss the change in energy of a graph G after an extra edge $\{u, v\}$ is added to it, obtaining the graph $G + e_{uv}$. The adjacency matrix of $G + e_{uv}$ is $\mathbf{A} + \mathbf{e}_u\mathbf{e}_v^\mathsf{T} + \mathbf{e}_v\mathbf{e}_u^\mathsf{T}$. As in Theorem 4.1 and Theorem 4.2, we shall express this change in energy as a Coulson–like integral formula.

We shall need the following lemma before proceeding.

Lemma 4.3 [14, Section 0.7.4] *If* $\mathbf{M}$ *is a* $p \times p$ *invertible matrix and* $\mathbf{x}, \mathbf{y}$ *are* $p \times 1$ *vectors such that* $\mathbf{y}^\mathsf{T}\mathbf{M}^{-1}\mathbf{x} \neq -1$, *then*

$$\left(\mathbf{M} + \mathbf{x}\mathbf{y}^\mathsf{T}\right)^{-1} = \mathbf{M}^{-1} - \frac{\mathbf{M}^{-1}\mathbf{x}\mathbf{y}^\mathsf{T}\mathbf{M}^{-1}}{1 + \mathbf{y}^\mathsf{T}\mathbf{M}^{-1}\mathbf{x}}.$$

Let us consider the matrix $\mathbf{R}_{G+e_{uv}}(x)$ associated with the graph $G+e_{uv}$. This is the matrix $\left(\mathrm{i}x\mathbf{I}-\mathbf{A}-\mathbf{e}_u\mathbf{e}_v^\intercal-\mathbf{e}_v\mathbf{e}_u^\intercal\right)^{-1}$. Let $\mathbf{H}=\mathrm{i}x\mathbf{I}-\mathbf{A}-\mathbf{e}_u\mathbf{e}_v^\intercal$ so that $\mathbf{R}_{G+e_{uv}}(x)=\left(\mathbf{H}-\mathbf{e}_v\mathbf{e}_u^\intercal\right)^{-1}$. By Lemma 4.3,

$$\mathbf{H}^{-1}=\mathbf{R}_G(x)+\frac{[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]}{1-\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]\mathbf{e}_u}=\mathbf{R}_G(x)+\frac{[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]}{1-[\mathbf{R}_G(x)]_{vu}}. \tag{15}$$

Furthermore, by the same lemma,

$$\left(\mathbf{H}-\mathbf{e}_v\mathbf{e}_u^\intercal\right)^{-1}=\mathbf{H}^{-1}+\frac{\mathbf{H}^{-1}\mathbf{e}_v\mathbf{e}_u^\intercal\mathbf{H}^{-1}}{1-\mathbf{e}_u^\intercal\mathbf{H}^{-1}\mathbf{e}_v}.$$

By (15), we can thus write $\mathbf{R}_{G+e_{uv}}(x)$ as

$$\begin{aligned}&\left(\mathbf{R}_G(x)+\frac{[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]}{1-[\mathbf{R}_G(x)]_{vu}}\right)\\ &+\frac{\left(\mathbf{R}_G(x)+\frac{[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]}{1-[\mathbf{R}_G(x)]_{vu}}\right)\mathbf{e}_v\mathbf{e}_u^\intercal\left(\mathbf{R}_G(x)+\frac{[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]}{1-[\mathbf{R}_G(x)]_{vu}}\right)}{1-\mathbf{e}_u^\intercal\left(\mathbf{R}_G(x)+\frac{[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]}{1-[\mathbf{R}_G(x)]_{vu}}\right)\mathbf{e}_v}.\end{aligned}$$

$$\begin{aligned}\mathbf{R}_{G+e_{uv}}(x)&=\mathbf{R}_G(x)+\frac{[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]}{1-[\mathbf{R}_G(x)]_{vu}}+\frac{1}{f(x)}\Bigg([\mathbf{R}_G(x)]\mathbf{e}_v\mathbf{e}_u^\intercal[\mathbf{R}_G(x)]\\ &+\frac{[\mathbf{R}_G(x)]\mathbf{e}_v\mathbf{e}_u^\intercal[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]}{1-[\mathbf{R}_G(x)]_{vu}}+\frac{[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]\mathbf{e}_v\mathbf{e}_u^\intercal[\mathbf{R}_G(x)]}{1-[\mathbf{R}_G(x)]_{vu}}\\ &+\frac{[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]\mathbf{e}_v\mathbf{e}_u^\intercal[\mathbf{R}_G(x)]\mathbf{e}_u\mathbf{e}_v^\intercal[\mathbf{R}_G(x)]}{(1-[\mathbf{R}_G(x)]_{vu})^2}\Bigg),\end{aligned}$$

$$\text{where}\qquad f(x)=1-[\mathbf{R}_G(x)]_{uv}-\frac{[\mathbf{R}_G(x)]_{uu}[\mathbf{R}_G(x)]_{vv}}{1-[\mathbf{R}_G(x)]_{vu}}. \tag{16}$$

Since $\mathbf{R}_G(x)$ is symmetric, $[\mathbf{R}_G(x)]_{uv}=[\mathbf{R}_G(x)]_{vu}$ and $[\mathbf{S}_G(x)]_{uv}=[\mathbf{S}_G(x)]_{vu}$. We now determine the trace of both sides of (16) using Lemma 2.1. In order to slightly shorten our notation, from this point onwards, we write $\mathbf{R}$ instead of $\mathbf{R}_G(x)$ and $\mathbf{S}$ instead of $\mathbf{S}_G(x)$.

$$\begin{aligned}\operatorname{tr}(\mathbf{R}_{G+e_{uv}}(x))&=\operatorname{tr}(\mathbf{R})+\frac{\mathbf{S}_{uv}}{1-\mathbf{R}_{uv}}+\frac{1}{f(x)}\left(\mathbf{S}_{uv}+\frac{\mathbf{S}_{vv}\mathbf{R}_{uu}+\mathbf{S}_{uu}\mathbf{R}_{vv}}{1-\mathbf{R}_{uv}}+\frac{\mathbf{S}_{uv}\mathbf{R}_{vv}\mathbf{R}_{uu}}{(1-\mathbf{R}_{uv})^2}\right)\\ &=\operatorname{tr}(\mathbf{R})+\frac{\mathbf{S}_{uv}((1-\mathbf{R}_{uv})^2-\mathbf{R}_{uu}\mathbf{R}_{vv})+\mathbf{S}_{uv}(1-\mathbf{R}_{uv})^2}{((1-\mathbf{R}_{uv})^2-\mathbf{R}_{uu}\mathbf{R}_{vv})(1-\mathbf{R}_{uv})}\\ &+\frac{(\mathbf{S}_{vv}\mathbf{R}_{uu}+\mathbf{S}_{uu}\mathbf{R}_{vv})(1-\mathbf{R}_{uv})+\mathbf{S}_{uv}\mathbf{R}_{vv}\mathbf{R}_{uu}}{((1-\mathbf{R}_{uv})^2-\mathbf{R}_{uu}\mathbf{R}_{vv})(1-\mathbf{R}_{uv})}\end{aligned}$$

$$\operatorname{tr}(\mathbf{R}_{G+e_{uv}}(x)) \quad = \quad \operatorname{tr}(\mathbf{R}) + \frac{2\,\mathbf{S}_{uv}(1-\mathbf{R}_{uv}) + \mathbf{S}_{vv}\mathbf{R}_{uu} + \mathbf{S}_{uu}\mathbf{R}_{vv}}{(1-\mathbf{R}_{uv})^2 - \mathbf{R}_{uu}\mathbf{R}_{vv}}. \tag{17}$$

But by Theorem 2.5, the energy of $G + e_{uv}$ is

$$E(G+e_{uv}) = \frac{1}{\pi}\int_{-\infty}^{\infty} n - \mathrm{i}x\operatorname{tr}(\mathbf{R}_{G+e_{uv}}(x))\,dx.$$

By (17), this can be expressed as

$$\begin{aligned} E(G+e_{uv}) &= \frac{1}{\pi}\int_{-\infty}^{\infty}\left[n - \mathrm{i}x\left(\operatorname{tr}(\mathbf{R}) + \frac{2\,\mathbf{S}_{uv}(1-\mathbf{R}_{uv}) + \mathbf{S}_{vv}\mathbf{R}_{uu} + \mathbf{S}_{uu}\mathbf{R}_{vv}}{(1-\mathbf{R}_{uv})^2 - \mathbf{R}_{uu}\mathbf{R}_{vv}}\right)\right]dx \\ &= \frac{1}{\pi}\int_{-\infty}^{\infty}\left[n - \mathrm{i}x\operatorname{tr}(\mathbf{R}) - \mathrm{i}x\left(\frac{2\,\mathbf{S}_{uv}(1-\mathbf{R}_{uv}) + \mathbf{S}_{vv}\mathbf{R}_{uu} + \mathbf{S}_{uu}\mathbf{R}_{vv}}{(1-\mathbf{R}_{uv})^2 - \mathbf{R}_{uu}\mathbf{R}_{vv}}\right)\right]dx \end{aligned}$$

$$= \frac{1}{\pi}\int_{-\infty}^{\infty}\left[n - \mathrm{i}x\operatorname{tr}(\mathbf{R})\right]dx + \frac{1}{\pi}\int_{-\infty}^{\infty}\left[-\mathrm{i}x\left(\frac{2\,\mathbf{S}_{uv}(1-\mathbf{R}_{uv}) + \mathbf{S}_{vv}\mathbf{R}_{uu} + \mathbf{S}_{uu}\mathbf{R}_{vv}}{(1-\mathbf{R}_{uv})^2 - \mathbf{R}_{uu}\mathbf{R}_{vv}}\right)\right]dx. \tag{18}$$

As before, the left hand side of (18), $E(G + e_{uv})$, and the first integral of the right hand side of (18), $E(G)$, are both convergent integrals. Thus, the last integral in (18) must also converge. We thus arrive at our result.

Theorem 4.4 *The difference between the energy of $G + e_{uv}$ and that of G is equal to*

$$E(G+e_{uv}) - E(G) =$$
$$\frac{1}{\mathrm{i}\pi}\int_{-\infty}^{\infty}\frac{x\big(2[\mathbf{S}_G(x)]_{uv}(1-[\mathbf{R}_G(x)]_{uv}) + [\mathbf{S}_G(x)]_{vv}[\mathbf{R}_G(x)]_{uu} + [\mathbf{S}_G(x)]_{uu}[\mathbf{R}_G(x)]_{vv}\big)}{(1-[\mathbf{R}_G(x)]_{uv})^2 - [\mathbf{R}_G(x)]_{uu}[\mathbf{R}_G(x)]_{vv}}\,dx.$$

If we apply the above argument to the graph $E(G - e_{uv})$, the graph obtained from G by removing edge $\{u, v\}$ from G, then the following theorem is deduced.

Theorem 4.5 *The difference between the energy of G and that of $G - e_{uv}$ is equal to*

$$E(G) - E(G-e_{uv}) =$$
$$\frac{1}{\mathrm{i}\pi}\int_{-\infty}^{\infty}\frac{x\big(2[\mathbf{S}_G(x)]_{uv}(1+[\mathbf{R}_G(x)]_{uv}) - [\mathbf{S}_G(x)]_{vv}[\mathbf{R}_G(x)]_{uu} - [\mathbf{S}_G(x)]_{uu}[\mathbf{R}_G(x)]_{vv}\big)}{(1+[\mathbf{R}_G(x)]_{uv})^2 - [\mathbf{R}_G(x)]_{uu}[\mathbf{R}_G(x)]_{vv}}\,dx.$$

Two graphs G_1 and G_2 satisfying $E(G_1) = E(G_2)$ are called *equienergetic graphs*. Clearly if $\phi(G_1, x) = \phi(G_2, x)$, then G_1 and G_2 are equienergetic. However, the converse of this statement is false. Indeed, several articles on the discovery and construction of equienergetic graphs having different characteristic polynomials may be found in [16, 1, 7, 19]. Theorem 4.5 provides a necessary and sufficient condition for two graphs differing by just one edge to be equienergetic.

Theorem 4.6 *The graphs G and $G \pm e_{uv}$ are equienergetic if and only if the integral*

$$\int_{-\infty}^{\infty} \frac{x\big(2[\mathbf{S}_G(x)]_{uv}(1 \mp [\mathbf{R}_G(x)]_{uv}) \pm [\mathbf{S}_G(x)]_{vv}[\mathbf{R}_G(x)]_{uu} \pm [\mathbf{S}_G(x)]_{uu}[\mathbf{R}_G(x)]_{vv}\big)}{(1 \mp [\mathbf{R}_G(x)]_{uv})^2 - [\mathbf{R}_G(x)]_{uu}[\mathbf{R}_G(x)]_{vv}}\, dx$$

is equal to zero.

Thus, if the expression to be integrated in Theorem 4.6 is an odd function, then G and $G \pm e_{uv}$ are equienergetic.

5 Conclusion

It is known that the energy of G is always larger than that of $G - v$, assuming that v is a vertex of G that is incident to at least one other vertex of G. Thus, the integrals displayed in Theorem 4.1 and Theorem 4.2 are positive quantities for such a vertex v in G, and are equal to zero if v is an isolated vertex.

The authors of [7] showed that the energy of a graph G may increase, decrease or stay the same after the deletion of one of its edges. We have provided a formula that calculates this energy discrepancy in Theorem 4.5. It is interesting to note that it uses not only entries from the resolvent $(z\mathbf{I} - \mathbf{A})^{-1}$ of G, but also entries from the square of this resolvent. Even though it is a relatively complicated formula, Theorem 4.5 sheds light on the problem of deducing how the energy of G changes upon the deletion of one of its edges.

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