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# Energy of a polynomial and the Coulson integral formula

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**Abstract** The energy of an arbitrary polynomial is defined in analogy to the energy of a graph, so that the Coulson integral formula remains valid. In particular, we extend the Coulson integral formula to the case when the zeros of the underlying polynomial are not real and simple. Some related proofs from a recent paper by Peña and Rada are corrected and their results generalized.

**Keywords** Energy (of graph) · Energy (of polynomial) · Coulson formula

## 1 Energy of polynomials

Motivated by chemical applications [1–4], the *energy* of a graph $G$ was defined in the 1970s as [5]

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

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where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the graph $G$ [6]. Since then, graph energy became a very popular topic of mathematical research; for details see the reviews [7,8], the recent papers [9–15], and the references quoted therein.

In view of the fact that the eigenvalues occurring on the right–hand side of Eq. 1 are the zeros of the characteristic polynomial of the graph $G$, the idea to extend this definition to arbitrary polynomials readily comes to the mind. Some early attempts along these lines were reported in [16], again motivated by chemical applications.

Let $\phi = \phi(\lambda)$ be a (complex or real) polynomial of degree $n$, written in the form

$$\phi(\lambda) = \sum_{k=0}^{n} a_k \, \lambda^{n-k}. \tag{2}$$

and let $z_1, z_2, \ldots, z_n$ be its zeros. Without loss of generality we may assume that $\phi$ is monic, i. e., that $a_0 = 1$. In the general case $z_1, z_2, \ldots, z_n$ are complex numbers.

Let $\Pi^+ = \{z : \operatorname{Re} z > 0\}$ and $\Pi^- = \{z : \operatorname{Re} z < 0\}$. Let $s^+$ (respectively $s^-$) be the sum of zeros of $\phi$ in $\Pi^+$ (respectively $\Pi^-$), counting multiplicities.

The eigenvalues of a simple (undirected) graph are real numbers, and their sum is equal to zero [6]. Therefore, in a trivial manner, the graph energy is equal to the right–hand sides of each of the following energy–like quantities:

$$E_+ = E_+(\phi) := 2\, s_+ \tag{3}$$

$$E_c = E_c(\phi) := s^+ - s^- \tag{4}$$

$$E_{re} = E_{re}(\phi) := \operatorname{Re}(s^+ - s^-) = \sum |\operatorname{Re} z_k| \tag{5}$$

$$E_a = E_a(\phi) := \sum |z_k|. \tag{6}$$

provided, of course, that $\phi$ is the characteristic polynomial.

The quantities $E_+$, $E_c$, $E_{re}$, and $E_a$, defined via Eqs. 3–6, may be viewed as possible extensions of the graph–energy concept to arbitrary polynomials.

In the general case the above four definitions are not equivalent. It is clear that $E_+ = E_c$ if and only if the sum of $z_k,\ 1 \le k \le n$, is equal to zero, i. e., $a_1 = 0$. Further, $E_{re} = E_c$ if and only if $\operatorname{Im} E_c = 0$, and $E_a = E_{re} = E_c$ if and only if all $z_k,\ 1 \le k \le n$, are real; otherwise $E_{re} < E_a$. In this paper our aim is to choose this extension in such a way that the *Coulson Integral Formula* (see [1,7,9,17]) remains valid.

As early as in 1940 Charles Coulson obtained a formula in which $E(G)$ was expressed in terms of the characteristic polynomial $\phi(G, \lambda)$ of the graph $G$ [1]:

$$E(G) = \frac{1}{\pi}\, v.p. \int_{-\infty}^{+\infty} \left[ n - i\, y \frac{\phi'(G, iy)}{\phi(G, iy)} \right] dy.$$

Let $P_\phi(z) = z\,\dfrac{\phi'}{\phi} - n$. In [10], using partial fraction decomposition of $P_\phi$, Cauchy residue formula, integration along semicircle and by applying the Jordan lemma, it was deduced that

$$v.p. \int_{-\infty}^{+\infty} P_\phi(iy)\, dy = \pi s^- - \pi s^+.$$

In other words, for an arbitrary polynomial $\phi$,

$$E_c(\phi) = \frac{1}{\pi}\, v.p. \int_{-\infty}^{+\infty} \left[ n - i\, y\, \frac{\phi'(iy)}{\phi(iy)} \right] dy \tag{7}$$

and thus, we consider $E_c(\phi)$, Eq. 4, as the most appropriate candidate for the *energy of a polynomial.*

## 2 Modifying the Coulson integral formula

Define $\gamma(t) = t^n\, \phi(i/t), -\infty < t < \infty$. Then $\gamma(t) = i^n\, \phi^*(t)$, where $\phi^*(t) = \sum_{k=0}^{n} a_k\, (-it)^k$. If the coefficients $a_k$ in (2) are real, we have $\phi^*(-t) = \overline{\phi^*(t)}$ and $|\gamma(-t)| = |\gamma(t)|$.

Let $\hat{\ln}$ be a branch of $Log$ along $\gamma$, such that $\hat{\ln}(\gamma(0)) = \pi i n/2$.

We will make use of the following proposition from Complex Analysis:

**Proposition 1** *If $f, g : [a, b] \to \mathbb{C}$ are non-zero differentiable functions, then for any branch* $\ln(fg)$ *of* $Log(fg)$

$$(\ln(fg))' = f'/f + g'/g.$$

Setting $y = 1/t$ and dividing the integral expression (7) for $E_c(\phi)$ onto two integrals over the intervals $[-\infty, 0]$ and $[0, +\infty]$, we get ($v.p.$ limit is preserved)

$$\begin{aligned} E_c(\phi) &= \frac{1}{\pi} \int_{-\infty}^{0} \left[ n - i\, y\, \frac{\phi'(iy)}{\phi(iy)} \right] dy + \frac{1}{\pi} \int_{0}^{+\infty} \left[ n - i\, y\, \frac{\phi'(iy)}{\phi(iy)} \right] dy \\ &= \frac{1}{\pi} \int_{0}^{-\infty} \left[ -\frac{n}{t} + \frac{i}{t^2}\, \frac{\phi'(i/t)}{\phi(i/t)} \right] \frac{dt}{t} + \frac{1}{\pi} \int_{+\infty}^{0} \left[ -\frac{n}{t} + \frac{i}{t^2}\, \frac{\phi'(i/t)}{\phi(i/t)} \right] \frac{dt}{t} \\ &= \frac{1}{\pi}\, v.p. \int_{-\infty}^{+\infty} \left[ \frac{n}{t} - i\, t^{-2}\, \frac{\phi'(i/t)}{\phi(i/t)} \right] \frac{dt}{t}. \end{aligned} \tag{8}$$

By partial integration, one can prove (see below)

$$E_c(\phi) = \frac{1}{\pi}\, v.p. \int_{-\infty}^{\infty} \left( \hat{\ln}(i^n\, \phi^*(t)) - \frac{\pi i n}{2} \right) \frac{dt}{t^2}. \tag{9}$$

Since $\mathrm{Re}\,\hat{\ln}(i^n \phi^*(t)) = \ln|\gamma(t)|$, we arrive at:

**Theorem 1** *Let $\phi$ be a polynomial of degree $n$ with leading coefficient 1, let $z_k$, $1 \le k \le n$, be its zeros, and let $\gamma(t) = t^n\, \phi(i/t)$. Then*

$$E_{re} = \frac{1}{\pi} \int_{-\infty}^{\infty} \ln|\gamma(t)|\, \frac{dt}{t^2} = \sum |Re\, z_k|. \tag{10}$$

*If $\phi$ is a real polynomial then also*

$$E_{re} = \frac{2}{\pi} \int_{0}^{\infty} \ln|\gamma(t)|\, \frac{dt}{t^2}. \tag{11}$$

*Proof* Suppose that $\phi$ has no zeros on the imaginary axis. Let $v(t) = \hat{\ln}(\gamma(t)) = \hat{\ln}[t^n\, \phi(i/t)]$. We have $v(0) = \pi i n/2$ and according to Proposition 1,

$$dv = \left( \frac{n}{t} - \frac{i}{t^2} \frac{\phi'(i/t)}{\phi(i/t)} \right) dt. \tag{12}$$

Define $\check{v} = v - v(0)$. Since $t^n\, \phi(i/t) = i^n\,(1 - a_1\, it) + O(t^2), t \to 0, \check{v}(t) = -a_1 it + O(t^2)$, so the $v.p.$ integral (9) converges.

By (8) and (12), $E_c(\phi) = \frac{1}{\pi} \int_{-\infty}^{+\infty} (1/t)\, d\check{v}$. By partial integration, setting $u(t) = 1/t$, we find that

$$E_c = \frac{1}{\pi}\, u\check{v}|_{-\infty}^{+\infty} + \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{t^2} \check{v}\, dt.$$

Since $t^n\, \phi(i/t)$ is a polynomial in $t$, $\mathrm{Im}\, \check{v}(t)$ is bounded and therefore $\frac{1}{\pi}\, \frac{\check{v}}{t}|_{-\infty}^{+\infty} = 0$. Hence $E_c(\phi) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{t^2} \check{v}\, dt$ and the formula (10) follows.

The analysis of the case when $\phi$ has zeros on the imaginary axis is routine and is skipped.

If $\phi$ is a real polynomial, then $\phi^*(-t) = \overline{\phi^*(t)},\ |\gamma(-t)| = |\gamma(t)|$, which yields (11). □

A graph is bipartite if and only if it contains no odd-membered cycles. If $G$ is bipartite, then its characteristic polynomial is of the form [6]

$$\phi(G, \lambda) = \sum_{k \ge 0} (-1)^k\, b_{2k}\, \lambda^{n-2k} \tag{13}$$

where $b_{2k} \geq 0,\ b_0 = 1$. Then the energy of $G$ satisfies [2,3]

$$E(G) = \frac{2}{\pi} \int_0^\infty \ln \sum_{k \geq 0} b_{2k}\, x^{2k} \frac{dx}{x^2}. \tag{14}$$

From (14) is evident that if for two bipartite graphs $G'$ and $G''$, the inequalities $b_{2k}(G') \geq b_{2k}(G'')$ hold for every $k \geq 1$, then $E(G') \geq E(G'')$. If at least one of these inequalities is strict, then $E(G') > E(G'')$.

## 3 On the Peña–Rada approach

Peña and Rada [11] have recently examined a special case of the topic that we consider in this paper, namely defining the energy of a digraph, so as to preserve the validity of the Coulson integral formula. They also outlined a proof of Theorem 1, applicable to the special case when $\phi$ is the characteristic polynomial of a digraph. Recall that the characteristic polynomial of a digraph is real, but its eigenvalues may be complex [6].

Let $G$ be a digraph on $n$ vertices and let $z_1, \ldots, z_n$ be its eigenvalues. If the energy of $G$ is defined as

$$E(G) = \sum_{k=1}^{n} |Re\, z_k|$$

then $E(G)$ is equal to the right–hand side of Eq. 7, which is a real number.

Consider the set $D_{n,h}$ of digraphs on $n$ vertices in which every (directed) cycle has length $h$. Peña and Rada [11] used that if $h \equiv 2\ (mod\ 4)$, then for $B \in D_{n,h}$,

$$E(B) = \frac{1}{\pi} \int_{-\infty}^{\infty} \ln \left( i^n \sum_{k \geq 0} b_{kh}\, x^{kh} \right) \frac{dx}{x^2} \tag{15}$$

and, in addition,

$$v.p. \int_{-\infty}^{\infty} \ln(i^n) \frac{dx}{x^2} = 0 \tag{16}$$

from which they deduced:

$$E(B) = \frac{2}{\pi} \int_0^\infty \ln \sum_{k \geq 0} b_{kh}\, x^{kh} \frac{dx}{x^2}. \tag{17}$$

It seems that one needs to make a correction in this approach, in the sense outlined in Sect. 2 and the “Appendix”. The problem is caused by the failure of the formula $\ln(ab) = \ln(a) + \ln(b)$ for complex numbers. Thus Eq. 17 does not directly follow from (15) and (16).

In order to obtain a rigorous proof of the Peña–Rada result, Eq. 17, we make use of Theorem 1 and our formula for energy. As noted after the proof of Theorem 1, the energy of bipartite graphs is given by Eq. 14. The characteristic polynomial of a digraph from $D_{n,h}$, $h \equiv 2\,(mod\,4)$, has the form (13) [11]). Therefore, for $B \in D_{n,h}$, $h \equiv 2\,(mod\,4)$, Eq. 14 reduces to 17.

## 4 Appendix

Let $\mathbb{C}^* = \mathbb{C} \setminus \{0\}$. Every $z \in \mathbb{C}^*$ can be written in the form $z = re^{i\varphi}$, $r > 0$, $\varphi \in \mathbb{R}$, where $r = |z|$ and $e^{i\varphi} = \cos\varphi + i \sin\varphi$. We define

$Arg\, z = \{\varphi \in \mathbb{R} : z = |z|e^{i\varphi}\}$ is a multiple-valued function. The function $Log\, z = \ln r + i\varphi$, $\varphi \in Arg\, z$, is also multiple-valued with infinitely many values. Those values all have the same real part, and their imaginary parts differ by integral multiples of $2\pi$.

The principal value is $\ln z = \ln r + i\varphi$, $r > 0$, $0 \leq \varphi < 2\pi$. It is a single-valued function, whose component functions are $u = \ln r$ and $v = \varphi$, and is not continuous at any point on the positive real axis.

It is continuous on a domain $r > 0$, $0 < \varphi < 2\pi$, consisting of all points in the plane except $z = 0$ and the points on the positive real axis.

If $a, b > 0$, then $\ln(ab) = \ln a + \ln b$. However, this is not always true for complex numbers, for instance:

$$\ln(-1+i) = \ln\sqrt{2} + i5\pi/4, \ (-1+i)^2 = 2i, \ \ln(-1+i)^2 = \ln 2 + i\pi/2$$
$$\ln(-1+i)^2 \neq 2\ln(-1+i).$$

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