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Coulson-type integral formulas for the general energy of polynomials with real roots☆

Lu Qiao, Shenggui Zhang*, Jing Li

Department of Applied Mathematics, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, P.R. China

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ABSTRACT

The energy of a graph is defined as the sum of the absolute values of its eigenvalues. In 1940 Coulson obtained an important integral formula which makes it possible to calculate the energy of a graph without knowing its spectrum. Recently several Coulson-type integral formulas have been obtained for various energies and some other invariants of graphs based on eigenvalues. For a complex polynomial $\phi(z)=\sum_{k=0}^{n}a_kz^{n-k}=a_0\prod_{k=1}^{n}(z-z_k)$ of degree n and a real number α, the general energy of $\phi(z)$, denoted by $E_\alpha(\phi)$, is defined as $\sum_{z_k\neq 0}|z_k|^\alpha$ when there exists $k_0\in\{1,2,\dots,n\}$ such that $z_{k_0}\neq 0$, and 0 when $z_1=\cdots=z_n=0$. In this paper we give Coulson-type integral formulas for the general energy of polynomials whose roots are all real numbers in the case that $\alpha\in\mathbb{Q}$. As a consequence of this result, we obtain an integral formula for the $2l$-th spectral moment of a graph. Furthermore, we show that our formulas hold when α is an irrational number with $0<|\alpha|<2$ and do not hold with $|\alpha|>2$.

1. Introduction

Let G be a graph of order n. The *spectrum* of G consists of the eigenvalues $\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_n$ of the *adjacency matrix* $A(G)$ of G, which are called the *eigenvalues* of G. It is well known that $\lambda_1=\max\{|\lambda_1|,\dots,|\lambda_n|\}$. The *energy* $E(G)$ of G is defined as the sum of the absolute values of the eigenvalues of G, which is an invariant related to total π-electron energy [16]. Many mathematicians and chemists have done lots of work in the theory of graph energy, and also have obtained many results on this invariant of graphs (see [8,11]). In 1940, Coulson [4] obtained an important integral formula which makes it possible to calculate the energy of a graph without knowing its spectrum. That is, for a graph G, its energy

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

where $\phi_A(G,x)$ is the characteristic polynomial of $A(G)$ (called the *characteristic polynomial* of G). This formula is said to be the *Coulson integral formula*, and has many applications in the theory of graph energy (see [2,3,8–11,17]).

The energy of graphs has many generalizations and extensions. Recently several Coulson-type integral formulas have been obtained for various energies and some other invariants of graphs based on eigenvalues (see [7,12–15]).

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* Corresponding author.
E-mail addresses: water6qiao@mail.nwpu.edu.cn (L. Qiao), sgzhang@nwpu.edu.cn (S. Zhang), jingli@nwpu.edu.cn (J. Li).

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Let

$$\phi(z) = \sum_{k=0}^{n} a_k z^{n-k} = a_0 \prod_{k=1}^{n} (z - z_k)$$

be a complex polynomial of degree n. In [12], the authors defined the following energy-like quantities of $\phi(z)$:

$$E_+(\phi) := 2 \sum_{\mathrm{Re} z_k > 0} z_k, \tag{1}$$

$$E_c(\phi) := \sum_{\mathrm{Re} z_k > 0} z_k - \sum_{\mathrm{Re} z_k < 0} z_k, \tag{2}$$

$$E_{re}(\phi) := \mathrm{Re}\left(\sum_{\mathrm{Re} z_k > 0} z_k - \sum_{\mathrm{Re} z_k < 0} z_k \right) = \sum |\mathrm{Re} z_k|, \tag{3}$$

$$E_a(\phi) := \sum |z_k|. \tag{4}$$

Clearly, the graph energy coincides the right-hand side of each of Eqs. (1)–(4). The authors of [12] extended the Coulson integral formula to the case when the roots of a polynomial are not real and simple. Shao et al. [15] proved both the complex form and real form of the Coulson integral formulas for $E_c(\phi)$ (called the (complex) energy of $\phi(z)$) by new approaches.

In [13], Qiao et al. further extended the energy of graphs to polynomials as follows.

Definition 1 [13]**.** Let

$$\phi(z) = \sum_{k=0}^{n} a_k z^{n-k} = a_0 \prod_{k=1}^{n} (z - z_k)$$

be a complex polynomial of degree n and α a real number. The general energy of $\phi(z)$, denoted by $E_\alpha(\phi)$, is defined as $\sum_{z_k \neq 0} |z_k|^\alpha$ when there exists $k_0 \in \{1, 2, \ldots, n\}$ such that $z_{k_0} \neq 0$, and 0 when $z_1 = \cdots = z_n = 0$.

In this paper, we obtain some Coulson-type integral formulas for the general energy of polynomials whose roots are all real numbers with $\alpha \in \mathbb{Q}$ in Section 3. Before that, in Section 2, we give some preliminaries we need from complex analysis. In Section 4, we present an integral formula for the $2l$-th spectral moment of a graph. In Section 5, We further show that our formulas hold when α is an irrational number with $0 < |\alpha| < 2$ and do not hold with $|\alpha| > 2$.

2. Preliminaries

We first introduce some basic concepts and results in complex analysis which will be used later. Let $w = \rho e^{i\theta}$, where $\rho \geq 0$ and $\theta \in [0, 2\pi)$. Then,

$$z^q - w = (z - \rho^{\frac{1}{q}} e^{i\frac{\theta}{q}})(z - \rho^{\frac{1}{q}} e^{i\frac{\theta+2\pi}{q}}) \cdots (z - \rho^{\frac{1}{q}} e^{i\frac{\theta+2(q-1)\pi}{q}}), \tag{5}$$

where $q \in \mathbb{Z}^+$.

Let D be a bounded domain. The boundary of D is denoted by ∂D.

The following three results in complex analysis are well known (see [6]).

Lemma 1 (Cauchy's Theorem)**.** *Let D be a bounded domain with piecewise smooth boundary. If $f(z)$ is analytic on D, and extends smoothly to ∂D, then*

$$\int_{\partial D} f(z) \mathrm{d}z = 0.$$

Lemma 2 (Cauchy Integral Formula)**.** *Let D be a bounded domain with piecewise smooth boundary. If $f(z)$ is analytic on D, and extends smoothly to the boundary of D, then*

$$f(z) = \frac{1}{2\pi i} \int_{\partial D} \frac{f(\zeta)}{\zeta - z} \mathrm{d}\zeta, \quad z \in D.$$

Lemma 3. *Suppose that Γ is a piecewise smooth curve. If $f(z)$ is a continuous function on Γ, then $\left| \int_\Gamma f(z) \mathrm{d}z \right| \leq \int_\Gamma |f(z)| \cdot |\mathrm{d}z|$. Further, if Γ has length L, and $|f(z)| \leq M$ on Γ, then*

$$\left| \int_\Gamma f(z) \mathrm{d}z \right| \leq ML.$$

We also need the following simple lemma. The proof is omitted here.