



# On $A_\alpha$ , Laplace and $ABC$ energies of Dendrimer and Bethe trees

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**Abstract.** In this paper, we obtain almost all  $A_\alpha$ , Laplace and  $ABC$  eigenvalues of Dendrimer trees and three reduction calculation formulae for the three corresponding energies. And we calculate all  $A_\alpha$ , Laplace and  $ABC$  eigenvalues and energies of Bethe trees.

## 1. Introduction

Dendrimers are widely used in sensing, catalysis, molecular electronics, photonics, nanomedicine and other fields [1, 7]. The energy of a graph is also an important topological index that can be used to approximate the total energy of  $\pi$ -electrons in conjugated hydrocarbons [4, 5].

A Dendrimer tree  $D_{n,k}$  [2] is an  $n + 1$  layer tree with the root  $u$  such that  $deg(v) = k$  for  $0 \leq d(u, v) < n$  and  $deg(v) = 1$  for  $d(u, v) = n$ , see Figure 1 for an example. A Bethe tree  $B_{n,k}$  [10] is obtained from a Dendrimer

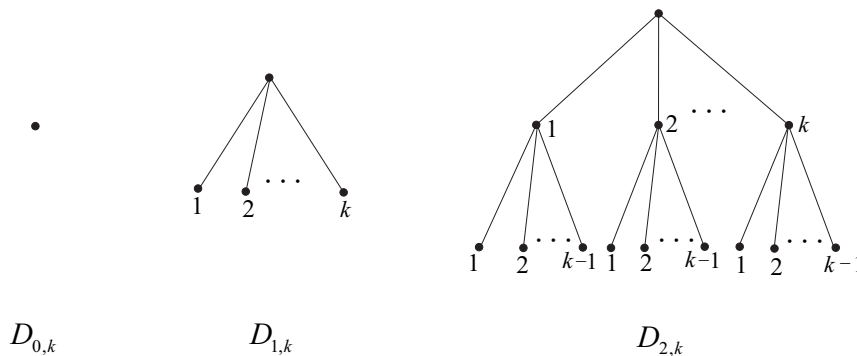


Figure 1: The Dendrimer trees  $D_{0,k}$ ,  $D_{1,k}$  and  $D_{2,k}$

tree  $D_{n,k}$  by deleting a child of the root  $u$  and all descendants of the child, see Figure 2 for an example.

Due to widespread application of these two types of trees in multiple disciplines and fields, their topological properties have attracted the attention of many scholars. In 2007, Rojo [10] derived an explicit

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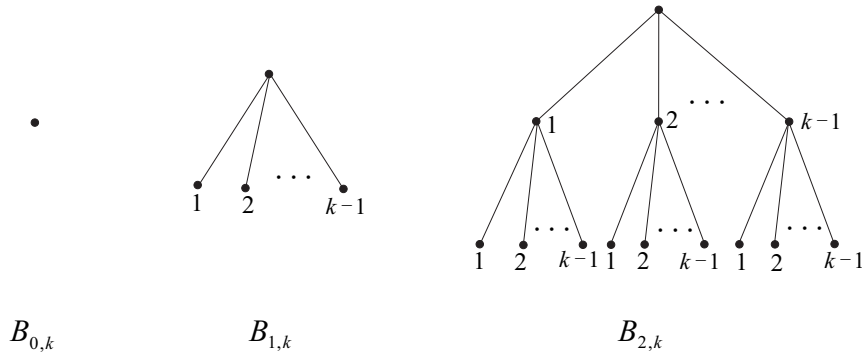


Figure 2: The Bethe trees  $B_{0,k}$ ,  $B_{1,k}$  and  $B_{2,k}$

formula for the eigenvalues of  $B_{n,k}$ . In 2017, Nikiforov [9] obtained the  $A_\alpha$ -characteristic polynomial and its spectrum of the generalized Bethe tree  $\mathcal{B}_k$ , which is a rooted tree of layer  $k + 1$  and vertices of the same level have the same degree. In 2021, Bokhary and Tabassum [2] gave the energy of  $D_{2,k}$  and  $D_{3,k}$  and compared the energies for distinct values of  $n$  and  $k$ . In 2022, Xu and Yan [11] obtained the characteristic polynomial and almost all eigenvalues of  $D_{n,k}$  and computed the energy of  $D_{3,k}$  and  $D_{4,k}$ .

The graph energy of a simple graph  $G$  is defined by Gutman in [4],

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

where  $\lambda_1(G), \lambda_2(G), \dots, \lambda_n(G)$  are the eigenvalues of the adjacency matrix of  $G$ . The  $A_\alpha$ -energy [12], Laplace energy [6], and  $ABC$  energy [3] of a graph are defined similar to the graph energy such that the sum of the absolute values of the eigenvalues of  $A_\alpha$ , Laplace and  $ABC$  matrices of the graph.

In this paper, we determine  $A_\alpha$ , Laplace and  $ABC$  characteristic polynomials and their eigenvalues for  $D_{n,k}$  and  $B_{n,k}$ .

## 2. Elementary

Let  $A(G), D(G)$  and  $Q(G)$  represent the adjacency matrix, diagonal matrix and signless Laplacian matrix of a graph  $G$ , respectively. For any real number  $\alpha \in [0, 1]$ , Nikiforov [8] defined  $A_\alpha$ -matrix and  $A_\alpha$ -characteristic polynomial as follows:

$$\begin{aligned} A_\alpha(G) &= \alpha D(G) + (1 - \alpha)A(G), \\ \phi(A_\alpha(G), \lambda) &= \det(\lambda I_n - A_\alpha(G)), \end{aligned}$$

where  $I_n$  is the identity matrix of order  $n$ . Obviously,  $A_0(G) = A(G)$ ,  $A_1(G) = D(G)$  and  $2A_{\frac{1}{2}}(G) = Q(G)$ .

For any integer  $0 \leq j \leq n$ , let  $N_{n-j}(T)$  be the number of vertices at layer  $j$  of a rooted tree  $T$  and  $m_s(T) = N_s(T)/N_{s+1}(T)$ . It is easy to calculate that





Since

$$(\lambda - k)\alpha - \frac{\beta^2 m_{n-1} P_{n-2}}{P_{n-1}} = \frac{(\lambda - \alpha k) P_{n-1} - \beta^2 k P_{n-2}}{P_{n-1}} = \frac{P_n - \beta^2 P_{n-2}}{P_{n-1}},$$

$$\phi_{A_\alpha(D_{n,k})}(\lambda) = \begin{vmatrix} P_0 I_{N_0} & -\beta J_{m_0} & 0 & & & 0 \\ & \frac{P_1}{P_0} I_{N_1} & -\beta J_{m_1} & & & \\ & & \frac{P_2}{P_1} I_{N_2} & & & \\ & & \ddots & \ddots & & \\ & & & \frac{P_{n-2}}{P_{n-3}} I_{N_{n-2}} & -\beta J_{m_{n-2}} & \\ & & & & \frac{P_{n-1}}{P_{n-2}} I_{N_{n-1}} & -\beta J_{m_{n-1}} \\ 0 & & & & 0 & \frac{P_n - \beta^2 P_{n-2}}{P_{n-1}} I_{N_n} \end{vmatrix}.$$

Therefore

$$\begin{aligned} \phi_{A_\alpha(D_{n,k})} &= P_0^{N_0} \left(\frac{P_1}{P_0}\right)^{N_1} \cdots \left(\frac{P_{n-2}}{P_{n-3}}\right)^{N_{n-2}} \left(\frac{P_{n-1}}{P_{n-2}}\right)^{N_{n-1}} \left(\frac{P_n - \beta^2 P_{n-2}}{P_{n-1}}\right)^{N_n} \\ &= P_0^{k(k-1)^{n-2}(k-2)} P_1^{k(k-1)^{n-3}(k-2)} \cdots P_{n-2}^{k(k-2)} P_{n-1}^{k-1} (P_n - \beta^2 P_{n-2}) \\ &= (P_n - \beta^2 P_{n-2}) P_{n-1}^{k-1} \prod_{j=0}^{n-2} P_j^{k(k-1)^{n-j-2}(k-2)}. \end{aligned}$$

**Corollary 3.2.** *The  $A_\alpha$ -eigenvalues of  $D_{n,k}$  are the roots of  $P_n - \beta^2 P_{n-2}$  and*

$$\alpha k + 2\beta \sqrt{k-1} \cos \frac{l\pi}{j+2},$$

moreover its multiplicity is

$$\begin{cases} k(k-1)^{n-j-2}(k-2), & j = 0, 1, \dots, n-2 \text{ and } l = 1, 2, \dots, j+1; \\ k-1, & j = n-1 \text{ and } l = 1, 2, \dots, n. \end{cases}$$

**Corollary 3.3.** *The  $A_\alpha$ -energy of  $D_{n,k}$  is*

$$\begin{aligned} E_{A_\alpha}(D_{n,k}) &= \alpha k \left[ \sum_{l=1}^{j+1} \sum_{j=0}^{n-2} k(k-2)(k-1)^{n-j-2} + \sum_{l=1}^n (k-1) \right] \\ &\quad + 2\beta \sqrt{k-1} \left[ k(k-2) \sum_{l=1}^{j+1} \sum_{j=0}^{n-2} (k-1)^{n-j-2} \left| \cos \frac{l\pi}{j+2} \right| + (k-1) \sum_{l=1}^n \left| \cos \frac{l\pi}{n+1} \right| \right] \\ &\quad + \varepsilon(P_n - \beta^2 P_{n-2}). \end{aligned}$$

where  $\varepsilon(P_n - \beta^2 P_{n-2})$  is the sum of the absolute values of the eigenvalues of  $P_n - \beta^2 P_{n-2}$ .

Following a similar procedure for the Dendrimer tree  $D_{n,k}$ , it is easier to calculate the  $A_\alpha$ -eigenvalues of the Bethe tree  $B_{n,k}$ .

**Theorem 3.4.** *The  $A_\alpha$ -characteristic polynomial of the Bethe tree  $B_{n,k}$  is*

$$\phi(A_\alpha(B_{n,k}), \lambda) = P_n \prod_{j=0}^{n-1} P_j^{(k-1)^{n-j-1}(k-2)}.$$

**Corollary 3.5.** *The  $A_\alpha$ -eigenvalues of  $B_{n,k}$  are*

$$\alpha k + 2\beta \sqrt{k-1} \cos \frac{l\pi}{j+2},$$

moreover its multiplicity is

$$\begin{cases} (k-1)^{n-j-1}(k-2), & j = 0, 1, \dots, n-1 \text{ and } l = 1, 2, \dots, j+1; \\ 1, & j = n, \text{ and } l = 1, 2, \dots, n+1. \end{cases}$$

**Corollary 3.6.** *The  $A_\alpha$ -energy of  $B_{n,k}$  is*

$$E_{A_\alpha}(B_{n,k}) = \alpha k \left[ (k-2) \sum_{j=0}^{n-1} \sum_{l=0}^{j+1} (k-1)^{n-j-1} + \sum_{l=1}^{n+1} 1 \right] + 2\beta \sqrt{k-1}(k-2) \left[ \sum_{j=0}^{n-1} \sum_{l=1}^{j+1} (k-1)^{n-j-1} \left| \cos \frac{l\pi}{j+2} \right| + \sum_{l=1}^{n+1} \left| \cos \frac{l\pi}{n+2} \right| \right].$$

#### 4. Adjacency eigenvalues and Laplace eigenvalues of $D_{n,k}$ and $B_{n,k}$

**Lemma 4.1.** *Let*

$$\begin{cases} P'_0 = \lambda; \\ P'_1 = \lambda^2 - (k-1); \\ P'_n = \lambda P'_{n-1} - (k-1)P'_{n-2} \text{ for } n \geq 2, \end{cases}$$

then

$$P'_n = \frac{1}{\sqrt{\lambda^2 - 4(k-1)}} \left[ \left( \frac{\lambda + \sqrt{\lambda^2 - 4(k-1)}}{2} \right)^{n+2} - \left( \frac{\lambda - \sqrt{\lambda^2 - 4(k-1)}}{2} \right)^{n+2} \right].$$

Setting  $\alpha = 0$  in Theorems 3.1 and 3.4, we have the following two corollaries.

**Corollary 4.2 ([11]).** *The characteristic polynomial of  $D_{n,k}$  is*

$$\phi_{D_{n,k}}(\lambda) = (P'_n - P'_{n-2})P'^{k-1}_{n-1} \prod_{j=0}^{n-2} P'_j{}^{k(k-1)^{n-j-2}(k-2)}.$$

The eigenvalues of  $D_{n,k}$  are the roots of  $P'_n - P'_{n-2}$  and

$$2\sqrt{k-1} \cos \frac{l\pi}{j+2},$$

moreover its multiplicity is

$$\begin{cases} k(k-1)^{n-j-2}(k-2), & j = 0, 1, \dots, n-2 \text{ and } l = 1, 2, \dots, j+1; \\ k-1, & j = n-1 \text{ and } l = 1, 2, \dots, n. \end{cases}$$

The energy of  $D_{n,k}$  is

$$E(D_{n,k}) = 2k(k-2)\sqrt{k-1} \sum_{l=1}^{j+1} \sum_{j=0}^{n-2} (k-1)^{n-j-2} \left| \cos \frac{l\pi}{j+2} \right| + 2(k-1)\sqrt{k-1} \sum_{l=1}^n \left| \cos \frac{l\pi}{n+2} \right| + \varepsilon(P'_n - P'_{n-2}).$$

**Corollary 4.3 ([10]).** *The characteristic polynomial of  $B_{n,k}$  is*

$$\phi_{B_{n,k}}(\lambda) = P'_n \prod_{j=0}^{n-1} P_j'^{k(k-1)^{n-j-1}(k-2)}.$$

The eigenvalues of  $B_{n,k}$  are

$$2\sqrt{k-1} \cos \frac{l\pi}{j+2},$$

moreover its multiplicity is

$$\begin{cases} (k-1)^{n-j-1}(k-2), & j = 0, 1, \dots, n-1 \text{ and } l = 1, 2, \dots, j+1; \\ 1, & j = n \text{ and } l = 1, 2, \dots, n+1. \end{cases}$$

The energy of  $B_{n,k}$  is

$$E(B_{n,k}) = 2(k-2)\sqrt{k-1} \sum_{l=1}^{j+1} \sum_{j=0}^{n-1} (k-1)^{n-j-1} \left| \cos \frac{l\pi}{j+2} \right| + 2\sqrt{k-1} \sum_{l=1}^{n+1} \left| \cos \frac{l\pi}{n+2} \right|.$$

**Lemma 4.4.** *Let*

$$\begin{cases} P''_0 = \lambda - 1; \\ P''_1 = (\lambda - k)(\lambda - 1) - (k - 1); \\ P''_n = (\lambda - k)P''_{n-1} - (k - 1)P''_{n-2} \text{ for } n \geq 2, \end{cases}$$

then

$$P''_n = \frac{1}{\sqrt{(\lambda-k)^2-4(k-1)}} \left[ \left( \frac{(\lambda-k) + \sqrt{(\lambda-k)^2-4(k-1)}}{2} \right)^{n+2} - \left( \frac{(\lambda-k) - \sqrt{(\lambda-k)^2-4(k-1)}}{2} \right)^{n+2} \right].$$

Recall that the Laplace matrix of  $G$  is  $L(G) = D(G) - A(G)$ .

**Theorem 4.5.** *The Laplace characteristic polynomial of the Dendrimer tree  $D_{n,k}$  is*

$$\phi_{L(D_{n,k})}(\lambda) = (P''_n - P''_{n-2})P''_{n-1} \prod_{j=0}^{n-2} P_j''^{k(k-1)^{n-j-2}(k-2)}.$$

The Laplace eigenvalues of  $D_{n,k}$  are the roots of  $P''_n - P''_{n-1}$  and

$$k + 2\sqrt{k-1} \cos \frac{l\pi}{j+2},$$

moreover its multiplicity is

$$\begin{cases} k(k-1)^{n-j-2}(k-2), & j = 0, 1, \dots, n-2 \text{ and } l = 1, 2, \dots, j+1; \\ k-1, & j = n-1 \text{ and } l = 1, 2, \dots, n. \end{cases}$$

The Laplace energy of  $D_{n,k}$  is

$$\begin{aligned} E_L(D_{n,k}) = & k \left[ k(k-2) \sum_{l=1}^{j+1} \sum_{j=0}^{n-2} (k-1)^{n-j-2} + \sum_{l=1}^n (k-1) \right] \\ & + 2\sqrt{k-1} \left[ k(k-2) \sum_{l=1}^{j+1} \sum_{j=0}^{n-2} (k-1)^{n-j-2} \left| \cos \frac{l\pi}{j+2} \right| + (k-1) \sum_{l=1}^n \left| \cos \frac{l\pi}{n+1} \right| \right] \\ & + \varepsilon(P''_n - P''_{n-2}). \end{aligned}$$

**Theorem 4.6.** *The Laplace characteristic polynomial of the Bethe tree  $B_{n,k}$  is*

$$\phi_{L(D_{n,k})}(\lambda) = P_n'' \prod_{j=0}^{n-1} P_j''^{(k-1)^{n-j-1}(k-2)}.$$

The Laplace eigenvalues of  $B_{n,k}$  are

$$k + 2\sqrt{k-1}\cos\frac{l\pi}{j+2},$$

moreover its multiplicity is

$$\begin{cases} (k-1)^{n-j-1}(k-2), & j = 0, 1, \dots, n-1 \text{ and } l = 1, 2, \dots, j+1; \\ 1, & j = n \text{ and } l = 1, 2, \dots, n+1. \end{cases}$$

The Laplace energy of  $B_{n,k}$  is

$$\begin{aligned} E_L(B_{n,k}) = & k \left[ (k-2) \sum_{j=0}^{n-1} \sum_{l=1}^{j+1} (k-1)^{n-j-1} + \sum_{l=1}^{n+1} 1 \right] \\ & + 2\sqrt{k-1} \left[ (k-2) \sum_{j=0}^{n-1} \sum_{l=1}^{j+1} (k-1)^{n-j-1} \left| \cos \frac{l\pi}{n+1} \right| + \sum_{l=1}^{n+1} \left| \cos \frac{l\pi}{n+2} \right| \right]. \end{aligned}$$

**Corollary 4.7.**

$$E_{A_\alpha(B_{n,k})} < E_L(B_{n,k}) = (k + 2\sqrt{k-1}) \left[ \frac{k(k-1)[(k-1)^n - 1]}{k-2} - nk + n + 1 \right].$$

**Proof.** Since

$$\sum_{l=1}^{j+1} \sum_{j=0}^{n-1} (k-1)^{n-j-1} \left| \cos \frac{l\pi}{j+2} \right| \leq \sum_{j=0}^{n-1} (j+1)(k-1)^{n-j-1} = \frac{(k-1)[(k-1)^n - 1]}{(k-2)^2} + \frac{n}{(k-2)},$$

we have

$$\begin{aligned} E_{A_\alpha(B_{n,k})} = & \alpha k \left[ (k-2) \sum_{j=0}^{n-1} \sum_{l=0}^{j+1} (k-1)^{n-j-1} + \sum_{l=1}^{n+1} 1 \right] \\ & + 2\beta\sqrt{k-1}(k-2) \left[ \sum_{j=0}^{n-1} \sum_{l=1}^{j+1} (k-1)^{n-j-1} \left| \cos \frac{l\pi}{j+2} \right| + \sum_{l=1}^{n+1} \left| \cos \frac{l\pi}{n+2} \right| \right] \\ < E_L(B_{n,k}) = & k \left[ (k-2) \sum_{j=0}^{n-1} \sum_{l=1}^{j+1} (k-1)^{n-j-1} + \sum_{l=1}^{n+1} 1 \right] \\ & + 2\sqrt{k-1} \left[ (k-2) \sum_{j=0}^{n-1} \sum_{l=1}^{j+1} (k-1)^{n-j-1} \left| \cos \frac{l\pi}{n+1} \right| + \sum_{l=1}^{n+1} \left| \cos \frac{l\pi}{n+2} \right| \right] \\ \leq & (k + 2\sqrt{k-1}) \left[ k(k-2) \sum_{j=0}^{n-1} \sum_{l=1}^{j+1} (k-1)^{n-j-1} + \sum_{l=1}^{n+1} 1 \right] \\ = & (k + 2\sqrt{k-1}) \left[ \frac{k(k-1)[(k-1)^n - 1]}{k-2} - nk + n + 1 \right]. \end{aligned}$$



**5. ABC energy of  $D_{n,k}$  and  $B_{n,k}$**

Chen [3] defined the ABC-matrix is  $ABC(G) = (abc_{ij})$  and ABC-characteristic polynomial of graph  $G$  as follows:

$$ABC(G) = (\omega_{ij}), \omega_{ij} = \begin{cases} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}, & i \text{ is adjacent to } j; \\ 0, & \text{otherwise,} \end{cases}$$

$$\phi(ABC(G), \lambda) = \det(\lambda I_n - ABC(G)).$$

It is not difficult to determine the ABC matrix of  $D_{n,k}$ .

$$ABC(D_{n,k}) = \begin{bmatrix} 0 & K_{m_0} & 0 & & 0 \\ K_{m_0}^T & 0 & K_{m_1} & & \\ & K_{m_1}^T & & & \\ & & \ddots & \ddots & \\ & & & K_{m_{n-2}} & K_{m_{n-1}} \\ 0 & & & K_{m_{n-2}}^T & 0 & K_{m_{n-1}}^T & 0 \end{bmatrix},$$

where  $K_{m_i}$  is the column  $m_i$  vector of  $\frac{\sqrt{2(k-1)}}{k}$  and  $K_{m_i}^T K_{m_i} = m_i \frac{2(k-1)}{k^2}$ .

**Lemma 5.1.** *Let*

$$\begin{cases} P_0''' = \lambda; \\ P_1''' = \lambda^2 - \frac{2(k-1)^2}{k^2}; \\ P_n''' = \lambda P_{n-1}''' - \frac{2(k-1)^2}{k^2} P_{n-2}''' \text{ for } n \geq 2, \end{cases}$$

then

$$P_n''' = \frac{1}{\sqrt{\lambda^2 - \frac{8(k-1)^2}{k^2}}} \left[ \left( \frac{\lambda + \sqrt{\lambda^2 - \frac{8(k-1)^2}{k^2}}}{2} \right)^{n+2} - \left( \frac{\lambda - \sqrt{\lambda^2 - \frac{8(k-1)^2}{k^2}}}{2} \right)^{n+2} \right].$$

Then again using a similar method for the calculation of the  $A_\alpha$ -energy of  $D_{n,k}$ , we have the following results.

**Theorem 5.2.** *The ABC characteristic polynomial of the Dendrimer tree  $D_{n,k}$  is*

$$\phi(ABC(D_{n,k}), \lambda) = \left( P_n''' - \frac{2(k-1)}{k^2} P_{n-2}''' \right) P_{n-1}'''^{k-1} \prod_{j=0}^{n-2} P_j'''^{(k-1)^{n-j-2}(k-2)}.$$

The ABC eigenvalues of  $D_{n,k}$  are the roots of  $P_n''' - \frac{2(k-1)}{k^2} P_{n-2}'''$  and

$$2\sqrt{2} \frac{k-1}{k} \cos \frac{l\pi}{j+2},$$

moreover its multiplicity is

$$\begin{cases} (k-1)^{n-j-2}(k-2), & j = 0, 1, \dots, n-2 \text{ and } l = 1, 2, \dots, j+1; \\ k-1, & j = n-1 \text{ and } l = 1, 2, \dots, n. \end{cases}$$

The ABC energy of  $D_{n,k}$  is

$$E_{ABC}(D_{n,k}) = 2\sqrt{2}\frac{k-2}{k} \sum_{j=1}^{n-2} \sum_{l=1}^{j+1} (k-1)^{n-j-1} \left| \cos \frac{l\pi}{j+2} \right| + 2\sqrt{2}\frac{(k-1)^2}{k} \sum_{l=1}^n \left| \cos \frac{l\pi}{n+1} \right| + \varepsilon \left( P_n''' - \frac{2(k-1)}{k^2} P_{n-2}''' \right).$$

**Theorem 5.3.** The ABC characteristic polynomial of the Bethe tree  $B_{n,k}$  is

$$\phi(ABC(B_{n,k}), \lambda) = P_n''' \prod_{j=0}^{n-1} P_j'''^{(k-1)^{n-j-1}(k-2)}.$$

The ABC eigenvalues of  $B_{n,k}$  are

$$2\sqrt{2}\frac{k-1}{k} \cos \frac{l\pi}{j+2},$$

moreover its multiplicity is

$$\begin{cases} (k-1)^{n-j-1}(k-2), & j = 0, 1, \dots, n-1 \text{ and } l = 1, 2, \dots, j+1; \\ 1, & j = n \text{ and } l = 1, 2, \dots, n+1. \end{cases}$$

The ABC energy of  $B_{n,k}$  is

$$E_{ABC}(B_{n,k}) = 2\sqrt{2}\frac{k-1}{k} \left[ \sum_{j=1}^{n-1} \sum_{l=1}^{j+1} (k-2)(k-1)^{n-j-1} \left| \cos \frac{l\pi}{j+2} \right| + \sum_{l=1}^{n+1} \left| \cos \frac{l\pi}{n+1} \right| \right].$$

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