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RESEARCH ARTICLE

Matrix Analysis of Hexagonal Model and Its Applications in Global Mean-First-Passage Time of Random Walks

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ABSTRACT Recent advances in graph-structured learning have demonstrated promising results on the graph classification task. However, making them scalable on huge graphs with millions of nodes and edges remains challenging due to their high temporal complexity. In this paper, by the decomposition theorem of Laplacian polynomial and characteristic polynomial we established an explicit closed-form formula of the global mean-first-passage time (GMFPT) for hexagonal model. Our method is based on the concept of GMFPT, which represents the expected values when the walk begins at the vertex. GMFPT is a crucial metric for estimating transport speed for random walks on complex networks. Through extensive matrix analysis, we show that, obtaining GMFPT via spectrums provides an easy calculation in terms of large networks.

INDEX TERMS Hexagonal model, Laplacian polynomial, decomposition theorem, GMFPT.

I. INTRODUCTION

Interactions between pairs of entities occur every day in real-world systems. Human interaction, financial systems, recommender systems, social networks, road networks, and networks of protein interactions are examples of such systems. In graph theory, these pairs of entities are called a network, in which the substances are vertices and the communication between any two substances are an edge [6]. Networks have rich applications in classical grid-structured data, such as photographs, to speed up calculations. The graph-structural data is useful in encoding networks of low-dimensional embeddings for classic machine learning and data mining algorithms [3]. Researchers follow this strategy to handle complex graph problems, such as graph categorization. The network arrangement problem is concerned with categorizing complicated network structures into multiple groups. It has many real-life phenomena, including text organization, predicting chemical venomousness, and categorizing public buildings in human interactions. Though the permuting indices and the encoding's runtime effectiveness are hurdles in graph classification, for a simple and less order graphs, it is easy to construct an adjacency matrix to check the properties of such graphs [14]. As a result, the best encoding strategy for simple and finite graph classification is indices over node permutations. The adjacency matrix strategy is also convenient in neural graphs to the limitations and worldwide locations of the set of nodes [32]. Prevailing graph classification methods frequently necessitate an adjacent assessment of the structures or rely entirely on algebraic and spectral symbol, which are difficult to calculate. Appropriate illustration approaches are mandatory to encrypt the atomic assembly of the display concisely, which is well-organized. However, transformation invariance, scalability, in addition the programming's runtime proficiency are hurdles in graph classification. Because of the deficiency in order of graph vertices, numerous adjacency matrices can represent the same graph. Consequently,

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the optimum programming method for graph classification is the best invariant further down transformations of the vertices. The current network classification methods frequently require an adjacent assessment of the structures or rely entirely on arranged algebraic spectral investigation, both of which are difficult to investigate. It has recently been used to quantify the robustness of networks in distributed networked control systems based on noisy data. In reality, it has many comparable descriptions, such as the spectrums of graphs and it can be used to extract graph representations.

It is renowned that hexagonal systems play a significant part in theoretical chemistry, since they are usual graph symbols of benzenoid hydrocarbon [11]. As a result, hexagonal systems have received a lot of attention. Kennedy and Quintas investigated the enumerations on perfect matchings in an arbitrary hexagonal chain model [17]. In [10] and [22], the authors determined the Wiener index (resp. Edge-Szeged index) of a hexagonal model. Li et al. [33] studied the normalized Laplacian of a penta-graphene with applications. For further studies on laplacian and normalized laplacian we refer [34], [35]. The reference [18] provided a comprehensive explanation of the distinctive polynomial of a hexagonal model. In [28], an explicit closed-form formula for the sum of a resistance distances of hexagonal chain is obtained with the help of Laplacian spectrum.

In this paper, motivated by [7], [8], [23], [28], [29], and [30], by Laplacian spectrums, we characterized an explicit closed-form formula for the GMFPT of HM_n.

II. PRELIMINARIES

The networks in this paper are simple, undirected, finite and connected. Let $N = (U_N, E_N)$ be a network, where U_N denotes the node set, and E_N its links respectively. We denote the *order* of N as $n = |U_N|$ and its *size* as $|E_N|$. For further notations we referred to [1], [4], [24], and [25].

Let $A(N)$ denotes an *adjacency matrix* of N, where the entry (i, j) contains 1 if and only if $ij \in E_N$ and 0, otherwise. Define the *Laplacian matrix* of N as $\Gamma(N) = D(N) - A(N)$. We assume that $\mu_1 < \mu_2 \leqslant \cdots \leqslant \mu_n$ be the spectrums of $\Gamma(N)$. It is obvious that if and only if N is a connected network, then $\mu_1 = 0$ and $\mu_2 > 0$. For further studies on $\Gamma(N)$, we refer to the following interesting papers [13], [20], [21] and the references within.

Assume that M is any $p_1 \times p_2$ square matrix, and $Q_1 \subset \{1, 2, \ldots, p_1\}$ and $Q_2 \subset \{1, 2, \ldots, p_2\}$. Denote $M(Q_1|Q_2)$ for the submatrix of M which is obtained by deleting the rows in Q_1 and the columns in Q_2. Particularly, we denote $M(Q_1|Q_2)$ by $M(i|j)$, where $Q_1 = \{i\}$ and $Q_2 = \{j\}$.

The fact that $\lambda_1 = 0$ is well known assumption in spectral graph theory, and $\lambda_2 > 0$ when the graph G is assumed to be connected. We denote the spectral of $\Gamma(G)$ with $Sp(G) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$. For more details on $\Gamma(G)$, we suggest [13].

For *distance*, among the nodes i, j of a graph G is defined as the dimension of a through *i-j* path in G [5].

Let L_n denotes the linear hexagonal chain with $4n + 2$ vertices. In this contribution, we concentrated on the

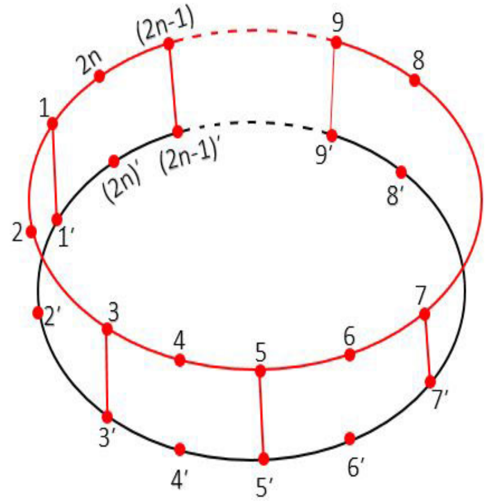

FIGURE 1. The hexagonal model HM_n.

hexagonal model HM_n (see Fig. 1). Sticking the two edges $1'1$ with $(2n+1)'(2n+1)$ of L_n and identifying the node 1 with node $(2n+1)$ (resp. node $1'$ and node $(2n+1)'$) yields the graph HM_n.

Let Φ denotes the *characteristic polynomial* of any $n \times n$ matrix then $\varphi(\Phi) = \det(tI - \Phi)$. The matrix I is called a unitary matrix having of Φ.

The *automorphism* of any network G is defined as a permutation of the nodes in G that maps links to links. Let Φ be an automorphism in any network G; thereby, one may define it as the product of transpositions and disjoint 1-cycles, that is,

$$\Phi = (t_1)(t_2)\cdots(t_m)(l_1, q_1)(l_2, q_2)\cdots(l_k, q_k).$$

We define, $\xi = \xi_0 \bigcup \xi_1 \bigcup \xi_2$, where $\xi_0 = \{w_1, w_2, \ldots, w_m\}$, $\xi_1 = \{u_1, u_2, \ldots, u_k\}$, $\xi_2 = \{v_1, v_2, \ldots, v_k\}$. This gives

$$\Gamma_G = \begin{array}{c c} & \begin{array}{ccc} \xi_0 & \xi_1 & \xi_2 \end{array} \\ \begin{array}{c} \xi_0 \\ \xi_1 \\ \xi_2 \end{array} & \begin{pmatrix} \Gamma_{\xi_{00}} & \Gamma_{\xi_{01}} & \Gamma_{\xi_{02}} \\ \Gamma_{\xi_{10}} & \Gamma_{\xi_{11}} & \Gamma_{\xi_{12}} \\ \Gamma_{\xi_{20}} & \Gamma_{\xi_{21}} & \Gamma_{\xi_{22}} \end{pmatrix} \end{array}.$$

Note that the automorphism g is G. Hence, $\Gamma_{\xi_{11}} = \Gamma_{\xi_{22}}$ and the below block matrix with respect to (G) gives

$$T = \begin{pmatrix} I_m & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} I_k & \frac{1}{\sqrt{2}} I_k \\ 0 & \frac{1}{\sqrt{2}} I_k & -\frac{1}{\sqrt{2}} I_k \end{pmatrix}.$$

Since, the unitary transformation $T\Gamma(G)T^T$ gives

$$T\Gamma(G)T^T = \begin{pmatrix} \Gamma_R(G) & 0 \\ 0 & \Gamma_S(G) \end{pmatrix}, \tag{1}$$

where

$$\Gamma_R(G) = \begin{pmatrix} \Gamma_{\xi_{00}} & \sqrt{2}\Gamma_{\xi_{01}} \\ \sqrt{2}\Gamma_{\xi_{10}} & \Gamma_{\xi_{11}} + \Gamma_{\xi_{12}} \end{pmatrix} \text{ and } \Gamma_S(G) = \Gamma_{\xi_{11}} - \Gamma_{\xi_{12}}. \tag{2}$$

In 1985 [27], the authors determined the following lemma of Laplacian polynomial for decomposition, which is stated as:

Lemma 2.1 ([27]): The matrices $\Gamma(N)$, $\Gamma_R(N)$ and $\Gamma_S(N)$ as defined in (2), then one has $\varphi(\Gamma(N)) = \varphi(\Gamma_R(N))\varphi(\Gamma_S(N))$.

Following Lemmas are well known matrix-tree theorem.

Lemma 2.2 ([16], [19]): Let G be an n-vertex connected graph of size m, then $R_{ij}(G) = n\sum_{k=2}^{n}\frac{1}{\lambda_k}$.

Lemma 2.3 ([1], [26]): The cycle is denoted by C_n and having n vertices, then $R_{ij}(C_n) = \frac{n^3-n}{12}$.

Rendering the considered vertices of a HM_n, as described in Fig. 1, an automorphism of HM_n is given as $g = (1, 1')(2, 2')\cdots(2n, (2n)')$. Thereby, $\xi_0 = \emptyset$, $\xi_1 = \{1, 2, \ldots, 2n\}$ and $\xi_2 = \{1', 2', \ldots, (2n)'\}$. From (1), we denote $\Gamma_R(T_n)$ by Γ_R and $\Gamma_S(T_n)$ with Γ_S. Then, one has

$$\Gamma_R = \Gamma_{\xi_{11}} + \Gamma_{\xi_{12}}, \qquad \Gamma_S = \Gamma_{\xi_{11}} - \Gamma_{\xi_{12}}.$$

Thus, $\Gamma_{\xi_{11}}$ and $\Gamma_{\xi_{12}}$ are constructed as follows:

$$\Gamma_{\xi_{11}} = \begin{pmatrix} 3 & -1 & 0 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 3 & -1 & \cdots & 0 & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 3 & -1 \\ -1 & 0 & 0 & 0 & \cdots & -1 & 2 \end{pmatrix}_{2n\times 2n,}$$

$$\Gamma_{\xi_{12}} = \begin{pmatrix} -1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}_{2n\times 2n.}$$

Hence

$$\Gamma_R = \begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 & -1 \\ -1 & 0 & 0 & 0 & \cdots & -1 & 2 \end{pmatrix}_{2n\times 2n,}$$

$$\Gamma_S = \begin{pmatrix} 4 & -1 & 0 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 4 & -1 & \cdots & 0 & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 4 & -1 \\ -1 & 0 & 0 & 0 & \cdots & -1 & 2 \end{pmatrix}_{2n\times 2n.}$$

Assume that the spectrums of a matrix Γ_S are μ_j, $j = 1, 2, \ldots, 2n$. Note that $\mu_j > 0$ for all j. In view of Lemma 2.1, one has the Laplacian spectrum of T_n is $\{\theta_1, \ldots, \theta_{2n}, \mu_1, \ldots, \mu_{2n}\}$.

Let

$$\begin{aligned}\varphi(\Gamma_S) &= \det(xI_{2n} - \Gamma_S) \\ &= x^{2n} + \alpha_1 x^{2n-1} + \cdots + \alpha_{2n-1}x + \alpha_{2n},\end{aligned}$$

where $\alpha_{2n} \neq 0$.

III. THE MFPT OF HM_n AND IMPORTANT LEMMAS

Given a graph G, the *MFPT* F_{ij} of any node j is the smallest number of steps of any random walk requires to reach at point j. The (MFPT) F_{ij} is defined as the expected value of F_j once walk starts at vertex i. MFPT is a vital quantity which is supposed to be useful to approximate the speed of any transport of the random walks of any graphs [15], [31]. The GMFPT denoted by $\langle F(G)\rangle$ actions the distribution competence of any walk, and obtained by averaging F_{ij} over $(|V_G|-1)$ probable end point and $|V_G|$ roots of elements [12], that is

$$\langle F(G)\rangle = \frac{1}{|V_G|(|V_G|-1)}\sum_{i\neq j} F_{ij}, \tag{3}$$

with the fact that $|V_G| \neq 1$. By [9], commuting time C_{ij} among the vertices i and j are accurately $2|E_G|r_{ij}$, i.e.,

$$C_{ij} = F_{ij} + F_{ji} = 2|E_G|r_{ij}. \tag{4}$$

Lemma 3.1: Assume that B be a $2n \times 2n$ matrix given below:

$$B = \begin{pmatrix} 4 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 4 & -1 & \cdots & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix}_{2n\times 2n.}$$

For $1 \leqslant i \leqslant 2n$, let

$$\begin{aligned}\chi_i &= B(\{i+1, i+2, \ldots, 2n\}|\{i+1, i+2, \ldots, 2n\}), \\ \chi_i' &= B(\{1, 2, \ldots, 2n-i\}|\{1, 2, \ldots, 2n-i\})\end{aligned}$$

be two submatrices of B. Assume that $\eta_i := \det\chi_i$ and $\eta_i' := \det\chi_i'$. We fix $\eta_0 = 1$, $\eta_0' = 1$. Then for $0 \leqslant i \leqslant 2n$, one has

$$\begin{aligned}\eta_i = \frac{1}{4}[&(3-(-1)^i+2\sqrt{2})(1+\sqrt{2})^i \\ &+(3-(-1)^i-2\sqrt{2})(1-\sqrt{2})^i]\end{aligned} \tag{5}$$

and

$$\begin{aligned}\eta_i' = \frac{1}{8}[&(4+(-1)^i\sqrt{2}+3\sqrt{2})(1+\sqrt{2})^i \\ &+(4-(-1)^i\sqrt{2}-3\sqrt{2})(1-\sqrt{2})^i].\end{aligned} \tag{6}$$

Proof: First, we show (5). To check that $\eta_1 = 4, \eta_2 = 7, \eta_3 = 24$ is straightforward. In case $3 \leqslant i \leqslant 2n$, we expand $\det \chi_i$ with regards to its last row

$$\eta_i = \begin{cases} 2\eta_{i-1} - \eta_{i-2}, & \text{for even } i; \\ 4\eta_{i-1} - \eta_{i-2}, & \text{for odd } i. \end{cases}$$

In case, $0 \leqslant i \leqslant n$, assume that $c_i = \eta_{2i}$ and for $0 \leqslant i \leqslant n-1$, let $d_i = \eta_{2i+1}$ and $c_0 = 1$, $d_0 = 4$. In case $i \geqslant 1$, we have

$$\begin{cases} c_i = 2d_{i-1} - c_{i-1}, \\ d_i = 4c_i - d_{i-1}. \end{cases} \tag{7}$$

From the first equation in (7), one has $d_{i-1} = \frac{1}{2}(c_i + c_{i-1})$, hence $d_i = \frac{1}{2}(c_{i+1} + c_i)$. Substituting the values of d_{i-1} and d_i in the second part of (7) gives $c_{i+1} = 6c_i - c_{i-1},\ i \geqslant 1$. By the same arguments one has $d_{i+1} = 6d_i - d_{i-1},\ i \geqslant 1$. Thus, η_i fulfill the following recurrence

$$\eta_i = 6\eta_{i-2} - \eta_{i-4},\ \ \eta_0 = 1,\ \ \eta_1 = 4,\ \ \eta_2 = 7,\ \ \eta_3 = 24. \tag{8}$$

Then the characteristic equation of (8) is $r^4 = 6r^2 - 1$, and its roots are $r_1 = \sqrt{2}+1$, $r_2 = -(\sqrt{2}+1)$, $r_3 = \sqrt{2}-1$ and $r_4 = -(\sqrt{2}-1)$. Hence, general solution of (8) is given by

$$\begin{aligned} \eta_i = {} & (\sqrt{2}+1)^i \zeta_1 + (-(\sqrt{2}+1))^i \zeta_2 + (\sqrt{2}-1)^i \zeta_3 \\ & + (-(\sqrt{2}-1))^i \zeta_4. \end{aligned} \tag{9}$$

Together with the IC,s in (8) give the followings

$$\begin{cases} \zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 1, \\ (\sqrt{2}+1)\zeta_1 + (-(\sqrt{2}+1))\zeta_2 + (\sqrt{2}-1)\zeta_3 \\ \ + (-(\sqrt{2}-1))\zeta_4 = 4, \\ (\sqrt{2}+1)^2\zeta_1 + (-(\sqrt{2}+1))^2\zeta_2 + (\sqrt{2}-1)^2\zeta_3 \\ \ + (-(\sqrt{2}-1))^2\zeta_4 = 7, \\ (\sqrt{2}+1)^3\zeta_1 + (-(\sqrt{2}+1))^3\zeta_2 + (\sqrt{2}-1)^3\zeta_3 \\ \ + (-(\sqrt{2}-1))^3\zeta_4 = 24. \end{cases}$$

The unique solution of this system can be found to be $\zeta_1 = \frac{3+2\sqrt{2}}{4}$, $\zeta_2 = -\frac{1}{4}$, $\zeta_3 = -\frac{1}{4}$, $\zeta_4 = \frac{3-2\sqrt{2}}{4}$. We get our result by putting ζ_1, ζ_2, ζ_3 and ζ_4 in (9). Through, the parallel directions as above, it is straightforward to obtain (6), which is omitted here. □

Lemma 3.2: $-\alpha_{2n-1} = \sum_{i=0}^{2n-1} \eta_i \eta'_{2n-1-i} - \sum_{i=0}^{2n-3} \eta'_i \eta_{2n-3-i}$.

Proof: For simplicity, let $\Gamma_S = (l_{ij})_{2n\times 2n}$. Then, for $2 \leqslant i \leqslant 2n-1$, we have

$$\Gamma_S(i|i) = \begin{pmatrix} l_{11} & -1 & \cdots & -1 \\ -1 & l_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & \cdots & l_{2n,2n} \end{pmatrix}_{(2n-1)\times(2n-1)}.$$

Therefore,

$$\begin{aligned} \det \Gamma_S(i|i) = {} & \sum_{\tau} sgn(\tau) l_{1\tau(1)} \cdots l_{(i-1)\tau(i-1)} l_{(i+1)\tau(i+1)} \\ & \cdots l_{(2n)\tau(2n)}, \end{aligned}$$

where the sum denotes the over all permutation $\tau(1), \ldots, \tau(i-1), \tau(i+1), \ldots, \tau(2n)$ of $1, \ldots, i-1, i+1, \ldots, 2n$. The $sgn(\tau)$ is 1 or -1 giving to τ is even or odd. To make it more simple, assume that $h(\tau) := sgn(\tau) l_{1\tau(1)} \cdots l_{(i-1)\tau(i-1)} l_{(i+1)\tau(i+1)} \cdots l_{(2n)\tau(2n)}$. We continue through in view of the subsequent three cases.

For $\tau(1) = 2n$ and $\tau(2n) = 1$. It is simple to verify that

$$\sum_{\substack{\tau\,:\,\tau(1)=2n,\\ \tau(2n)=1}} h(\tau) = -\det N(i-1|i-1) = -\eta'_{i-2}\eta_{2n-1-i}.$$

If $\tau(1) \neq 2n$, $\tau(2n) = 1$, or $\tau(1) = 2n$ and $\tau(2n) \neq 1$, then we just consider the former subcase. Through parallel direction, we may show the later subcase, which we omitted here. Notice that $\tau(1) \neq 1$. If $\tau(1) \in \{3, \ldots, 2n-1\}$, then $l_{1\tau(1)} = 0$. Thus, $h(\tau) = 0$. Whence $\tau(1) = 2$, thereby $l_{1\tau(1)} = -1$. After a few simple calculations, we have $\det \Gamma_S(\{1, i, 2n\}|\{1, 2, i\}) = 0$. Hence $h(\tau) = 0$. Thus,

$$\sum_{\substack{\tau\,:\,\tau(1)\neq 2n,\\ \tau(2n)=1}} h(\tau) = 0.$$

If $\tau(1) \neq 2n$ and $\tau(2n) \neq 1$, then we consider the entries $(1, 2n)$ and $(2n, 1)$ of Γ_S as 0. Hence

$$\sum_{\substack{\tau\,:\,\tau(1)\neq 2n,\\ \tau(2n)\neq 1}} h(\tau) = \det F(i|i) = \eta_{i-1}\eta'_{2n-i}.$$

Thus, for $2 \leqslant i \leqslant 2n-1$, one has $\det \Gamma_S(i|i) = \eta_{i-1}\eta'_{2n-i} - \eta'_{i-2}\eta_{2n-1-i}$. Therefore,

$$\begin{aligned} -\alpha_{2n-1} &= \eta_{2n-1} + \eta'_{2n-1} + \sum_{i=2}^{2n-1} \det \Gamma_S(i|i) \\ &= \sum_{i=0}^{2n-1} \eta_i \eta'_{2n-1-i} - \sum_{i=0}^{2n-3} \eta'_i \eta_{2n-3-i}. \end{aligned} \tag{10}$$

This completes the proof. □

Hence, we build the square matrices F and N, here F is a matrix obtained from Γ_S by substituting $(1, 2n)$-entry and the $(2n, 1)$-entry by 0. Let $N = \Gamma_S(\{1, 2n\}|\{1, 2n\})$.

Assume that

$$\begin{aligned} F_i &= F(\{i+1, i+2, \ldots, 2n\}|\{i+1, i+2, \ldots, 2n\}), \\ N_i &= N(\{i+1, i+2, \ldots, 2n\}|\{i+1, i+2, \ldots, 2n\}) \end{aligned}$$

be two i-th order principal submatrices of F and N. One can check it easily that $\det F_i = \eta_i$ and $\det N_i = \eta'_i$, where η_i and η'_i are defined in Lemma 3.1. We proceed by showing the following Lemmas.

Lemma 3.3: Let Γ_S is a matrix as defined above. Then

$$\det \Gamma_S = \left[(\sqrt{2}+1)^n - (\sqrt{2}-1)^n\right]^2.$$

Proof: We take determinant of Γ_S with its last row and obtained that $\det \Gamma_S = 2\eta_{2n-1} - \eta'_{2n-2} - \eta_{2n-2} - 2$. Based on Lemma 3.1, we get the desired result. $\square$

Now, we are ready to obtain α_{2n-1}.

Lemma 3.4: Let α_{2n-1} be defined as above. Then

$$-\alpha_{2n-1} = \frac{3\sqrt{2}n}{4}(\sqrt{2}+1)^{2n} - \frac{3\sqrt{2}n}{4}(\sqrt{2}-1)^{2n}.$$

Proof: Note that the number $-\alpha_{2n-1}$ is over all sum of the principal minors with $2n-1$ order of a matrix Γ_S (see [1, P5]). Thus,

$$-\alpha_{2n-1} = \sum_{t=1}^{2n} \det \Gamma_S(t|t).$$

Now we come back to show Lemma 2.3. Let $\mu_1(x)$ (resp. $\mu_2(x)$) is the ordinary generating function of $\{\eta_i\}$ (resp. $\{\eta'_i\}$), which is,

$$\mu_1(x) = \sum_{i\geqslant 0} \eta_i x^i, \quad \mu_2(x) = \sum_{i\geqslant 0} \eta'_i x^i. \tag{11}$$

In view of (10) and (11), and to determine $-\alpha_{2n-1}$, it is enough to obtain the coefficients of r^{2n-1} and r^{2n-3} in $\mu_1(r)\mu_2(r)$. We may rewrite $\mu_1(r)$ and $\mu_2(r)$ as

$$\begin{aligned}\mu_1(r) &= \sum_{i\geqslant 0} \eta_i r^i = 1 + 4r + 7r^2 + 24r^3 + \sum_{i\geqslant 4} \eta_i r^i \\ &= 1 + 4r + 7r^2 + 24r^3 + \sum_{i\geqslant 4}(6\eta_{i-2} - \eta_{i-4})r^i \\ &= 1 + 4r + 7r^2 + 24r^3 + 6r^2 \sum_{i\geqslant 4} \eta_{i-2} r^{i-2} \\ &\quad - r^4 \sum_{i\geqslant 4} \eta_{i-4} r^{i-4} \\ &= 1 + 4r + 7r^2 + 24r^3 \\ &\quad + 6r^2(\mu_1(r) - 1 - 4r) - r^4\mu_1(r)\end{aligned}$$

and

$$\begin{aligned}\mu_2(r) &= \sum_{i\geqslant 0} \eta'_i r^i = 1 + 2r + 7r^2 + 12r^3 + \sum_{i\geqslant 4} \eta'_i r^i \\ &= 1 + 2r + 7r^2 + 12r^3 + \sum_{i\geqslant 4}(6\eta'_{i-2} - \eta'_{i-4})r^i \\ &= 1 + 2r + 7r^2 + 12r^3 + 6r^2 \sum_{i\geqslant 4} \eta'_{i-2} r^{i-2} \\ &\quad - r^4 \sum_{i\geqslant 4} \eta'_{i-4} r^{i-4} \\ &= 1 + 2r + 7r^2 + 12r^3 + 6r^2(\mu_2(r) - 1 - 2r) \\ &\quad - r^4\mu_2(r).\end{aligned}$$

Thus,

$$\mu_1(r) = \frac{1+4r+r^2}{1-6r^2+r^4}, \quad \mu_2(r) = \frac{1+2r+r^2}{1-6r^2+r^4}. \tag{12}$$

Let

$$\begin{aligned}F(r) &= \frac{1}{2}(\mu_1(r)\mu_2(r) - \mu_1(-r)\mu_2(-r)) \\ &= \frac{6(r+r^3)}{(1-6r^2+r^4)^2}.\end{aligned}$$

Then we claim the coefficient of r^{2n-1} in $F(r)$ is the same as the coefficient of r^{2n-1} in $\mu_1(r)\mu_2(r)$. In fact,

$$\begin{aligned}&\frac{1}{2}\Big(\sum_{i=0}^{2n-1} \eta_i\eta'_{2n-1-i} - \sum_{i=0}^{2n-1}(-1)^i\eta_i(-1)^{2n-1-i}\eta'_{2n-1-i}\Big) \\ &= \sum_{i=0}^{2n-1} \eta_i\eta'_{2n-1-i},\end{aligned}$$

as desired. Similarly, the coefficient of r^{2n-3} in $F(r)$ is the same as the coefficient of r^{2n-3} in $\mu_1(r)\mu_2(r)$. Hence, in order to determine $-\alpha_{2n-1}$, it suffices for us to determine the coefficients of r^{2n-1} and r^{2n-3} in $F(r)$. $\square$

By a direct calculation, we have

$$\begin{aligned}F(r) &= \frac{3(r-1)}{4(r^2-2r-1)^2} - \frac{3}{8(r^2-2r-1)} \\ &\quad + \frac{3(r+1)}{4(r^2+2r-1)^2} + \frac{3}{8(r^2+2r-1)}.\end{aligned}$$

Notice that $1+\sqrt{2}$ and $1-\sqrt{2}$ are the roots of r^2-2r-1. Hence, assume that

$$\begin{aligned}\frac{3(r-1)}{4(r^2-2r-1)^2} &= \frac{a}{(r-1-\sqrt{2})^2} + \frac{b}{r-1-\sqrt{2}} \\ &\quad + \frac{c}{(r-1+\sqrt{2})^2} + \frac{d}{r-1+\sqrt{2}},\end{aligned} \tag{13}$$

where a, b, c, d belongs to the real numbers. Linking both sides of (13) gives $a = -c = \frac{3}{16\sqrt{2}}$ and $b = d = 0$, that is $\frac{3(r-1)}{4(r^2-2r-1)^2} = \frac{3}{16\sqrt{2}}\big[\frac{1}{(r-1-\sqrt{2})^2} - \frac{1}{(r-1+\sqrt{2})^2}\big]$. Note that

$$\begin{aligned}\frac{1}{(r-1-\sqrt{2})^2} &= \Big(\frac{1}{1+\sqrt{2}}\Big)^2\Big(\frac{1}{1-\frac{r}{1+\sqrt{2}}}\Big)^2 \\ &= \Big(\frac{1}{1+\sqrt{2}}\Big)^2\Big(\sum_{i=0}^{\infty}(\frac{r}{1+\sqrt{2}})^i\Big)^2.\end{aligned}$$

Hence, coefficient of r^{2n-1} in $\frac{1}{(r-1-\sqrt{2})^2}$ is

$$\begin{aligned}&\Big(\frac{1}{1+\sqrt{2}}\Big)^2 \sum_{i=0}^{2n-1}\Big(\frac{1}{1+\sqrt{2}}\Big)^i\Big(\frac{1}{1+\sqrt{2}}\Big)^{2n-1-i} \\ &= 2n\Big(\frac{1}{1+\sqrt{2}}\Big)^{2n+1}.\end{aligned}$$

Through a parallel directions, we get that the coefficient of r^{2n-1} in $\frac{1}{(r-1+\sqrt{2})^2}$ is $2n(\frac{1}{1-\sqrt{2}})^{2n+1}$. Thus, the coefficient of r^{2n-1} in $\frac{3(r-1)}{4(r^2-2r-1)^2}$ is

$$\frac{3n}{8\sqrt{2}}\Big[\frac{1}{(1+\sqrt{2})^{2n+1}} - \frac{1}{(1-\sqrt{2})^{2n+1}}\Big]. \tag{14}$$

Bear in mind that

$$-\frac{3}{8(r^2-2r-1)} = -\frac{3}{16\sqrt{2}}\Big(\frac{1}{r-1-\sqrt{2}}-\frac{1}{r-1+\sqrt{2}}\Big),$$

$$\frac{3(r+1)}{4(r^2+2r-1)^2} = \frac{3}{16\sqrt{2}}\Big[\frac{1}{(r+1-\sqrt{2})^2}-\frac{1}{(r+1+\sqrt{2})^2}\Big],$$

$$\frac{3}{8(r^2+2r-1)} = \frac{3}{16\sqrt{2}}\Big(\frac{1}{r+1-\sqrt{2}}-\frac{1}{r+1+\sqrt{2}}\Big).$$

Then by a parallel discussion as above we can get the coefficients of r^{2n-1} in $\frac{-3}{8(r^2-2r-1)}$, $\frac{3(r+1)}{4(r^2+2r-1)^2}$ and $\frac{3}{8(r^2+2r-1)}$ are, respectively, $\frac{3}{16\sqrt{2}}[(\frac{1}{1+\sqrt{2}})^{2n}-(\frac{1}{1-\sqrt{2}})^{2n}]$,

$$\frac{3n}{8\sqrt{2}}\left[\left(\frac{1}{\sqrt{2}-1}\right)^{2n+1}+\left(\frac{1}{\sqrt{2}+1}\right)^{2n+1}\right]$$

and

$$-\frac{3}{16\sqrt{2}}\left[\left(\frac{1}{\sqrt{2}-1}\right)^{2n}-\left(\frac{1}{\sqrt{2}+1}\right)^{2n}\right].$$

Together with (14) the coefficient of r^{2n-1} in $F(r)$ is

$$\sum_{i=0}^{2n-1}\eta_i\eta'_{2n-1-i} = \frac{3n}{4\sqrt{2}}\left[(\sqrt{2}+1)^{2n+1}+(\sqrt{2}-1)^{2n+1}\right] + \frac{3}{8\sqrt{2}}\left[(\sqrt{2}-1)^{2n}-(\sqrt{2}+1)^{2n}\right].$$

Through the same directions, we establish the coefficient of r^{2n-3} in $F(r)$ is

$$\sum_{i=0}^{2n-3}\eta'_i\eta_{2n-3-i} = \frac{3(n-1)}{4\sqrt{2}}\left[(\sqrt{2}+1)^{2n-1}+(\sqrt{2}-1)^{2n-1}\right] + \frac{3}{8\sqrt{2}}\left[(\sqrt{2}-1)^{2n-2}-(\sqrt{2}+1)^{2n-2}\right].$$

By a direct calculation, $\sum\limits_{i=0}^{2n-1}\eta_i\eta'_{2n-1-i} - \sum\limits_{i=0}^{2n-3}\eta'_i\eta_{2n-3-i} = \frac{3\sqrt{2}n}{4}[(\sqrt{2}+1)^{2n}-(\sqrt{2}-1)^{2n}]$. Hence, in view of (3.5), one has

$$-\alpha_{2n-1} = \frac{3\sqrt{2}n}{4}(\sqrt{2}+1)^{2n} - \frac{3\sqrt{2}n}{4}(\sqrt{2}-1)^{2n},$$

as desired.

Lemma 3.5: Let HM_n be a hexagonal model having n hexagons. Then the sum of resistance distance of HM_n

$$R_{ij}(HM_n) = 2R_{ij}(C_{2n}) - 4n\frac{\alpha_{2n-1}}{\det\Gamma_S}. \tag{15}$$

Proof: Note that $|V_{HM_n}| = 4n$. By Lemma 2.2, one has

$$R_{ij}(HM_n) = 4n\left(\sum_{i=1}^{2n-1}\frac{1}{\theta_i}+\sum_{j=1}^{2n}\frac{1}{\mu_j}\right),$$

here θ_i $(1\leqslant i\leqslant 2n-1)$ and μ_j $(1\leqslant j\leqslant 2n)$ represents the spectrums of the matrices Γ_R and Γ_S.

On the one hand, in view of Lemma 2.2 we have

$$4n\sum_{i=1}^{2n-1}\frac{1}{\theta_i} = 2\cdot 2n\sum_{i=1}^{2n-1}\frac{1}{\theta_i} = 2R_{ij}(C_{2n}). \tag{16}$$

On the other hand, $\mu_1, \mu_2, \ldots, \mu_{2n}$ are the roots of

$$\det(rI_{2n}-\Gamma_S) = r^{2n}+\alpha_1 r^{2n-1}+\cdots+\alpha_{2n-1}r+\alpha_{2n} = 0.$$

We immediately obtain that $\frac{1}{\mu_1}, \frac{1}{\mu_2}, \ldots, \frac{1}{\mu_{2n}}$ are the roots of

$$\alpha_{2n}r^{2n}+\alpha_{2n-1}r^{2n-1}+\cdots+\alpha_1 r+1 = 0.$$

By Vieta's Theorem, one has

$$\sum_{j=1}^{2n}\frac{1}{\mu_j} = -\frac{\alpha_{2n-1}}{\alpha_{2n}} = -\frac{\alpha_{2n-1}}{\det\Gamma_S}. \tag{17}$$

Together with (16) and (17), our result follows immediately. □

In order to obtain $R_{ij}(HM_n)$, it suffices to determine α_{2n-1} and $\det\Gamma_S$ in (15). Based on Lemmas 3.1-3.5, we obtain

Lemma 3.6: Let HM_n be a zig-zag polyhex nanotube with n hexagons. Then

$$R_{ij}(HM_n) = \frac{4n^3-n}{3} + 3\sqrt{2}n^2\frac{(\sqrt{2}+1)^n+(\sqrt{2}-1)^n}{(\sqrt{2}+1)^n-(\sqrt{2}-1)^n}.$$

IV. PROOF OF THEOREM

Note that $|E_{HM_n}| = 5n$ and $|V_{HM_n}| = 4n$. From (3) and (4), the GMFPT for HM_n is

$$\begin{aligned}\langle F(HM_n)\rangle &= \frac{1}{|V_{HM_n}|(|V_{HM_n}|-1)}\sum_{i\neq j}F_{ij}\\ &= \frac{2|E_{HM_n}|}{|V_{HM_n}|(|V_{HM_n}|-1)}R_{ij}(HM_n)\\ &= \frac{10n}{4n(4n-1)}R_{ij}(HM_n)\\ &= \frac{5}{2(4n-1)}\Big[\frac{4n^3-n}{3}\\ &\quad + 3\sqrt{2}n^2\frac{(\sqrt{2}+1)^n+(\sqrt{2}-1)^n}{(\sqrt{2}+1)^n-(\sqrt{2}-1)^n}\Big].\end{aligned}$$

Hence, we get our desired result.

V. NUMERICAL CONSEQUENCES AND DISCUSSIONS

In this section, by using Matlab, we give some graphical interpretations between the number of hexagons (n) and $\langle F(HM_n)\rangle$. We also investigated the effect of $\langle F(HM_n)\rangle$ for $n = 3$ and 4. For the sake of simplicity, we assume $\langle F(HM_n)\rangle = M_g$. In Fig. 2, it shows that M_g increases as we increase the hexagons (n). In Fig. 3, it shows that M_g increases for both $n = 3$ and $n = 4$, but the slope of M_g for $n = 4$ is larger than for $n = 3$. This means that the GMFPT works efficiently for the large nodes. Hence, we developed a unified strategy for obtaining the scaling properties of $\langle F(HM_n)\rangle$

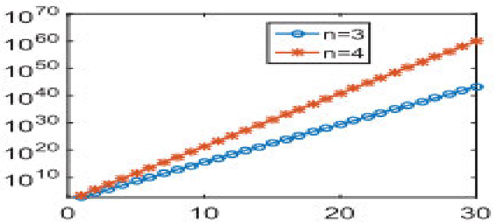

FIGURE 2. $\langle F(HM_n)\rangle = M_g$ **versus** n.

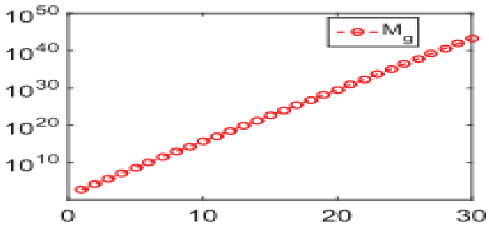

FIGURE 3. **The comparison** $\langle F(HM_n)\rangle = M_g$ **versus** n.

and achieved an organized study for GMFPT. Since, the study of spectrums are crucial in determining the scaling of GMFPT. Therefore, we used a closed-form formula for GMFPT and all pairs of nodes. Finally, looking at GMFPT in a network, we found that as the number of hexagons grows, so does GMFPT. This demonstrates that hexagons and network invariants have a direct relationship. The GMFPT between source and target exhibits search efficiency when we analyze many random walks equally. We demonstrated in Fig.2 and Fig.3 that GMFPT works efficiently for the large nodes.

VI. CONCLUDING REMARKS

In this contribution, we obtained the GMFPT of HM_n. Note that Carmona, Encinas and Mitjana studied the resistance distances for ladder-like graphs [7]. Very recently, Barrett, Evans and Francis [2] studied the effective resistances in straight linear 2-trees (i.e., linear triangle chain) and some related problems. It is quite motivating to study the effective resistances for the Möbius hexagonal ring, and the Möbius pentagonal ring. We will do it in the near future.

Declarations

Conflicts of interest/Competing interests: The authors declare no any conflict of interest/competing interests.

Data availability: Not applicable

Code availability: Not applicable

Authors' contributions: *(All author contributed equally to this work.)*

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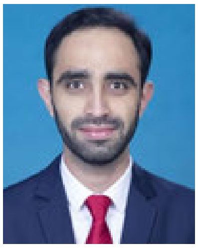

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