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RESISTANCE DISTANCES AND THE GLOBAL CYCLICITY INDEX OF FULLERENE GRAPHS

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A fullerene graph is a cubic 3-connected plane graph with exact 12 pentagons and other hexagons. In the present work, by Rayleigh's short-cut method and Foster's formulas, it is shown that in a fullerene graph resistance distances between pairs of adjacent vertices lie within a rather narrow interval ranging from $\frac{48}{79}$ to $\frac{5}{7}$ with their average value being $\frac{2(n-1)}{3n}$; and resistance distances between pairs of vertices at distance two lie within the small interval $\left[\frac{66}{79},\frac{8}{7}\right]$ with their average value being $\frac{n-2}{n}$. As a byproduct, bounds for the global cyclicity index of fullerene graphs are obtained.

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1. Introduction

Let $G=(V(G),E(G))$ be a connect graph. A novel intrinsic metric on G, *resistance distance,* was introduced by Klein and Randić in 1993 [1]. The term resistance distance was used because of the physical interpretation: one imagines unit resistors on each edge of G and takes the resistance distance between vertices i and j to be the net effective resistance between vertices i and j, denoted by $\Omega_G(i,j)$. It is shown [1] that $\Omega_G(i,j)$ equals the length $d_G(i,j)$ of the shortest path between i and j if and only if there is a unique single path between i and j, while if there is more than one path (even of different lengths), then $\Omega_G(i,j)$ is strictly less than $d_G(i,j)$. On the basis of the above property, the *global cyclicity index* (also interpreted as a "total excess bond conductance") was suggested [2]:

$$C(G)=\sum_{i\sim j}^{G}(\Omega_G^{-1}(i,j)-d_G^{-1}(i,j))=\sum_{i\sim j}^{G}(\Omega_G^{-1}(i,j)-1),$$

where $i\sim j$ denotes that i is adjacent to j and the summation is over all edges of G. Besides being an important component of electrical circuit theory and an intrinsic graph metric, resistance distance is a relevant tool to characterize wave- or fluid-like communication between two vertices [3], and thus it is well studied in physical, mathematical and chemical literatures. For more information, the readers are referred to [4-25] and references therein.

Fullerenes are carbon-cage molecules exclusively consisting of carbon atoms arranged on a sphere with 12 five-membered faces and other six-membered faces. These molecules are of great importance in chemistry. The icosahedral C_{60} molecule, Buckminsterfullerene, proposed firstly by

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Kroto et al. [26] and confirmed by later experiments [27, 28], is the archetype of fullerenes. A *fullerene graph* as a molecular graph of a fullerene is a three-regular and three-connected plane graph where exactly 12 faces are pentagons and remaining faces are hexagons. So far, resistance distances have been computed for some special fullerene graphs, such as C_{60} and C_{70} isomers and so on [4,7,13]. However, there hasn't been any study which takes resistance distances of general fullerene graphs into consideration. In this paper, we will make some effort toward this end and resistance distances between pairs of adjacent vertices and pairs of vertices at distance two of fullerene graphs will be studied.

2. Main results

In this section, resistance distances between pairs of adjacent vertices and pairs of vertices at distance two in fullerene graphs are investigated. As a byproduct, bounds for the global cyclicity index of fullerene graphs are obtained.

We first introduce some classical results in electrical network theory which will be crucial for obtaining the main results of the present paper.

1. *Series connection rule*: resistors that are connected in series can be replaced by a single resistor whose resistance is the sum of resistors.

2. *Parallel connection rule*: resistors that are connected in parallel can be replaced by a single resistor whose conductance (the inverse of resistance) is the sum of conductances.

3. *Rayleigh's short-cut method* [29]: Shorting certain sets of vertices together can only decrease the resistance distance of the network between two given vertices. Cutting certain edges can only increase the resistance distance between two given vertices.

4. *Foster's first formula* [30]: the sum of resistance distances between all pairs of adjacent vertices of a graph with n vertices is equal to $n-1$.

5. *Foster's second formula* [31]:

$$\sum \frac{\Omega_G(i,j)}{d_v} = n-2,$$

where $\Omega_G(i,j)$ is measured across the end-vertices of two adjacent edges iv and vj, d_v is the degree of vertex v, and the summation is taken all adjacent edges iv and vj.

Before giving our main result, it is also necessary to introduce formulas for computing resistance distances of weighted wheel graphs.

The wheel graph W_n is a graph that contains a cycle of order n, and for which every graph vertex in the cycle is connected to one other vertex (which is known as the center). In W_n, the vertices corresponding to the cycle C_n are labeled from 1 to n in cyclic order, and the center is labeled as $n+1$. Explicit formulas for computing resistance distances in W_n have been obtained by Bapat and Gupta [25]. In fact, they also considered a more generalized case that the wheel graph is a weighted wheel in which the edges connect $n+1$ and i, $i \in \{1,2,\ldots,n\}$, called the spokes of the wheel, have the same weight α (the weight of the edge denote the resistance of the edge).

Let

$$\gamma = 2+\frac{1}{\alpha},\ \mu = \frac{\gamma+\sqrt{\gamma^2-4}}{2},\ \nu = \frac{\gamma-\sqrt{\gamma^2-4}}{2},$$

and define $G_k(\alpha)$ as the generalized Fibonacci number

$$G_k(\alpha) = \frac{\mu^k - \nu^k}{\mu - \nu}.$$

Then resistance distances in weighted wheel graph W_n can be computed as follows.

Lemma 1. [25] Let $n \geq 3$ be a positive integer. The following results hold for W_n:

(1) The resistance distance between vertex $n+1$ and vertex i, $i \in \{1,2,\ldots,n\}$ is

$$\Omega_{W_n}(i,n+1)=\Omega_{W_n}(n+1,i)=\frac{G_n^2}{G_{2n}-G_n}.$$

(2) The resistance distance between vertices $i, j\in\{1,2,\dots,n\}$ is

$$\Omega_{W_n}(i,j)=\frac{G_n^2}{G_{2n}-2G_n}[2-\frac{G_{2k}}{G_k}]+G_k,$$

where $k=\begin{cases}|j-i|, & if\ |j-i|\le\left\lfloor\frac{n}{2}\right\rfloor\\ n-|j-i|, & if\ |j-i|>\left\lfloor\frac{n}{2}\right\rfloor\end{cases}.$

Theorem 2. Let F be a fullerene graph with n vertices. Then for any two adjacent vertices i and j,

$$\frac{48}{79}\le\Omega_F(i,j)\le\frac{5}{7}.$$

Moreover, the average value of resistance distances between pairs of adjacent vertices is $\frac{2(n-1)}{3n}$.

Proof. First consider the lower bound. Choose a facial cycle C which contains ij as an edge. Define

$$S=\{v\in V(F)|v\in V(C)\ or\ v\ has\ a\ neighbor\ in\ C\}.$$

Short all the vertices in $V(F)-S$ together and denote the resulted graph by F'. Then by Rayleigh's short-cut method,

$$\Omega_F(i,j)\ge\Omega_{F'}(i,j).$$

Now we compute $\Omega_{F'}(i,j)$. Clearly, by simplifying resistors connected in parallel and in series according to series and parallel connection rules, we could finally get a weighted wheel graph W as shown in Fig. 1 (for simplicity, we do not mark out weights on edges whose weights are equal to 1). Thus

$$\Omega_{F'}(i,j)=\Omega_W(i,j).$$

To compute $\Omega_W(i,j)$, we distinguish the following two cases.

Case 1. C is a hexagon. In this case, W is W_6 with $\alpha=\frac{3}{2}$. Thus

$$\gamma=2+\frac{1}{\alpha}=2+\frac{2}{3}=\frac{8}{3},\mu=\frac{\gamma+\sqrt{\gamma^2-4}}{2}=\frac{4+\sqrt{7}}{3},\nu=\frac{\gamma-\sqrt{\gamma^2-4}}{2}=\frac{4-\sqrt{7}}{3},$$

$$G_k=\frac{\mu^k-\nu^k}{\mu-\nu}=\frac{3^{-(k-1)}[(4+\sqrt{7})^k-(4-\sqrt{7})^k]}{2\sqrt{7}}.$$

Then by Lemma 1, the resistance distance between i and j is

$$\Omega_{W_6}(i,j)=\frac{G_6^2}{G_{12}-2G_6}[2-\frac{G_2}{G_1}]+G_1=\frac{237}{385}.$$

Case 2. C is a pentagon. In this case, w is W_5 with $\alpha=\frac{3}{2}$. Then G_k is the same as given in Case 1 and thus by Lemma 1, the resistance distance between i and j can be computed as

$$\Omega_{W_5}(i,j)=\frac{G_5^2}{G_{10}-2G_5}[2-\frac{G_2}{G_1}]+G_1=\frac{48}{79}.$$

Comparing the result in Case 1 with the result in Case 2, we can draw the conclusion that $\Omega_W(i, j) \geq \frac{48}{79}$ and the lower bound is proved.

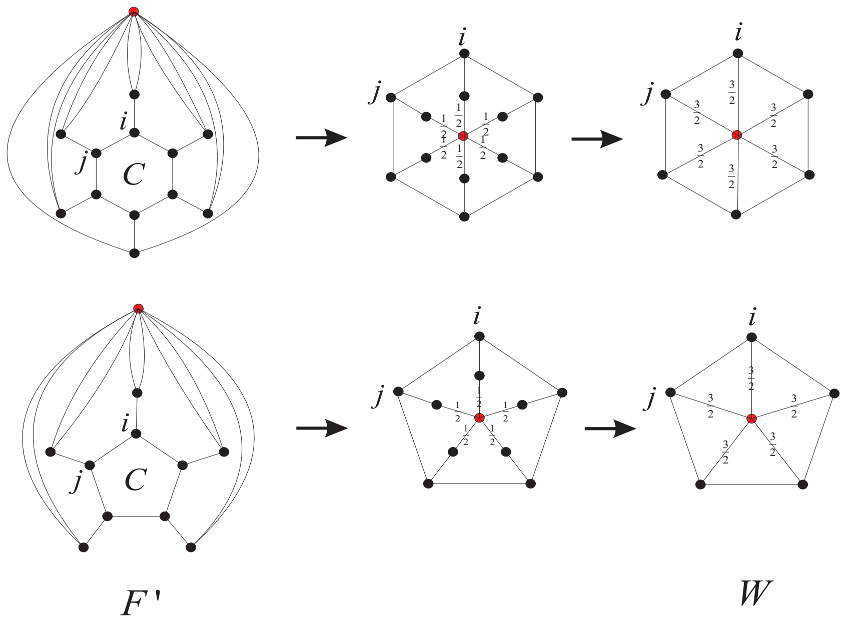

Fig. 1. Calculating the resistance distance between i and j in F' in the proof of Theorem 2. Graphs in the first row correspond to the case that C is a hexagon and graphs in the second row correspond to the case that C is a pentagon.

For the upper bound, let C' be the facial cycle which has a common edge ij with C. Consider the sub-graph induced by C and C', denoted by F''. Then by Rayleigh's short-cut method, we have

$$\Omega_F(i, j) \leq \Omega_{F''}(i, j).$$

On the other hand, by the series and parallel connection rules,

$$\Omega_{F''}(i, j) = \frac{1}{\frac{1}{1} + \frac{1}{|V(C_1)| - 1} + \frac{1}{|V(C_2)| - 1}} \leq \frac{1}{1 + \frac{1}{5} + \frac{1}{5}} = \frac{5}{7}.$$

Thus the upper bound is proved.

Note that F has $\frac{3n}{2}$ pairs of adjacent vertices. Then the average value of resistance distances between pairs of adjacent vertices is a straightforward consequence of Foster's first formula.

From Theorem 1, bounds for the global cyclicity index of fullerene graphs may be easily determined.

Theorem 3. Let F be a fullerene graph with n vertices. Then

$$\frac{3}{5} n \leq C(F) \leq \frac{31}{32} n.$$

Now we turn to resistance distances between pairs of vertices at distance two.

Theorem 4. Let F be a fullerene graph with n vertices. Then for any two adjacent vertices i and j at distance two,

$$\frac{66}{79} \leq \Omega_F(i, j) \leq \frac{8}{7}.$$

Moreover, the average value of resistance distances between pairs of vertices at distances two is $\frac{n-2}{n}$.

Proof. Frist we show the lower bound. Since i and j are at distance two, we could find a path $P = ikj$ of length two connecting i and j. Clearly that P must be contained in a facial cycle C. As in the proof of Theorem 2, according to C, we could define S, construct the sub-graph F' and simplify F' to weighted wheel graph W in the same way. Then by Rayleigh's short-cut method,

$$\Omega_F(i,j) \geq \Omega_{F'}(i,j) = \Omega_W(i,j).$$

Now we distinguish two cases:

Case 1. C is a hexagon. In this case, W is W_6 with $\alpha = \frac{3}{2}$. Thus by Lemma 1,

$$\Omega_{W_6}(i,j) = \frac{G_6^2}{G_{12} - 2G_6}[2 - \frac{G_4}{G_2}] + G_2 = \frac{48}{55}.$$

Case 2. C is a pentagon. In this case, w is W_5 with $\alpha = \frac{3}{2}$. Then by Lemma 1,

$$\Omega_{W_5}(i,j) = \frac{G_5^2}{G_{10} - 2G_5}[2 - \frac{G_4}{G_2}] + G_2 = \frac{66}{79}.$$

Thus it is easily obtained that $\Omega_F(i,j) \geq \frac{66}{79}$.

For the upper bound, let C' and C'' be the two facial cycles each of which has a common edge with C such that their common edge is contained in P. Denote the sub-graph induced by C, C' and C'' by F_1, and the sub-graph obtained from F_1 by deleting the common edge kl of C' and C'' by F_2, see Fig. 2. Then by Rayleigh's short-cut method,

$$\Omega_F(i,j) \leq \Omega_{F_1}(i,j) \leq \Omega_{F_2}(i,j).$$

By series and parallel connection rules, it is easy to obtain that

$$\Omega_{F_2}(i,j) = \frac{1}{\frac{1}{|V(C')|-2+|V(C'')|-2} + \frac{1}{2} + \frac{1}{|V(C)|-2}} \leq \frac{1}{\frac{1}{6-2+6-2} + \frac{1}{2} + \frac{1}{6-2}} = \frac{8}{7}$$

And thus the upper bound is proved.

Note that there are $3n$ pairs of vertices at distance two and the sum of resistance distances at distance two is $3(n-2)$ by Foster's second formula. Thus the average value is derived.

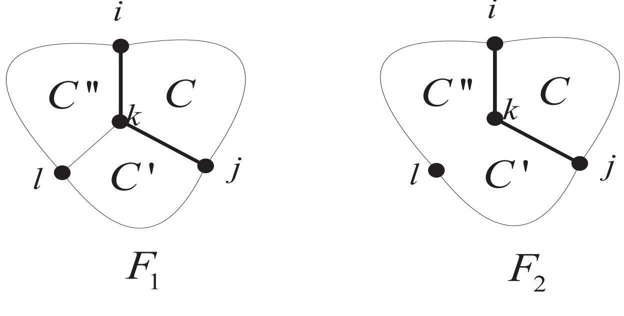

Fig. 2. Illustration of sub-graphs F_1 and F_2 in the proof of Theorem 4. The path $P = ikj$ is illustrated in bold line.

Acknowledgements

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