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Traversing every edge in each direction once, but not at once: Cubic (polyhedral) graphs

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Abstract

A *retracting-free bidirectional circuit* in a graph G is a closed walk which traverses every edge exactly once in each direction and such that no edge is succeeded by the same edge in the opposite direction. Such a circuit revisits each vertex only in a number of steps. Studying the class Ω of all graphs admitting at least one retracting-free bidirectional circuit was proposed by Ore (1951) and is by now of practical use to nanotechnology. The latter needs in various molecular polyhedra that are constructed from a single chain molecule in the retracting-free way. Some earlier results for simple graphs, obtained by Thomassen and, then, by other authors, are specially refined by us for a cubic graph Q. Most of such refinements depend only on the number n of vertices of Q.

1. Preliminaries

Let $Q = (V, E)$ be a simple cubic graph with the vertex set V and edge set E $\big(|V| = n, |E| = m = 3n/2\big)$. A *spanning tree* T of Q is a subtree covering all the vertices of Q $\big(|V(T)| = n; |E(T)| = n - 1\big)$. Its *cotree* $Q - E(T)$ $\big(\big|V\big(Q - E(T)\big)\big| = n; \big|E\big(Q - E(T)\big)\big| = (n + 2)/2\big)$ is a graph Q less all edges belonging to T.

A *symmetric digraph* $S(G)$ of an undirected graph G is obtained by substituting a pair of opposite arcs for every edge in G. It is worth noting that $S(G)$ and G share the same adjacency

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matrix A. In a graph-theoretical literature, one may also encounter phrases with some abuse of a rigorous language, *e.g.*: "an arc of a graph", "arcs of an edge", *etc.*. This indicates that both appearances of a graph (undirected or directed) may tolerate each other in a certain context.

An *Eulerian circuit* is a circuit that circularly traverses every edge of a graph G (res. arc of a digraph D) exactly once. A graph is called an *Eulerian graph* if it admits at least one Eulerian circuit. A simple graph is Eulerian iff all vertex degrees of G are even. A digraph D is an *Eulerian digraph* if an indegree $d^-(v)$ of each vertex $v \in V(D)$ is equal to its outdegree $d^+(v)$. Evidently, the symmetric digraph $S(G)$ is an Eulerian one. An Eulerian circuit in $S(G)$ is tantamount to a bidirectional circuit in a graph G, which traverses each edge of G exactly once in each direction. Therefore, one may easily replace in many instances G by $S(G)$, or vice versa, for convenience of considerations.

In 1951, Ore [1] posed a problem, asking for a characterization of graphs that admit closed walk which traverses every edge exactly once in each direction and such that no edge is succeeded by the same edge in the opposite direction. The problem was partially solved in [2] and [3], and completely solved almost 40 years later by Thomassen [4]. The further results were obtained in [5–8]. We denote by Ω the class of all graphs about which Ore posed his question [1]. The underlined closed walks [1–4] are called *retracting-free bidirectional circuits*, which is a remake of the terminology used by Thomassen [4]. Studying the class Ω [1–8] is, in particular, of practical use to nanotechnology [9–12]. The latter needs in various molecular polyhedra that are constructed from a single chain molecule traversing a geometric polyhedron's frame in the retracting-free way [9–12].

Here, we turn the main section.

2. The main part

Let $\delta(G)$ and $\Delta(G)$ be the minimum and maximum vertex degrees of a graph G, respectively. Thomassen proved the following (Theorem 3.3 of [4]):

Theorem 1. *A graph G admits a closed walk which traverses every edge exactly once in each direction and such that no edge is succeeded by the same edge in the opposite direction if and only if $\delta(G) > 1$ and G has a spanning tree T such that each component of the cotree $G - E(T)$ has an even number of edges or contains a vertex v of degree ≥ 4.*

We derive the following corollary of Theorem 1:

Corollary 1.1. *A cubic graph Q admits a closed walk which traverses every edge exactly once in each direction and such that no edge is succeeded by the same edge in the opposite direction if and only if Q has a spanning tree T such that each (connected) component of the cotree $Q - E(T)$ has an even number of edges and is either a proper cycle or path of length ≥ 0.*

Proof. Valencies of vertices in a spanning tree $T(Q)$ may be only $1, 2, 3$. Hence, vertex valencies of $Q - E(T)$ may be only $0, 1, 2$. This proves that possible (connected) components of the latter graph are either cycles or paths. Theorem 1 determines the number of edges in each component to be even. This completes the proof. □

The next corollary is useful for applications.

Corollary 1.2. *Let a cubic graph Q admit a closed walk which traverses every edge exactly once in each direction and such that no edge is succeeded by the same edge in the opposite direction ($Q \in \Omega$). Then, Q has an odd number $|E(Q)| = 3h$ of edges (where $h = 3, 5, 7, \ldots$).*

Proof. By virtue of Theorem 1, a cotree $Q - E(T)$ has an even number of edges. However, a spanning tree T has an odd number of edges. The number of all edges in a graph Q is exactly the sum of these two numbers. But "an odd number" + "an even number" equals "an odd number". The latter is divisible by 3 (in a cubic graph Q) and is ≥ 9 (where the equality holds for a triangular prism), which completes the proof. $\qquad\square$

It is of use to estimate the number of components of each type in a cotree $Q - E(T)$. Here, we state an independent assertion, *viz.*:

Lemma 2. *Let T be an arbitrary spanning tree of a simple cubic graph Q. Then, $Q - E(T)$ contains exactly $(n - 2)/2$ paths, while the other (connected) components, if any, are proper cycles. (Recall that, for $\forall Q \in \Omega$, Corollary 1.1 imposes the restriction on each component of $Q - E(T)$ to have an even number of edges.)*

Proof. Let F be an arbitrary forest on n_F vertices, with a total number m_F of edges. An arbitrary tree T^* has n_{T^*} vertices and $n_{T^*} - 1$ edges, while the difference between the numbers is $n_{T^*} - (n_{T^*} - 1) = 1$ for each tree. Consequently, the difference $n_F - m_F$ is equal to the number of all trees in F. An arbitrary cycle C has n_C vertices and n_C edges, which gives a zero difference for any cycle and, similarly, 0 for any family of cycles. Taking into account both circumstances, we may interpret the difference between the number of vertices of a cotree $Q - E(T)$ and the number of its edges as the number of all trees (*i.e.*, paths) in $Q - E(T)$. Direct calculation gives: $n - (n + 2)/2 = (n - 2)/2$. This completes the proof. $\qquad\square$

Denote by c_k and p_l the numbers of cycles of length k and the number of paths of length l in $Q - E(T)$, respectively, where $k = 4, 6, 8, \ldots, 2h$ and $l = 0, 2, 4, \ldots, 2h$ ($h \in \mathbb{N} \setminus 2\mathbb{N}$). Besides, let $c := \sum_{k=4}^{2h} c_k$ and $p := \sum_{l=0}^{2h} p_l = (n - 2)/2$. Some simple relations can be deduced, *e.g.*:

Lemma 3. *Let $Q \in \Omega$ and let $Q - E(T)$ obey Corollary 1.1. Then,*

$$\sum_{k=4}^{n} kc_k + \sum_{l=0}^{n} (l - 1)p_l = 2 \quad (k, l \in 2\mathbb{N}). \tag{1}$$

Proof. Taking into account that $E\big(Q - E(T)\big) = (n + 2)/2$, we obtain

$$\sum_{k=4}^{n} kc_k + \sum_{l=0}^{n} lp_l = \frac{n + 2}{2} \quad (k, l \in 2\mathbb{N}). \tag{2}$$

By virtue of Lemma 2, $\sum_l^n p_l = (n-2)/2$ $(l \in 2\mathbb{N})$. Therefore,

$$\sum_{k=4}^n kc_k + \left(\sum_{l=0}^n lp_l - \sum_{l=0}^n p_l\right) = \sum_{k=4}^n kc_k + \sum_{l=0}^n (l-1)p_l = \frac{n+2}{2} - \frac{n-2}{2} = 2 \quad (k, l \in 2\mathbb{N}), \quad (3)$$

which affords the proof. $\qquad\qquad\square$

Nanosynthesists deal with a larger class $\Xi \supset \Omega$ of polyhedral graphs. Namely, a graph $H \in \Xi$ admits retracting-free double circuits traversing every edge twice, but not necessarily in each direction, as is for graphs of Ω. The minimum graph from $\Xi \setminus \Omega$ is that of tetrahedron [9–12]. The following result is due to Sabidussi [13] and was later independently proven by Eggleton and Skilton ([3; Theorem 9]).

Lemma 4. *A connected graph G has a retracting-free double tracing iff G has no pendent points.*

Lemma 4 has the following important corollary:

Corollary 4.1. *Let Ξ be the class of all polyhedral graphs that admit retracting-free double circuits traversing every edge twice, but not necessarily in each direction. Then, Ξ is exactly the class of all polyhedral graphs (having all valencies ≥ 3).*

Let $S(G)$ be the symmetric digraph of a graph G as above. Precedentially, Chinese mathematicians studied the *line digraph* [14, 15], as a direct generalization of the usual (undirected) *line graph*. Following this, the *arc graph $\Gamma(G)$ of a graph G $\big(digraph\ S(G)\big)$* is defined [16] as a digraph whose vertex set is the set of all arcs of $S(G)$, and two arcs qu and vw, of $S(G)$, are adjacent (as vertices) in $\Gamma(G)$ iff $u = v$, whether or not $q = w$. The number of all bidirectional circuits of G is equal to the number of all *Hamiltonian cycles* of $\Gamma(G)$ (visiting each vertex exactly once); see [14–16]. In order to consider just the retracting-free circuits traversing every edge exactly once in each direction, if any in G, it is needed to construct a certain spanning subdigraph $\Theta(G) \subset \Gamma(G)$, already used in statistical physics (without a reference) for counting *nonselfbacktracking (nonselfreversing) walks on G*. (This might be a synonym for 'retracting-free walks', but with the permission of eventually traversing any edge in either direction an arbitrary number of times.) The vertex set of $\Theta(G)$ is also the set of all arcs of $S(G)$, and two incident arcs uv and vw are adjacent (as vertices) in Θ iff $u \neq w$ (that is, not as in Γ, in which the instance of $u = w$ is also used under construction).

We specifically state the following.

Lemma 5. *Let $\Gamma(G)$ be the arc graph of a simple graph G. The number of retracting-free bidirectional circuits, of G, traversing every edge exactly once in each direction is equal to the number of Hamiltonian cycles of a subdigraph $\Theta(G) \subset \Gamma(G)$. (Thus, for all graphs $G \in \Omega$, $\Theta(G)$ is a Hamiltonian digraph.)*

By definition, the indegree $\mathfrak{d}_j^-$ and outdegree $\mathfrak{d}_j^+$ of vertex in the subdigraph $\Theta(G) \subset \Gamma(G)$, respectively, are equal to $d_j^- - 1$ and $d_j^+ - 1$, where d_j^- and d_j^+ are the indegree and outdegree of vertex j in $\Gamma(G)$. In particular, if G is a simple cubic graph Q, then $\mathfrak{d}_j^- = \mathfrak{d}_j^+ = 2$ $(j \in \{1, 2, \ldots, 3n\})$, in $\Theta(Q)$. Thus, all components of $\Theta(Q)$ are Eulerian.

Let J_s and I_s be $s \times s$ matrices of all ones (the former) and a unit diagonal matrix (the latter). The *subfactorial* $!s$ *of* s ($s \in \mathbb{N}^+$) is defined as

$$!s := \mathrm{per}(J_s - I_s) \quad (s \in \mathbb{N}^+), \tag{4}$$

where I_s can equivalently be replaced by any $s \times s$ permutation matrix P (giving the same value).

In order to proceed, we need to perform some technical manipulations with the adjacency matrix $A\big(\Theta(G)\big)$ of a digraph $\Theta(G)$. These manipulations reduce $A\big(\Theta(G)\big)$ to some derivative matrix $\big[A\big(\Theta(G)\big)\big]'$, obtained by specially permuting rows and columns of $A\big(\Theta(G)\big)$. Such a transformation produces a matrix having the same permanent: $\mathrm{per}(A) = \mathrm{per}(A')$, which will be used by us in the proof of the next statement. Here, we use the following four-step argument.

1. Recall that the set $V(\Theta)$ vertices of $\Theta(G)$ is the set $E_\uparrow(S)$ of arcs of the symmetric digraph $S(G)$. Numerate all arcs of $E_\uparrow(S)$ in such a way that all d_j^- arcs ij entering a vertex j of $S(G)$ be numbered consecutively ($i, j \in \{1, 2, \ldots, |V(G)|\}$). Accordingly, the matrix $A\big(\Theta(G)\big)$ has such a form $A = A_1$ that is partioned into $d_j \times |E_\uparrow(S)|$ blocks B_j, each associated with the respective vertex $j \in V(G)$; $A_1 = \big[B_1^\mathsf{T} \, B_2^\mathsf{T} \, \cdots B_{|V(G)|}^\mathsf{T}\big]^\mathsf{T}$, where T denotes the matrix transposition.

2. Note that each block B_j ($j \in \{1, 2, \ldots, |V(G)|\}$ has exactly $|E_\uparrow(S)| - d_j^-$ all-zero columns, and the other d_j^- columns have exactly $d_j^- - 1$ ones (1's) each, while keeping their zero entries in d_j^- different rows.

3. According to the numeration of arcs in $S(G)$, two different blocks B_i and B_j, of A_1, keep their 1's in disjoint (B_i- and B_j-sets of) columns of A_1. Owing to this, we can permute the columns of each block B_j $\big($or of the entire matrix $A\big(\Theta(G)\big)\big)$ so that all 1's of B_j be collected in its d_j^- consecutive columns. This makes another matrix A_2. It is essential that all 1's of the former B_j-rows of A_1 are thus collected in a $d_j^- \times d_j^-$ block of A_2. Without any loss of generality, we may permute the columns in such a way that A_2 have a block-diagonal form. $\big($Mention that $d_j^- = d_j^+$ in $S(G)$.$\big)$

4. Recall that every such square block, keeping all units of the respective rows of A_2, contains exactly one 0 in each row and each column. This allows us to permute rows of A_2 in each block so that all 0's thereof comprise an all-zero diagonal (with all other entries being 1's), to produce a matrix A_3. This is just our target derivative matrix: $\big[A\big(\Theta(G)\big)\big]' = A_3$.

Now, by analogy with Proposition 6 for $\mathrm{per}\big(\Gamma(G)\big)$ in [16], we can state the following:

Lemma 6. *Let* $\mathrm{per}\big[A\big(\Theta(G)\big)\big]$ *be the permanent of the adjacency matrix of the subdigraph* $\Theta(G) \subset \Gamma(G)$*, as above. Then,*

$$\mathrm{per}\big[A\big(\Theta(G)\big)\big] = \prod_{i=1}^{n}(!d_i), \tag{5}$$

where $!d_i$ *is the subfactorial of the valency of the* i*-th vertex of a simple graph* G*.* $\big($*Cf.* $\mathrm{per}\big(\Gamma(G)\big) = \prod_{i=1}^{n}(d_i!)$ *[16].*$\big)$

Proof. It is similar to the Proof of Proposition 6 in [16]. Sketch it. By not simultaneously permuting of rows and columns of $A\big(\Theta(G)\big)$, this matrix may be reduced to a block-diagonal form A', where each block is of form $J_{d_i} - I_{d_i}$ ($i = 1, 2, \ldots, n$). Since permuting rows and/or columns of

a matrix do not alter its permanent, $\operatorname{per}\big[A\big(\Theta(G)\big)\big]$ is equal to the product of permanents of all diagonal blocks of A', which is $\prod_{i=1}^{n}(!d_i)$. Whence we arrive at the proof. $\qquad\square$

Corollary 6.1. *Let* $\operatorname{per}\big[A\big(\Theta(Q)\big)\big]$ *be the permanent of the adjacency matrix of the subdigraph* $\Theta(Q) \subset \Gamma(Q)$, *where* Q *is a simple cubic graph. Then,* $\operatorname{per}\big[A\big(\Theta(Q)\big)\big] = 2^n$, *where* n *is the number of vertices of* Q. *(The result just depends on* n, *and not the construction of* Q.)

Proof. In the Proof of Lemma 6, substitute a concrete value 2 for each diagonal-block permanent $\operatorname{per}(J_{d_j} - I_{d_j}) = (!3) = 2$ (associated with a diagonal block in the block-diagonal form A'), which immediately affords the proof. $\qquad\square$

There is another way to calculate the power-of-two value of $\operatorname{per}\big[A\big(\Theta(Q)\big)\big]$. To this end, represent the adjacency matrix $A\big(\Theta(Q)\big)$ of $\Theta(Q)$ as the sum of two permutation matrices:

$$A\big(\Theta(Q)\big) = P_1 + P_2, \tag{6}$$

where P_1 and P_2 are two permutation matrices (which are arbitrary chosen to obey the equality). The following statement is due to [17] (eq. (1.23) on p. 325):

Theorem 7. *Let* P_1 *and* P_2 *be two* $(s \times s)$ *permutation matrices* $(s \geq 2)$, *and let* ξ_1 *and* ξ_2 *be two (real) constants. Then,*

$$\operatorname{per}\big(\xi_1 P_1 + \xi_2 P_2\big) = \prod_{j=1}^{k}\big(\xi_1^{l_j} + \xi_2^{l_j}\big), \tag{7}$$

where l_j *is the length of the* j-*th cycle in permutation* $P_1^{-1}P_2$, *and* k *is the number of all cycles in* $P_1^{-1}P_2$.

Of use to us is the following corollary [17] (eq. (1.26) on p. 326):

Corollary 7.1. *Let* P_1 *and* P_2 *be two* $(s \times s)$ *permutation matrices* $(s \geq 2)$. *Then,*

$$\operatorname{per}(P_1 + P_2) = 2^k, \tag{8}$$

where k *is the number of all cycles in permutation* $P_1^{-1}P_2$.

Taking into account that $\Theta(Q)$ is a digraph whose all in- and outdegrees are equal to 2, we immediately conclude that the instance of the permanent $\operatorname{per}\big[A\big(\Theta(Q)\big)\big]$ determines $k = n$ in (7). Thus, while representing $A\big(\Theta(Q)\big)$ as an appropriate sum of two permutation matrices, P_1 and P_2, we beforehand know that $P_1^{-1}P_2$ always has exactly n cycles (by Corollary 6.1). Here, we specially show that under all possible variations of the pair (P_1, P_2), the assortment of cycles in $P_1^{-1}P_2$ is the same.

For demonstration of the above assertion, make some easy calculations. Meaning that our target permanent $\operatorname{per}\big[A\big(\Theta(Q)\big)\big]$ has the form $\operatorname{per}(P_1 + P_2)$ for a certain choice of (P_1, P_2), calculate $(P_1 + P_2)^{\mathsf{T}}(P_1 + P_2)$, where T denotes the matrix transposition. We obtain:

$$(P_1 + P_2)^{\mathsf{T}}(P_1 + P_2) = (P_1^{-1} + P_2^{-1})(P_1 + P_2) = 2I + P_1^{-1}P_2 + P_2^{-1}P_1, \tag{9}$$

where the last two (mutually transposed) matrices are mutual inverses: $(P_2^{-1}P_1) = (P_1^{-1}P_2)^{-1}$. Hence, we come to the following technical lemma:

Lemma 8. *The matrix $B = (P_1^{-1}P_2 + P_2^{-1}P_1)$ is the adjacency matrix of an undirected graph H, without loops and multiple edges. Accordingly, H is the disjoint union of n undirected cycles, each of which is the union of two oppositely oriented cycles. (Where n is the number of vertices of Q.)*

Proof. Since B is the sum of inverses, it is a symmetric matrix. This proves that H is undirected. The absence of loops and multiple edges is evident. In the former instance, B has all diagonal entries equal to zero. In the latter, entries of the two permutation matrices in the sum do not have 1's in the same positions. That is, B is a $(0, 1)$-matrix. Thus, we have proved both parts of our first claim.

Now, recall that all cycles of a fixed permutation exactly coincide, with accuracy to orientation, with respective cycles of its inverse permutation. Hence, we deduce that undirected cycles of the graph B exactly coincide with respective directed cycles of either permutation (and are the unions of cycles with opposite orientations). Thus, we deduce that the graph H is the disjoint union of exactly n undirected cycles.

Lastly, realize that the adjacency matrix B does not depend on a choice of a 'pertinent' pair (P_1, P_2) and is always the same for all such pairs may be. This completes the proof. $\square$

One can easily determine the assortment of cycles in H using well-known spectral methods [18]. Once we know Q, we can determine $\Theta(Q)$, then, $A\big(\Theta(Q)\big)$, calculate $\big[(A(\cdots))^{\mathsf{T}}A(\cdots)\big]$, and the eigenvalues of the last matrix. Further, spectral graph theory allows to find the assortment of cycles [18] in H using these eigenvalues.

Just in case, remark that the matrix $P_1^{-1}P_2$ (res. $P_2^{-1}P_1$) corresponds to an even permutation π, since, in our context, this is a $3n \times 3n$ matrix representing a permutation π with exactly n cycles.

Besides, note that knowing the value 2^n allows us to calculate the number of all covers of $\Theta(Q)$ by oriented cycles, which is also the number of all vertex covers of a simple cubic graph Q by retracting-free bidirectional (sub)circuits of lengths $\leq 3n$. This may eventually come in handy for estimating the number of possible synthetic roots to obtain nanopolyhedra using more than one chain molecule, if this will stand for reason.

An *undirected version* $\big(\Theta(Q)\big)^*$ of the digraph $\Theta(Q)$ is obtained by erasing an orientation of every arc in the latter (thereby, every arc becomes an undirected edge). The adjacency matrix A^* of $\big(\Theta(Q)\big)^*$ is:

$$A^* = A\big[\big(\Theta(Q)\big)^*\big] = A\big(\Theta(Q)\big) + [A\big(\Theta(Q)\big)]^{\mathsf{T}}. \tag{10}$$

Evidently, the Hamiltonicity of $\Theta(Q)$ always implies the Hamiltonicity of $\big(\Theta(Q)\big)^*$, while the converse is not in general true. To us, it is of use to know when the converse statement may be true. So far, this is an open problem. We have nothing better to do than to look for any previous results in the literature, which may somehow be relevant to the subject.

One known fact is that the Hamiltonicity of a simple graph G implies certain spectral properties of the latter [19], which includes also the roots of the *chromatic polynomial* $P(G, t)$ [20]. In some instances, the Hamiltonicity of G guarantees that G has more than one Hamiltonian cycle [21]. There were studied in detail *Hamiltonian ladders* (defined by the *Cartesian product $G \times K_2$ of G and K_2*) [22], which are a generalization of graphs of prisms.

In particular, van den Heuvel (Corollary 3 in [19]) proved the following:

Theorem 9. *Let G be an r-regular graph on p vertices. If G contains a Hamiltonian cycle, then*

$$\lambda_i(G) - (r-2) \leq \lambda_i(C_p) \leq \lambda_i(G) + (r-2) \quad (i = 1, 2, \ldots, p), \tag{11}$$

where $\lambda_i(...) \ (i = 1, 2, \ldots, p)$ is the i-th (in a nonincreasing order) eigenvalue of G (or cycle C_p).

For $\big(\Theta(Q)\big)^*$, $p = 3n$ and $r = 4$. Hence, we deduce:

Corollary 9.1. *Let $\big(\Theta(Q)\big)^*$ be a 4-regular graph on $3n$ vertices, as above. If $\big(\Theta(Q)\big)^*$ contains a Hamiltonian cycle, then*

$$\lambda_i\big[\big(\Theta(Q)\big)^*\big] - 2 \leq \lambda_i(C_{3n}) \leq \lambda_i\big[\big(\Theta(Q)\big)^*\big] + 2 \quad (i = 1, 2, \ldots, 3n). \tag{12}$$

If G is a graph and t is a nonnegative integer, then $P(G, t)$ denotes the number of colorings of G such that all colors are one of the integers $1, 2, \ldots, t$. As $P(G, t)$ is a polynomial, it is defined for all real numbers t. We say that t is a *chromatic root of G* if $P(G, t) = 0$. Thomassen [20] proved:

Theorem 10. *If the chromatic polynomial $P(G, t)$ of a graph G has a noninteger root less than or equal to*

$$t_0 = \frac{2}{3} + \frac{1}{3}\sqrt[3]{26 + 6\sqrt{33}} + \frac{1}{3}\sqrt[3]{26 - 6\sqrt{33}} = 1.29559\ldots, \tag{13}$$

then the graph has no Hamiltonian path. This result is best possible in the sense that it becomes false if t_0 is replaced by any larger number.

It is interesting to know if Theorems 9 and 10 may also be generalized to directed graphs, as is $\Theta(Q)$. So far, this is an open question.

Acknowledgments

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