Making Walks Count: From Silent Circles to Hamiltonian Cycles

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1 Introduction

Leonhard Euler (1707–1783) famously invented graph theory in 1735, when he was faced with a puzzle, which some of the inhabitants of Königsberg amused themselves with. They were looking for a way to walk across each of their seven bridges once and only once, but they could not find any. Euler reduced the problem to its bare bones and showed that such a puzzle would have a solution if and only if every "node" (i.e., every land mass) in the underlying "graph" was at the origin of an even number of "edges" (each corresponding a bridge) with at most two exceptions—which could only be at the start or at the end of the journey. Since this was not the case at Königsberg, the puzzle had no solution.

Except for tiny examples like that historical one, a sketch on paper is rarely an adequate description of a graph. One convenient representation of a directed graph (often called *digraph* for short) is given by its *adjacency matrix* A, where the element $A_{i,j}$ is the number of edges that go from node i to node j (in a simple graph, that number is either 0 or 1). An undirected graph, like the Königsberg graph, can be viewed as a digraph with a symmetric adjacency matrix (as every undirected edge between two nodes corresponds to a pair of directed edges going back and forth between the nodes).

A fruitful bonus of using adjacency matrices for representation of graphs is that the ordinary multiplication of such matrices is surprisingly meaningful: the n-th power of the adjacency matrix of a graph describes *walks* along n successive edges (not necessarily distinct) in this graph. This observation leads to a method called the *transfer-matrix method* (e.g., see [2, Section 4.7]) that employs the linear algebra techniques to enumerate walks very efficiently. In the present work, we shall perform a few spectacular enumerations using the transfer-matrix method.

The element $A_{i,j}$ of the adjacency matrix A can be viewed as the number of walks of length 1 from node i to node j. What is the number of such walks of length 2? Well, it is clearly the number of ways to go from i to some node k along one edge and then from that node k to node j along a second edge. This amounts to the sum over k of all products $A_{i,k} \cdot A_{k,j}$, which is immediately recognized as a matrix element of the square of A, namely $(A^2)_{i,j}$. More generally, the above is the pattern for a proof by induction on n of the following theorem.

Theorem 1 ([2, Theorem 4.7.1])**.** *The number $(A^n)_{i,j}$ equals the number of walks of length n going from node i to node j in the digraph with the adjacency matrix A.*

A walk is called *closed* if it starts and ends at the same node. Theorem 1 immediately implies the following statement for the number of closed walks.

Corollary 2. *In a digraph with the adjacency matrix A, the number of closed walks of length n equals* $\mathrm{tr}(A^n)$*, the trace of A^n.*

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It is often convenient to represent a sequence of numbers $a_0, a_1, a_2, \ldots$ as a *generating function* $f(z)$ (of indeterminate z) such that the coefficient of z^n in $f(z)$ equals a_n for all integers $n \geq 0$ (e.g., see [4] for a nice introduction to generating functions). In other words, $f(z) = a_0 + a_1 \cdot z + a_2 \cdot z^2 + \cdots$. The generating function for the number of closed walks has a neat algebraic expression:

Theorem 3 ([2, Corollary 4.7.3]). *For any $m \times m$ matrix A,*

$$\sum_{n=0}^{\infty} \operatorname{tr}(A^n) \cdot z^n = m - \frac{zF'(z)}{F(z)},$$

where $F(z) = \det(I_m - z \cdot A)$, and I_m is the $m \times m$ identity matrix.

We will show how to put these nice results to good use by reducing some enumeration problems to the counting of walks or closed walks in certain digraphs.

2 Silent Circles

One of our motivations for the present work was the elegant solution to a problem originally posed by Philip Brocoum, who described the following game as a preliminary event in a drama class he once attended at MIT. The game was played repeatedly by all the students until silence was achieved.[1]

An even number ($2n$) of people stand in a circle with their heads lowered. On cue, everyone looks up and stares either at one of their two immediate neighbors (left or right) or at the person diametrically opposed. If two people make eye contact, both will scream! What is the probability that everyone will be silent? For $n > 1$,[2] since each person has 3 choices, there are 3^{2n} possible configurations (which are assumed to be equiprobable). The problem then becomes just to count the number of *silent configurations*.

Let us first do so in the slightly easier case of an *n-prism* of people (we will come back to the original question later). This is a fancy way to say that the people are now arranged in two concentric circles each with n people, where every person faces a "partner" on the other circle and is allowed to look either at that partner or at one of two neighbors on the same circle.

The key idea is to notice that the silent configurations are in an one-to-one correspondence with the closed walks of length n in a certain digraph on 8 nodes. Indeed, there are $3^2 - 1 = 8$ different ways for the two partners in a pair to not make an eye contact with each other. We call each such way a *gaze* and denote it with a pair of arrows, one over another, indicating sight directions of the partners. We build the *gaze digraph*, whose nodes are the different gazes. There is a (directed) edge from node i to node j if and only if gaze j can be clockwise next to gaze i in a silent configuration. The gaze digraph and its adjacency matrix A are shown in Fig. 1.

Let t_n be the number of "silent" n-gonal prisms. By Corollary 2, we have $t_n = \operatorname{tr}(A^n)$. Theorem 3 further implies (by direct calculation) that

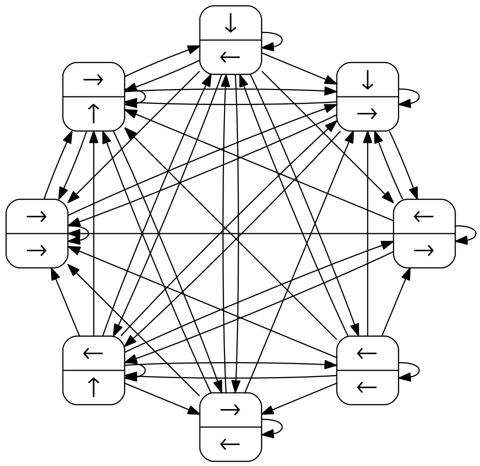
$$\sum_{n=0}^{\infty} t_n \cdot z^n = \frac{8 - 56z + 96z^2 - 50z^3 + 4z^4}{1 - 8z + 16z^2 - 10z^3 + z^4}.$$

From this generating function, we can easily derive a recurrence relation for t_n. Namely, multiplying of the generating function by $1 - 8z + 16z^2 - 10z^3 + z^4$, we get

$$(1 - 8z + 16z^2 - 10z^3 + z^4) \cdot \sum_{n=0}^{\infty} t_n \cdot z^n = 8 - 56z + 96z^2 - 50z^3 + 4z^4.$$

[1] Presumably, the teacher would participate only if the number of students was odd.

[2] The case $n = 1$ is special, since the two immediate neighbors and the diametrically opposite person all coincide.



	→ →	← ←	← ↑	↓ →	← →	→ ←	→ ↑	↓ ←
→ →	1	0	0	1	0	0	1	0
← ←	1	1	1	1	1	1	1	1
← ↑	1	1	1	1	1	1	1	1
↓ →	1	0	1	1	1	0	1	0
← →	1	0	1	1	1	0	1	0
→ ←	1	0	0	1	0	1	1	1
→ ↑	1	0	0	1	0	1	1	1
↓ ←	1	1	1	1	1	1	1	1

Figure 1: The gaze digraph and its adjacency matrix A.

For $n \geq 5$, the equality of coefficients of z^n in the left-hand and right-hand sides gives

$$t_n - 8t_{n-1} + 16t_{n-2} - 10t_{n-3} + t_{n-4} = 0.$$

The values of t_n form the sequence `A141384` in the OEIS [3].

Returning to the original question, we remark that each gaze is formed by two diametrically opposite people from the same circle. For $n > 1$, a silent configuration for a circle of $2n$ is therefore defined by a walk on $n + 1$ nodes, where the starting and ending nodes represent the same pair of people but in different order. It follows that the starting and ending gazes must be obtained from each other by a vertical flip. The entries in the adjacency matrix corresponding to such gaze flips are colored green: the number s_n of such walks equals the sum of elements in these entries in the matrix A^n. Since the minimal polynomial of A is

$$x^5 - 8x^4 + 16x^3 - 10x^2 + x,$$

the sequence s_n (sequence `A141221` in the OEIS [3]) satisfies the recurrence relation:

$$s_n = 8s_{n-1} - 16s_{n-2} + 10s_{n-3} - s_{n-4}, \qquad n \geq 6,$$

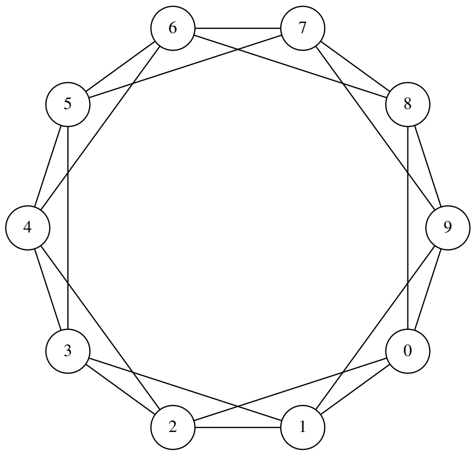
which matches that for t_n. Taking into account the initial values of s_n for $n = 2, 3, 4, 5$, we further deduce the generating function

$$\sum_{n=2}^{\infty} s_n \cdot z^n = \frac{30z^2 - 84z^3 + 58z^4 - 6z^5}{1 - 8z + 16z^2 - 10z^3 + z^4}.$$

We give initial numerical values of the sequences t_n and s_n along with the corresponding probabilities of silent configurations in the table below. Quite remarkably we have $t_n = s_n + 2$ for all $n > 1$. It further follows that both probabilities $t_n/3^{2n}$ and $s_n/3^{2n}$ grow as $(\alpha/9)^n \approx 0.5948729^n$, where

$$\alpha = \frac{1}{3}\left(7 + 2 \cdot \sqrt{22} \cdot \cos\left(\frac{\arctan(\sqrt{5319}/73)}{3}\right)\right) \approx 5.353856$$

is the largest zero of the minimal polynomial of A.



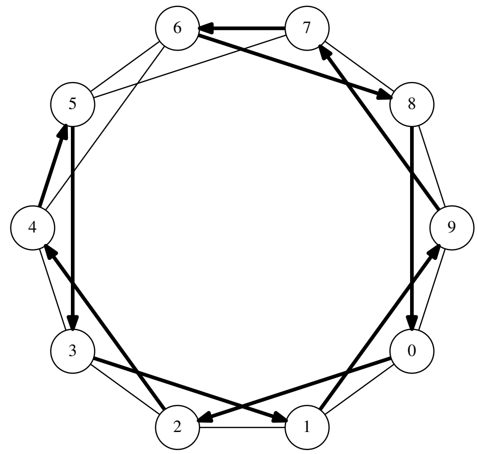


Figure 2: **(a)** The antiprism graph $C_{10}^{1,2}$. **(b)** A directed Hamiltonian cycle in $C_{10}^{1,2}$ that does not visit either of the edges $(4,6)$, $(5,6)$, $(5,7)$, i.e., has signature 000 at node 4.

n	2	3	4	5	6	7	8	9	10
t_n	32	158	828	4408	23564	126106	675076	3614144	19349432
$t_n/3^{2n}$	0.395	0.217	0.126	0.075	0.044	0.026	0.016	0.009	0.006
s_n	30	156	826	4406	23562	126104	675074	3614142	19349430
$s_n/3^{2n}$	0.370	0.214	0.126	0.075	0.044	0.026	0.016	0.009	0.006

3 Hamiltonian Cycles in Antiprism Graphs

An *antiprism graph* represents the skeleton of an antiprism. The n-antiprism graph (defined for $n \geq 3$) has $2n$ nodes and $4n$ edges and is isomorphic to the circulant graph $C_{2n}^{1,2}$; that is, its nodes can be placed along a circle and enumerated with numbers from 0 to $2n-1$ such that each node i ($i = 0, 1, \ldots, 2n-1$) is connected to nodes $i \pm 1 \bmod 2n$ and $i \pm 2 \bmod 2n$ (Fig. 2a).

A *cycle* is a closed walk without repeated edges, up to a choice of a starting/ending node. A cycle is *Hamiltonian* if it visits every node in the graph exactly once. A recurrence formula for the number of Hamiltonian cycles in $C_{2n}^{1,2}$ was first obtained in [1]. Here we present a simpler derivation for the same formula.

For a subgraph G of $C_{2n}^{1,2}$, we define the *visitation signature* of G at node i as a triple of binary digits describing whether edges $(i, i+2)$, $(i+1, i+2)$, $(i+1, i+3)$ belong to (visited by) G, where digits 1/0 mean visited/non-visited. Then a Hamiltonian cycle Q (viewed as a subgraph) in $C_{2n}^{1,2}$ has one of the following two types:

(T1) there exists i such that the visitation signature of Q at i is 000;

(T2) for every i, the visitation signature of Q at i is not 000.

It is not hard to see that for each fixed i, there exist exactly two directed Hamiltonian cycles (of opposite directions) that has visitation signature 000 at i (an example of such a cycle for $n = 5$ and $i = 4$ is given in Fig. 2b). Moreover, the value of i is unique for such cycles. So the total

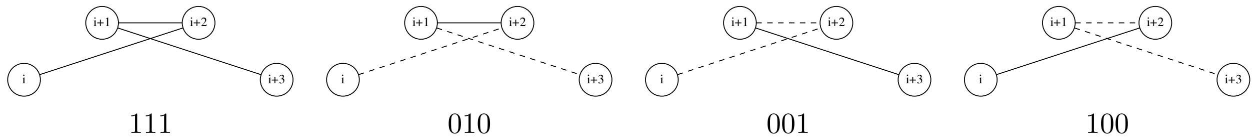


Figure 3: Possible visitation signatures for a Hamiltonian cycle of type (T2) in $C_{2n}^{1,2}$. Visited and non-visited edges are shown as solid and dashed, respectively.

number of directed Hamiltonian cycles of type (T1) equals $4n$. Their generating function is

$$\sum_{n=3}^{\infty} 4n \cdot z^n = \frac{4z^3(3-2z)}{(1-z)^2}. \tag{1}$$

Now we focus on computing the number of Hamiltonian cycles of type (T2), for which we need the following lemma.

Lemma 4. *A subgraph Q of $C_{2n}^{1,2}$ is a Hamiltonian cycle of type (T2) if and only if (i) every node of $C_{2n}^{1,2}$ is incident to exactly two edges in Q; and (ii) the visitation signature of Q at every node is* 111*,* 001*,* 010*, or* 100 *(shown in Fig. 3).*

Proof. If Q is a Hamiltonian cycle of type (T2), then condition (i) trivially holds. Condition (ii) can also be easily established by showing that no other visitation signature besides 111, 001, 010, and 100 is possible in Q. Indeed,

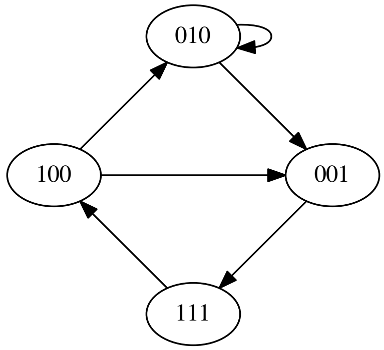
- the signature 000 cannot happen anywhere in Q by the definition of type (T2);
- the signature 011 at node i implies the signature 000 at node $i-1$;
- the signature 110 at node i implies the signature 000 at node $i+1$;
- the signature 101 at node i implies the presence of edges $(i, i+1)$ and $(i+2, i+3)$ in Q; that is, Q must coincide with the cycle $(i, i+2, i+3, i+1, i)$, a contradiction to $n \geq 3$.

Now, let Q be a subgraph of $C_{2n}^{1,2}$ satisfying conditions (i) and (ii). Let $Q' \subset Q$ be a connected component of Q. Since every node is incident to two edges from Q, Q' represents a cycle in $C_{2n}^{1,2}$.

We claim that for any $i \in \{0, 1, \dots, 2n-1\}$, Q' either contains node $i+1$ or both nodes i and $i+2$. If this is not so, then starting at a node belonging Q' and increasing its label by 1 or 2 modulo $2n$ (keeping the node in Q'), we can find a node i in Q' such that neither $i+1$, nor $i+2$ are in Q'. Then Q' (and Q) contains edges $(i-2, i)$ and $(i-1, i)$, and since every node in Q is incident to exactly two edges, Q does not contain edges $(i-1, i+1)$, $(i, i+1)$, and $(i, i+2)$. That is, the visitation signature of Q at node $i-1$ is 000, a contradiction.

We say that Q' *skips* node i if it contains nodes $i-1$ and $i+1$, but not i. It is easy to see that if Q' does not skip any nodes, then it contains all nodes $0, 1, \dots, 2n-1$, in which case $Q' = Q$ represents a Hamiltonian cycle. If Q' skips a node i, consider a connected component Q'' of Q that contains i. It is easy to see that the nodes of Q' and Q'' must interweave, i.e., $Q' = (i-1, i+1, i+3, \dots)$ and $Q' = (i, i+2, i+4, \dots)$. Then the signature of Q at node i is 101, a contradiction proving that Q' cannot skip nodes. □

Lemma 4 allows us to compute the number of Hamiltonian cycles of type (T2) in $C_{2n}^{1,2}$ as the number of subgraphs Q satisfying conditions (i) and (ii). To compute the number of such subgraphs, we construct a directed graph S on the allowed visitation signatures as nodes, where there is a



	111	010	001	100
111	0	0	0	1
010	0	1	1	0
001	1	0	0	0
100	0	1	1	0

Figure 4: The signature graph S and its adjacency matrix.

directed edge (s_1, s_2) whenever the signatures s_1 and s_2 can happen in Q at two consecutive nodes. The graph S and its adjacency matrix A_S are shown in Fig. 4.

By Lemma 4 and Corollary 2, the number of Hamiltonian cycles of type (T2) in $C_{2n}^{1,2}$ equals $\mathrm{tr}(A_S^{2n})$. Correspondingly, the total number of directed Hamiltonian cycles h_n in $C_{2n}^{1,2}$ equals $4n + 2\,\mathrm{tr}(A_S^{2n})$; its generating function (derived from (1) and Theorem 3) is

$$\sum_{n=3}^{\infty} h_n \cdot z^n = \frac{4z^3(3-2z)}{(1-z)^2} + \frac{2z^3(10+11z+5z^2)}{1-z-2z^2-z^3} = \frac{2z^3(16-19z-15z^2+3z^3+9z^4)}{(1-z)^2(1-z-2z^2-z^3)}.$$

It further implies that the sequence h_n satisfy the recurrence relation:

$$h_n = 3h_{n-1} - h_{n-2} - 2h_{n-3} + h_{n-5}, \qquad n \geq 8$$

with the initial values $32, 58, 112, 220, 450, \ldots$ for $n = 3, 4, \ldots$ (sequence `A124353` in the OEIS [3]).

4 Hamiltonian Cycles and Paths in Arbitrary Graphs

Similarly to cycles, a path (i.e., a non-closed walk without repeated edges) in a graph is called *Hamiltonian* if it visits every node of the graph exactly once. Enumeration of Hamiltonian paths/cycles in an arbitrary graph represents a famous NP-complete problem. That is, one can hardly hope for existence of an efficient (i.e., polynomial-time) algorithm for this enumeration and thus has to rely on less efficient algorithms of (sub)exponential time complexity. Below we describe such not-so-efficient but very neat and simple algorithm,[3] which is based on the transfer-matrix method and another basic combinatorial enumeration method called inclusion-exclusion (e.g., see [2, Section 2.1]).

We denote the number of (directed) Hamiltonian cycles and paths in a graph G by $\mathrm{HC}(G)$ and $\mathrm{HP}(G)$, respectively.

Theorem 5. *Let G be a graph with a node set $V = \{v_1, \ldots, v_n\}$ and A be the adjacency matrix of G. Then*

$$\mathrm{HP}(G) = \sum_{S \subset V} (-1)^{|S|} \cdot \mathrm{SUM}\left(A_{V \setminus S}^{n-1}\right) \tag{2}$$

[3] We are not aware if this algorithm has been described in the literature before, but based on its simplicity we suspect that this may be the case.

and

$$\mathrm{HC}(G) = \frac{1}{n} \sum_{S \subset V} (-1)^{|S|} \cdot \mathrm{tr}\left(A^n_{V \setminus S}\right), \tag{3}$$

where $\textsc{sum}(M)$ *is the sum of all*[4] *elements of a matrix* M.

Proof. First, we notice that a Hamiltonian path in G is the same as a walk of length $n-1$ that visits every node. Indeed, a walk of length $n-1$ visits n nodes, and if it visits every node in G, then it must visit each node only once. That is, such a walk is a Hamiltonian path.

For a subset $S \subset V$, we define P_S as the set of all walks of length $n-1$ in G that do not visit any node from S. Then by the inclusion-exclusion, the number of Hamiltonian paths $\mathrm{HP}(G)$ is given by

$$\mathrm{HP}(G) = \sum_{S \subset V} (-1)^{|S|} \cdot |P_S|.$$

To use this formula for computing $\mathrm{HP}(G)$, it remains to evaluate $|P_S|$ for every $S \subset V$, which can be done as follows. Let $G_{V \setminus S}$ be the graph obtained from G by removing all nodes (along with their incident edges) present in S, and let $A_{V \setminus S}$ be the adjacency matrix of $G_{V \setminus S}$. Then the elements of P_S are nothing else by the walks of length $n-1$ in the graph $G_{V \setminus S}$. Hence, by Theorem 1, $|P_S|$ equals $\textsc{sum}\left(A^{n-1}_{V \setminus S}\right)$, which implies formula (2).

Similarly, a Hamiltonian cycle in G can be viewed as a closed walk of length n that starts/ends at node v_1 and visits every node. Hence, the number $\mathrm{HC}(G)$ of Hamiltonian cycles in G can be computed by the formula

$$\mathrm{HC}(G) = \sum_{S \subset V \setminus \{v_1\}} (-1)^{|S|} \cdot \left(A^n_{V \setminus S}\right)_{1,1}.$$

Similar formulae hold if we view closed walks as starting/ending at node v_i. Averaging over $i = 1, 2, \dots, n$ gives us formula (3). $\square$

Formulae (2) and (3) can be used for practical computing $\mathrm{HP}(G)$ and $\mathrm{HC}(G)$, although they have exponential time complexity as they sum 2^n terms (indexed by the subsets $S \subset V$). On a technical side, we remark that the matrix $A_{V \setminus S}$ can be obtained directly from the adjacency matrix A of G by removing the rows and columns corresponding to the nodes in S.

In an undirected graph G, the number of undirected Hamiltonian paths and cycles is given by $\frac{1}{2}\,\mathrm{HP}(G)$ and $\frac{1}{2}\,\mathrm{HC}(G)$, respectively.

5 Simple Cycles and Paths of a Fixed Length

Our approach for enumerating Hamiltonian paths/cycles can be further extended to enumerating *simple* (i.e., visiting every node at most once) paths/cycles of a fixed length. We refer to simple paths and cycles of length k as k-paths and k-cycles, respectively. We denote the number of (directed) k-cycles and k-paths in a graph G by $\mathrm{SC}_k(G)$ and $\mathrm{SP}_k(G)$, respectively.

Theorem 6. *Let* G *be a graph with a node set* $V = \{v_1, \dots, v_n\}$ *and* A *be the adjacency matrix of* G. *Then, for an integer* $k \geq 1$,

$$\mathrm{SC}_k(G) = \frac{1}{k} \sum_{T \subset V} \binom{n-|T|}{k-|T|} \cdot (-1)^{k-|T|} \cdot \mathrm{tr}\left(A^k_T\right) \tag{4}$$

[4]Alternatively, we can define $\textsc{sum}(M)$ as the sum of all *non-diagonal* elements of M; formula (2) still holds in this case.

and

$$\mathrm{SP}_k(G) = \sum_{T\subset V} \binom{n-|T|}{k+1-|T|} \cdot (-1)^{k+1-|T|} \cdot \textsc{sum}\left(A_T^k\right). \tag{5}$$

Proof. If a k-cycle c visits nodes from a set $U \subset V$, $|U| = k$, then c represents a Hamiltonian cycle in the subgraph G_U of G induced by U. Hence, the number of k-cycles in G equals

$$\mathrm{SC}_k(G) = \sum_{U\subset V,\ |U|=k} \mathrm{HC}(G_U).$$

By formula (3), we further have

$$\begin{aligned}
\mathrm{SC}_k(G) &= \sum_{U\subset V,\ |U|=k} \frac{1}{k} \sum_{S\subset U} (-1)^{|S|} \cdot \mathrm{tr}\left(A_{U\setminus S}^k\right) \\
&= \frac{1}{k} \sum_{T\subset V} \sum_{U:\ T\subset U\subset V,\ |U|=k} (-1)^{k-|T|} \cdot \mathrm{tr}\left(A_T^k\right) \\
&= \frac{1}{k} \sum_{T\subset V} \binom{n-|T|}{k-|T|} \cdot (-1)^{k-|T|} \cdot \mathrm{tr}\left(A_T^k\right),
\end{aligned}$$

which proves (4). (Here T stands for the set $U \setminus S$.)

If a k-path p visits nodes from a set $U \subset V$, $|U| = k+1$, then p represents a Hamiltonian path in the subgraph G_U of G induced by U. Similarly to the above, we can employ formula (2) to obtain (5). □

In an undirected graph G, the number of undirected k-cycles and k-paths is given by $\frac{1}{2}\,\mathrm{SC}_k(G)$ and $\frac{1}{2}\,\mathrm{SP}_k(G)$, respectively.

Using formula (4), we have computed the number of k-cycles in the graph of the regular 24-cell for various values of k (sequence `A167983` in the OEIS [3]).

Acknowledgments

The work of MAA supported by the National Science Foundation under grant no. IIS-1462107.

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