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Paired Domination of Certain Nanotubes

Research Article

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Abstract: A vertex subset D of a graph G is a dominating set if every vertex of G is either in D or is adjacent to a vertex in D. The paired-domination problem on G asks for a minimum-cardinality dominating set S of G such that the subgraph induced by S contains a perfect matching. A set S of vertices in G is a total dominating set of G if every vertex of V is adjacent to some vertex in S. In this paper we construct a minimum paired dominating set for H-Naphtalenic Nanotorus, TUC_4C_8 (S) nanotube and V-phenylenic nanotube and hence we determine the total dominating set.

Keywords: Nanotubes, Perfect Matching, Paired Domination.

1. Introduction

A matching in a graph $G = (V, E)$ is a subset M of edges, no two of which have a vertex in common. A matching M is said to be perfect if every vertex in G is an endpoint of one of the edges in M. Thus a perfect matching in G is a 1-regular spanning subgraph of G. In the literature it is also known as a 1-factor of G. The perfect matching problem is known to be in randomized NC. Finding a perfect matching has received considerable attention in the field of parallel algorithms. Though deterministic parallel algorithms are known for planar bipartite graphs, no deterministic algorithm exists for the non-bipartite case. The structural formulae of chemical compounds are molecular graphs where vertices represent atoms and edges represent chemical bonds. A kekule structure in a molecular graph is nothing but a perfect matching in the graph. A vertex subset D of a graph G is a dominating set if every vertex of G is either in D or is adjacent to a vertex in D.

The domination number $\gamma(G)$ is the minimum cardinality of a dominating set of G. A subset S of V is a paired-dominating set (PDS) of G, if S is a dominating set and the subgraph induced by the vertices of S contains a perfect matching. The paired-domination number $\gamma_{pr}(G)$ is the minimum cardinality of a paired-dominating set. If S is a paired-dominating set with a perfect matching M, then two vertices v_j and v_k are said to be paired in S if the edge $v_jv_k \in M$.

Historically, the first domination-type problems came from chess. Apart from chess, domination in graphs has applications to several other fields. Domination arises in facility location problems, where the number of facilities is fixed and one attempts to minimize the distance that a person needs to travel to get to the closest facility. Concepts from domination also appear in problems involving finding sets of representatives in monitoring communication or electrical networks an in land surveying. The physical and chemical properties of molecules are well correlated with graph theoretical invariants that

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are termed as topological indices or molecular descriptors. One of such graph theoretical invariants is domination number. It has been shown that this number discriminates well even the slightest changes in trees and hence it is very suitable for the analysis of the RNA structures [10]. Paired domination was introduced by Haynes and Slater [7] and it was motivated by the variant of the area monitoring problem in which each guard has another guard as a backup (i.e., pairs of guards protecting each other).

The concept of paired dominating sets has applications in mobile ad hoc wireless networks and has been proposed as a virtual backbone for routing in wireless ad hoc networks [6]. The paired-domination problem is known to be NP-complete. It is NP-complete for bipartite graphs [11]. Panda et al. propose a linear time algorithm to compute a minimum paired-dominating set of a chordal bipartite graph, a well-studied subclass of bipartite graphs [11].

Chellali et al. [2] provide sharp upper bounds on the total and paired-domination numbers of trees that improve known bounds for some cases. Lappas et al. [9] provide an $O(n)$-time algorithm for the paired-domination problem on permutation graphs. Chen et al. [3] study the paired-domination problem for block graphs. Cheng et al. [4] have solved the paired-domination problem for interval and circular arc graphs. Kang et al. [8] have investigated the paired-domination problem in inflated graphs.

2. Nanotube

Nanotechnology is defined as the study and use of structures between 1 nanometer and 100 nanometers in size. Nanotechnology creates many new materials and devices with a wide range of applications in medicine, electronics, and computer. Nanotechnology is expected to revolutionize the 21st century as space, entertainment and communication technology revolutionized the 20th century. It involves different structures of nanotubes. Nanotechnology is the study of manipulating matter on an atomic and molecular scale. Most of the nanotechnology products that are in the market today are gradually improved products in which some form of nanotechnology enabled material is used in the manufacturing process. There are many applications of nanotechnology in the area of medicine, chemistry, energy, agriculture, information and communication, heavy industry and consumer goods. Nanotube was accidentally discovered by a Japanese researcher at NEC in 1990 while making Buckyballs [5].

Nanotubes can easily penetrate membrances such as cell walls. In fact, the long, narrow shape of nanotubes make them look like miniature needles, thus it makes sense that they can function like a needle at the cellular level. Medical researchers are using this property by attaching molecules to the naotubes that are attracted to cancer cells to deliver drugs directly to diseased cells [13]. Nanotubes are three dimensional cylindrical structures formed out of the two dimensional sheets.In this paper we determine the paired domination for V-phenylenic nanotube, $TUC_4C_8(S)$ nanotube and H-Naphtalenic Nanotorus.

3. V-phenylenic VPH[p, q] Nanotube

V-Phenylenic nanotubes $VPH[p, q]$ are molecular graphs that are covered by C_6, C_4 and C_8 [1]. In this section, the paired domination number of V-phenylenic $VPH[p, q]$ nanotube is computed. In the V-phenylenic $VPH[p, q]$ nanotube, p represents the number of hexagons in each column and q represents the number of hexagons in each row. In otherwords, p represents the number of rows and q represents the number of columns. The number of vertices in V-phenylenic $VPH[p,$

$q]$ nanotube is $6pq$. See Fig. 1 (a). The edges of V-phenylenic $VPH[p,\ q]$ nanotube can be divided into 4 types namely horizontal, vertical, acute and obtuse edges.

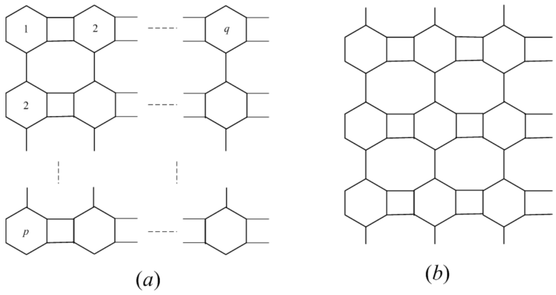

Figure 1. **(a) V-phenylenic $VPH[p,\ q]$ nanotube (b) V-phenylenic $VPH[3,3]$ nanotorus**

Theorem 3.1. *Let G be a V-phenylenic VPH[p, q] nanotube. Then* $\gamma_{pr}(G) = 2pq$.

Proof. In each row i, $1 \leq i \leq p$, select the left-hand side vertical edges in each hexagon as shown in Fig. 2. The end vertices of each selected vertical edges form a paired dominating set S. Let (u_1, v_1) and (u_2, v_2) be the two selected vertical edges such that $d(u_1, v_1) = d(u_2, v_2) = 3$. Let us consider the vertices a, b, c and d between the edges (u_1, v_1) and (u_2, v_2). Now the vertex a is dominated by u_1, the vertex b is dominated by u_2, the vertex c is dominated by v_2 and the vertex d is dominated by v_1. Moreover every vertex in G is adjacent to exactly one vertex in S and the subgraph induced by the set S contains only independent edges. Thus $\gamma_{pr}(G) = 2pq$. □

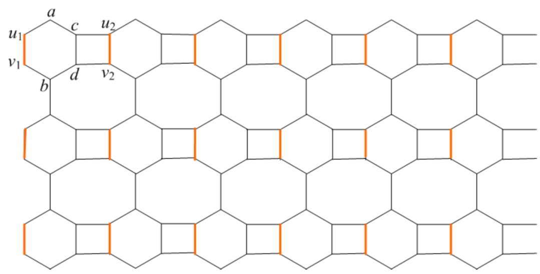

Figure 2. **V-phenylenic $VPH[3,\ 6]$ nanotube**

Theorem 3.1 can be extended to V-phenylenic $VPH[p,\ q]$ nanotorus. V-phenylenic $VPH[p,\ q]$ nanotorus can be obtained by adding the wraparound edges between the two degree vertices in each column as shown in Fig. 1 (b). Thus we have the following theorem.

Theorem 3.2. *Let G be a V-phenylenic VPH[p, q] nanotorus. Then* $\gamma_{pr}(G) = 2pq$.

4. H-Naphtalenic Nanotorus

Carbon nanotubes (CNTs) are peri-condensed Benzenoids, which are ordered in graphite like, hexagonal pattern. They may be derived from graphite by rolling up the rectangular sheets along certain vectors. All benzenoids, including graphite and CNTs are aromatic structures.

A H-Naphtalenic Nanotorus are obtained by the sequence C_6, C_6, C_4, C_6 and $C_6 \ldots C_6$, C_6, C_4, C_6, C_6 and the repeat unit C_6, C_6, C_4. See Fig. 3. Each row i is divided into two levels L_i^1 and L_i^2. The vertices of L_i^1 and L_i^2 are labeled from left to right as shown in the Fig. 3.

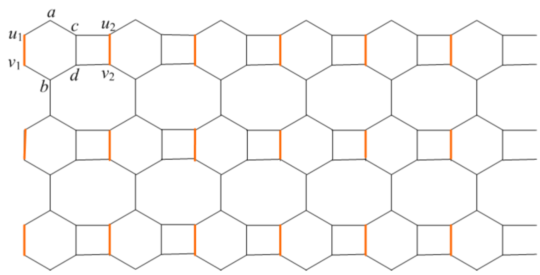

Figure 3. **H-Naphtalenic Nanotorus**

Theorem 4.1. *Let G be a H-Naphtalenic nanotorus. Then G has a paired dominating set.*

Proof. Select the vertices $6n-4$ and $6n-5$, $n \geq 1$ from L_i^1 and select the vertices $6n-1$ and $6n-2$, $n \geq 1$ from L_i^2. Now we need to prove that these vertices form a paired domination and it is minimum. It is easy to see that the selected vertices in L_i^1 and L_i^2 form an independent edges. Let S be the set of all selected independent edges. If (α, β) and $(\gamma, \delta) \in S \cap L_i^1$ then $d(\beta, \gamma) = 5$. Let a, b, c and d be the vertices between the edges (α, β) and (γ, δ). Now the vertex a is dominated by β, the vertex d is dominated by δ and the vertices b and c are dominated by L_i^2 and L_{i-1}^1, viceversa. Thus every vertex in G are dominated by exactly one vertex from the set S. Thus we obtained a minimum paired dominating set. □

5. $TUC_4C_8(p, q)$ nanotube

The nanotube $TUC_4C_8(p, q)$ [12] is a trivalent decoration made by alternating squares C_4 and octagons C_8 as shown in Fig. 4. In this section let q, an even number, represent the number of rows as shown in Fig. 4. Let p represent the number of squares induced by row i and row $i+1$, i odd, $1 \leq i \leq q-1$. We describe the edges of the nanotube as follows to find perfect matchings in the nanotube:

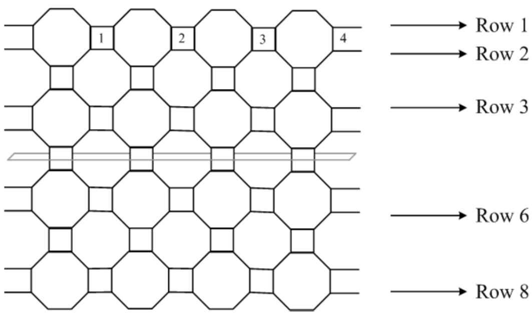

Figure 4. $TUC_4C_8(4, 8)$ **nanotube**

Consider a plane which cuts nanotube horizontally as shown in Fig. 4. Edges of nanotube parallel to the plane are called horizontal edges, those edges perpendicular to the plane are called vertical edges, those edges that make an acute angle with the plane are called acute edges and those that make an obtuse angle with the plane are called obtuse edges. See Fig. 4. We note that every vertical edge of an octagon merges with the vertical edge of a square. On the other hand every horizontal edge of an octagon not lying on the first row or the last row merges with a horizontal edge of a square.

Theorem 5.1. *Let G be the $TUC_4C_8(p, q)$ nanotube, $p \equiv 0 \mod 6$. Then $\gamma_{pr}(G) = \frac{4pq}{3}$.*

Proof. Select the horizontal edges of the square in row i, $i \equiv 0, 1 \mod 6$ and select the horiontal edges of the octagon in the row i, $i \equiv 3, 4 \mod 6$. These horizontal edges are independent. The end vertices of the horizontal edges of the square will dominate three vertices namely one vertex from the octagon and two vertices from the vertices induced by octagon and square. Similarly the end vertices of the horizontal edges of the octagon will dominate three vertices. For any edge (u, v) the end vertices of the neighboring edges are not selected. See Fig. 5.

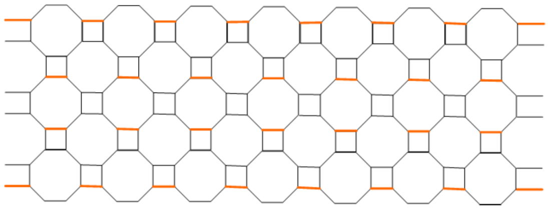

Figure 5. $TUC_4C_8(7, 6)$ **nanotube**

In each selected row, 2p edges are selected and for every 6 rows 4 rows are selected. Thus $\gamma_{pr}(G) = \frac{4pq}{3}$. □

6. Conclusion

In this paper we determine the paired domination for V-phenylenic nanotubes, $TUC_4C_8(S)$ nanotubes and H-Naphtalenic Nanotorus. It would be an interesting line of research to determine the paired domination for other nanotubes.

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