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Enumerating independent vertex sets in grid graphs

Seungsang Oh [a,*,1], Sangyop Lee [b,c,2]

[a] Department of Mathematics, Korea University, Seoul 02841, Republic of Korea
[b] Department of Mathematics, Chung-Ang University, Seoul 06974, Republic of Korea
[c] Korea Institute for Advanced Study, Seoul 02455, Republic of Korea

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ABSTRACT

A set of vertices in a graph is called independent if no two vertices of the set are connected by an edge. In this paper we use the state matrix recursion algorithm, developed by Oh, to enumerate independent vertex sets in a grid graph and even further to provide the generating function with respect to the number of vertices. We also enumerate bipartite independent vertex sets in a grid graph. The asymptotic behavior of their growth rates is presented.

1. Introduction

The Merrifield–Simmons index and the Hosoya index of a graph, respectively introduced by Merrifield and Simmons [11–13] and by Hosoya [8], are two prominent examples

* Corresponding author.
E-mail addresses: seungsang@korea.ac.kr (S. Oh), sylee@cau.ac.kr (S. Lee).

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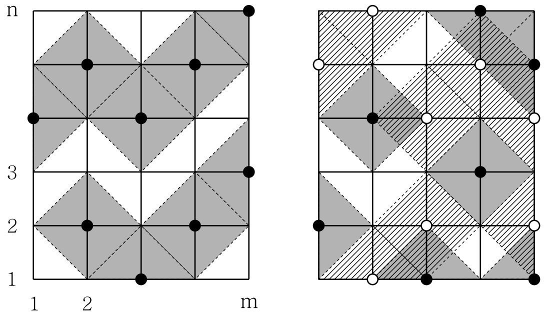

Fig. 1. Independent and bipartite independent vertex sets.

of topological indices for the study of the relation between molecular structure and physical/chemical properties of certain hydrocarbon compound, such as the correlation with boiling points [5]. An *independent* set of vertices/edges of a graph G is a set of which no two vertices of the set are connected by a single edge. The Merrifield–Simmons index is defined as the total number, denoted by $\sigma(G)$, of independent vertex sets, while the Hosoya index is defined as the total number of independent edge sets. Especially, finding the Merrifield–Simmons index of graphs is known as the Hard Square Problem in lattice statistics.

One of important problems is to determine the extremal graphs with respect to these two indices within certain prescribed classes. For example, among trees with the same number of vertices, Prodinger and Tichy [17] proved that the star maximizes the Merrifield–Simmons index, while the path minimizes it. The situation for the Hosoya index is absolutely opposite; the star minimizes the Hosoya index, while the path maximizes it [5]. A good summary of results for extremal graphs of various types can be found in a survey paper [18]. The interested reader is referred, however, to other articles [1,2,6,20–22] that treat several classes of graphs such as fullerene graphs, trees with prescribed degree sequence, graphs with connectivity at most k and the generalized Aztec diamonds.

We also consider a bipartite vertex set $\mathcal{V}$ in a graph G in which some vertices of $\mathcal{V}$ are colored black and the others are white. We say that $\mathcal{V}$ is a *bipartite independent vertex set* if the vertices of the same color are independent (vertices with different colors may not be independent). The total number of bipartite independent vertex sets in G will be called the bipartite Merrifield–Simmons index and denoted by $\beta(G)$. See the drawings in Fig. 1 for examples.

Recently several important enumeration problems on two-dimensional square lattice models have been solved by means of the *state matrix recursion algorithm*, developed by Oh in [14]. This algorithm provides recursive matrix-relations to enumerate monomer and dimer coverings [14], multiple self-avoiding walks and polygons [15], and knot mosaics in quantum knot mosaic theory [16]. Furthermore, these recursive formulae also produce their generating functions. Based upon these results, this algorithm shows considerable promise for further two-dimensional lattice model enumerations.