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Some new characterizations of Hamiltonian cycles in triangular grid graphs

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ABSTRACT

In the studies that have been devoted to the protein folding problem, which is one of the great unsolved problems of science, some specific graphs, like the so-called triangular grid graphs, have been used as a simplified lattice model. Generation and enumeration of Hamiltonian paths and Hamiltonian circuits (compact conformations of a chain) are needed to investigate the thermodynamics of protein folding. In this paper, we present new characterizations of the Hamiltonian cycles in labeled triangular grid graphs, which are graphs constructed from rectangular grids by adding a diagonal to each cell. By using these characterizations and implementing the computational method outlined here, we confirm the existing data, and obtain some new results that have not been published. A new interpretation of Catalan numbers is also included.

1. Introduction

A Hamiltonian cycle in a graph G is a cycle that visits each vertex of G exactly once. In polymer science, the study of Hamiltonian paths (compact conformations of a chain) has been advocated as a first approximation for understanding qualitatively the excluded-volume mechanisms at work behind protein folding. Hamiltonian cycles are a mathematical idealization of polymer melts, too. In addition, the number of Hamiltonian cycles on a graph corresponds to the entropy of a polymer system [8]. The entropy per site is

$$\frac{S}{N} = \frac{1}{N} \ln C_{N,P},$$

where $C_{N,P}$ is the number of Hamiltonian circuits in a N-point lattice with periphery P. For example, the graph we study in this paper has $N = (n+1)\cdot(m+1)$ vertices, if $C_{N,P} \sim a_m \theta_m^n$ for some positive real numbers a_m and θ_m, where θ_m denotes the largest eigenvalue of the adjacency matrix for a certain multidigraph that will be introduced later, then the entropy per site is

$$\lim_{n\to\infty} \frac{\ln C_{N,P}}{(n+1)(m+1)} = \ln \sqrt[m+1]{\theta_m}.$$

For the application of Hamiltonian chains we refer the reader to [1,4,20] and the references therein.

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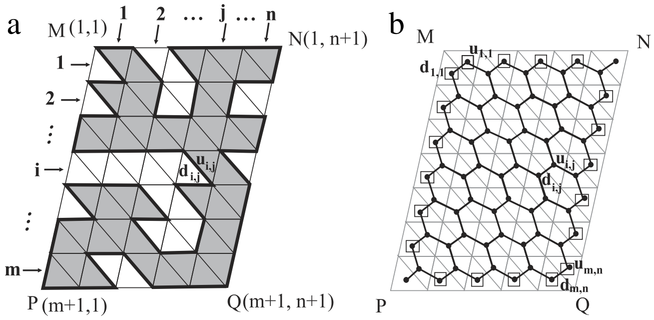

Fig. 1. A Hamiltonian graph on $T_{7,5}$ and its dual graph $W_{7,5}$.

Enumeration of Hamiltonian cycles and related problems in rectangular grids had been extensively studied. See, for examples, [2,4–6,11–14,17–19,25,26]. A common thread among these papers is the introduction of an encoding method, and the use of a transfer matrix (with the exception in [2,17]) to study the transition between the underlying structures within the Hamiltonian cycles. See [7,22] for more applications of transfer matrices in enumerative combinatorics.

Construct a graph from a rectangular grid graph by adding a diagonal in each square (or cell) within the graph. Although we could have named such a graph a triangulated rectangular grid, we follow [14,20] to call it a ***triangular grid graph***. In this paper, we study the generation and enumeration of Hamiltonian cycles in a triangular grid graph. The results in [14,20] were obtained by encoding the vertices. We are guided by the principle that solving problems in a new way is very desirable because, not only could it verify existing results obtained by other methods, but a new approach may lead to properties that are interesting from a mathematical standpoint, although they may still be unexplained from the chemical perspective.

Here is an illustration of our viewpoint. In [3] we posed a conjecture that, for each fixed m, the numbers of contractible (as Jordan curves) and non-contractible Hamiltonian cycles on the cylinder grid graph $C_m \times P_n$ behave the same way asymptotically as n grows. This conjecture is supported by the exact enumeration up to $m = 10$. This property of the cylinder grid graph could not have been discovered by coding the vertices of the graph, but instead by coding the squares of the grid.

We shall propose two methods to encode the triangles within the triangular grid graph $T_{m,n}$ in a rather natural way. By studying the possible connection between consecutive columns within a Hamiltonian cycle, we are able to obtain, for fixed m, the generating function of the number of Hamiltonian cycles in $T_{m,n}$ for $n \geq 1$. As m grows, it is natural for the generating functions to become lengthy and awkward. Nevertheless, a generating function provides a compact formula to record, in an indirect way, the *entire* sequence under consideration. It also allows us to analyze the asymptotic behavior of the sequence. Consequently, generating functions are more desirable than merely listing a finite number of entries within the sequence.

The algorithm presented in this article does not aspire to being the best algorithm for enumerating Hamiltonian cycles on the triangular grid graph, in terms of computational efficiency or implementation. Those who are interested in better efficiency for solving this problem could consult [14]. Our main goal is to solve this enumeration problem on a relatively simple triangular grid graph, and use it as our first step towards more complicated triangular grid graphs. We aim at discovering properties of these graphs like the one mentioned above of the cylinder grid graph.

2. Preliminaries

Start with a rectangular grid $P_{m+1} \times P_{n+1}$. It has mn cells. Label its vertices (i, j), where $1 \leq i \leq m+1$, and $1 \leq j \leq n+1$. Call the four corners $(1, 1)$, $(1, n+1)$, $(m+1, 1)$, and $(m+1, n+1)$ the vertices M, N, P and Q respectively. Construct the triangular grid $T_{m,n}$ by adding diagonals that join (i, j) to $(i+1, j+1)$, whenever $i \leq m$ and $j \leq n$. Each diagonal divides a square cell into two triangular cells $u_{i,j}$ and $d_{i,j}$ (for "up" and "down"), above and below the diagonal respectively. See Fig. 1a. We call them ***windows*** of the triangular grid, and write $w_{i,j}$ if we are not concerned with its position (hence, $w_{i,j}$ could be either an up window or a down window). In this way, instead of m windows in each column of the rectangular grid $P_{m+1} \times P_{n+1}$, we obtain $2m$ windows in each column of $T_{m,n}$. We note that authors of [14] used $T_{n+1,m+1}$ to denote the same graph.

Observe that any Hamiltonian cycle encircles a connected region consisting of adjacent windows. This prompts us to study the dual of $T_{m,n}$. The dual graph $W_{m,n}$ comprised of vertices corresponding to the windows of $T_{m,n}$, and two vertices in the dual are adjacent if the corresponding windows in $T_{m,n}$ share a common edge. The dual graph $W_{7,5}$ of the triangular grid $T_{7,5}$ is displayed in Fig. 1b. For the sake of clarity, the vertices in $W_{m,n}$ are also labeled as $u_{i,j}$ and $d_{i,j}$, and, in general, $w_{i,j}$ if we disregard its position. The interior windows enclosed by a Hamiltonian cycle on $T_{m,n}$ yield a tree in $W_{m,n}$, but the exterior windows produce a forest in $W_{m,n}$.

To facilitate our discussion, we define R as the set of windows (called ***roots***) in $T_{m,n}$ with exactly one edge on the boundary of the rectangular grid:

$$R = \{d_{i,1} \mid 1 \leq i < m\} \cup \{u_{1,j} \mid 1 \leq j < n\} \cup \{d_{m,j} \mid 1 < j \leq n\} \cup \{u_{i,n} \mid 1 < i \leq m\}.$$

The vertices in $W_{7,5}$ that represent the roots of $T_{7,5}$ are marked with squares in Fig. 1b. Notice that these are the vertices with degree 2 in $W_{m,n}$.