EPJ Web of Conferences **173**, 02016 (2018) https://doi.org/10.1051/epjconf/201817302016
Mathematical Modeling and Computational Physics 2017

Near-Perfect Matchings on Cylinders $C_m \times P_n$ of Odd Order

Sergey N. Perepechko[1,⋆]

[1] *Petrozavodsk State University, Russia*

Abstract. A close relationship was established between the number of perfect and near-perfect matchings on cylinders $C_m \times P_n$. Generating functions are obtained for the number of near-perfect matchings in these graphs for fixed odd $m \leqslant 13$. A conjecture is put forth on the properties of the denominators of generating functions for arbitrary odd m.

1 Introduction

One of the classical lattice models of statistical mechanics is the dimer problem. In this model, the rigid dimers (diatomic molecules) are treated as the edges of a graph together with the vertices incident to it. Each lattice node cannot be occupied by more than one atom, so the edges must be non-adjacent.

In the dimer model, close-packed lattice coverings containing the maximum possible number of dimers are studied. The combinatorial interpretation of the model leads to the need to enumerate the maximum matchings in certain set of lattice graphs.

For many kinds of lattices of even order, used in applications, the maximum matchings are perfect matchings. Near-perfect matchings are a natural analogue of perfect matchings in graphs of odd order. A near-perfect matching is one in which exactly one vertex is unmatched. A vertex of the graph, which is not saturated by a matching, will be called *vacancy*.

A significant part of the work related to the enumeration of matchings deals with perfect matchings. At the same time, the quantitative characteristics of other kinds of matchings require further study. In this paper cylinders $C_m \times P_n$ are considered when both parameters m and n are odd. Among the works of the past years devoted to the study of such graphs, the paper [1] is of the greatest interest. This paper gives a closed-form expression for the number of near-perfect matchings when the vacancy is on the boundary of a cylinder. In [2] Kong briefly mentions the results of numerical calculations on cylinders for a fixed value of the parameter m. The author reports about the similarity of asymptotic expansions for the total number of near-perfect matching on cylinders and rectangular lattices $P_m \times P_n$, while omitting the details of the computations.

In our work we use a universal method for enumerating matchings. This allows us to avoid many of the restrictions inherent to the Pfaffian technique, and to study in detail the dependence of the number of near-perfect matchings on the vacancy location. The results of investigation clearly demonstrate that parity considerations are just as important for solving this problem as for counting perfect matchings.

Extending the results of numerical calculations by Kong, we reveal a deep connection between the number of near-perfect and perfect matchings on the cylinder with the same value of m. In fact, for

⋆e-mail: persn@newmail.ru

fixed m and changing n, the number of near-perfect matchings and the number of perfect matchings are solutions of the same recurrence relation if the vacancy location does not change. Based on this result, we can conjecture the form of the denominator of the generating function for the total number of near-perfect matchings on the cylinder for any odd m.

2 Basic notation

Consider the graph $G_{m,n} = C_m \times P_n$. This graph can be viewed as n copies of C_m placed sequentially with edges joining the corresponding vertices of C_m. We number all the cycles C_m by integers from 1 to n. The ordinal number put in parentheses will be indicated as superscript as shown at the left of Figure 1. The union of graphs $\cup_{k=1}^{n} C_m^{(k)}$ forms a spanning subgraph of $G_{m,n}$.

Let $\mathcal{V}$ be the set of vertices of $G_{m,n}$ and $K_m^{v}(n)$, $(v \in \mathcal{V})$ – the number of near-perfect matchings on the cylinder when the vacancy is fixed at the node v. We denote by $\mathcal{V}_k$ the set of vertices of the cycle $C_m^{(k)}$. Consider two graphs $G_{m,n} - v'_k$ and $G_{m,n} - v''_k$, where $v'_k, v''_k \in \mathcal{V}_k$, $v'_k \neq v''_k$. Since these graphs are isomorphic, then $K_m^{v'_k}(n) = K_m^{v''_k}(n)$. Let's introduce the notation $\hat{K}_m^{(k)}(n) = K_m^{v_k}(n)$, $(v_k \in \mathcal{V}_k)$. The set of values of $\hat{K}_m^{(k)}(n)$, $(k = 1, 2, \ldots, n)$ will be called the profile of near-perfect matchings on cylinder $G_{m,n}$. This function satisfies the simple symmetry relation $\hat{K}_m^{(k)}(n) = \hat{K}_m^{(n+1-k)}(n)$, $(k = 1, 2, \ldots, \lfloor n/2 \rfloor)$.

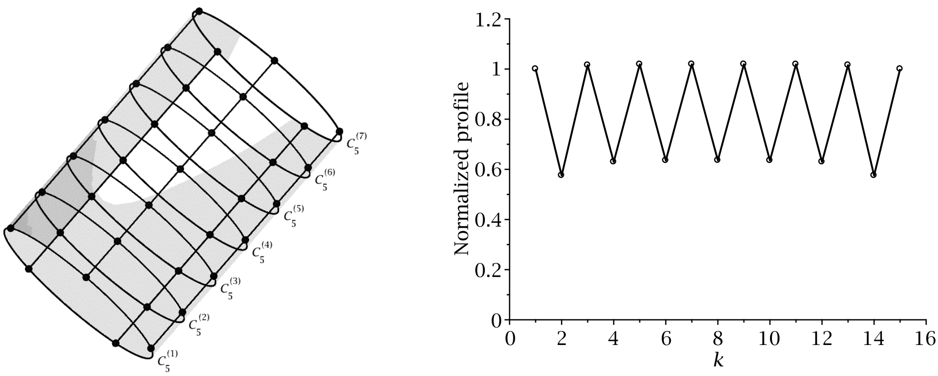

Figure 1. Cylinder $C_5 \times P_7$ and normalized profile of near-perfect matchings on $C_5 \times P_{15}$

The exponential dependence of the number of near-perfect matchings on both parameters of the graph makes it difficult to compare different profiles. It is convenient to introduce *normalized* profiles by dividing all $\hat{K}_m^{(k)}(n)$ by $\hat{K}_m^{(1)}(n)$. An example of such a profile for a small cylinder is shown at the right in Figure 1. The main advantage of the normalized profiles is their weak dependence on the parameters m and n.

For the existence of a near-perfect matching in the graph, its order must be odd, so in the future the parameter m will always be considered odd. The different kinds of maximum matchings discussed in this paper will be distinguished by superscripts as follows:

B – vacancy occurs at the boundary,
$\hat{K}_m^{B}(n) = \hat{K}_m^{(1)}(2n+1)$ – the number of near-perfect matchings on $G_{m,2n+1}$ graph with one fixed vacant node on the boundary. $G_m^{B}(z) = \sum_{n=0}^{\infty} \hat{K}_m^{B}(n)\, z^n$ – generating function for the sequence $\{\hat{K}_m^{B}(n)\}$.

P – perfect matchings,
$K_m^{P}(n)$ – the number of perfect matchings on the $G_{m,2n}$ graph. $G_m^{P}(z) = \sum_{n=0}^{\infty} K_m^{P}(n)\, z^n$ – generating function for the sequence $\{K_m^{P}(n)\}$.

N – near-perfect matchings,
$\hat{K}_m^N(n) = m \cdot \sum_{k=1}^{2n+1} \hat{K}_m^{(k)}(2n+1)$ – the total number of near-perfect matchings on $G_{m,2n+1}$ graph.
$G_m^N(z) = \sum_{n=0}^{\infty} \hat{K}_m^N(n)\, z^n$ – generating function for the sequence $\{\hat{K}_m^N(n)\}$.

3 Counting matchings

The method proposed by Wilf was used to count matchings [3]. This method allows us to reduce the problem of counting perfect matchings in a graph of order n to evaluating the coefficients of a certain polynomial in n variables. It is attractive due to its universality and ease of implementation in computer algebra systems. In our implementation of the algorithm we used a 64-bit version of Maple 17. Due to the extensive set of library functions built into this CAS, the program code turned out to be very compact.

To generate the graphs studied, the `GraphTheory` package was used. The same package was used to perform all operations on graphs. Calling routine `CartesianProduct(PathGraph(n), CycleGraph(m))` with odd m and n created a cylinder of odd order. To calculate the profile of near-perfect matchings, one vertex belonging to the cycle $C_m^{(k)}$ was selected for each value of k from 1 to $\lceil n/2 \rceil$. This vertex, together with the edges incident to it, was removed from the cylinder. Then, to evaluate $\hat{K}_m^{(k)}(n)$, the algorithm by Wilf was applied to the resulting even-order graph. The second half of the profile was reconstructed on the basis of symmetry considerations. To accelerate the computations, the values of $\hat{K}_m^{(k)}(n)$ for different k were calculated in parallel. To do this, the tools of the `Threads` package were used.

After calculating the profile of near-perfect matchings on the graph $G_{m,n}$, we can find the value of $\hat{K}_m^N(\lfloor n/2 \rfloor)$, which was of primary interest in the paper by Kong. Then the parameter n was increased by 2 and all calculations were repeated on the graph $G_{m,n+2}$. Multiple repetition of the calculations made it possible to obtain initial segments of the sequences $\{\hat{K}_m^{(k)}(n)\}$ and $\{\hat{K}_m^N(n)\}$. In those cases when these segments turned out to be sufficiently long, it was possible to derive recurrence relations. For example, the sequence $\{\hat{K}_3^B(n)\}$ satisfies a second-order relation $\hat{K}_3^B(n+1) = 5\hat{K}_3^B(n) - \hat{K}_3^B(n-1)$. However, $\{K_3^P(n)\}$ also satisfies the same recurrence relation, which indicates close connections between perfect and near-perfect matchings.

For Cartesian product graphs and fixed values of m, the method by Wilf has properties which are typical for algorithms from the complexity class **FPT**. The resources required to compute $\hat{K}_m^{(k)}(n)$ depend exponentially on m and are polynomial in n. In turn, the upper bound of the order of the recurrence relations satisfied by the sequence $\{K_m^P(n)\}$ is equal to $2^{\lfloor m/2 \rfloor}$, and this boundary as a rule is achieved [4]. To derive such relation, the initial segment must contain more than $2^{\lfloor m/2 \rfloor + 1}$ elements. Under such circumstances, obtaining analytical expressions is possible only for small m. At moderate values of m, we must limit ourselves to the numerical values of the number of near-perfect matchings.

All calculations were carried out on a personal computer with an Intel Core i7-980 3.33 GHz processor and 24 GB RAM. The computer was running a 64-bit version of Windows 7. Calculations were performed in the 64-bit version of Maple 17. Available facilities make it possible to find linear recurrence relations and generating functions $G_m^B(z), G_m^N(z)$ on cylinders for $m \leqslant 13$. Profiles of near-perfect matchings were evaluated on $G_{m,n}$ graphs for $15 \leqslant m \leqslant 19$ and $n \leqslant n^*$, where $n^* = 135$ for $m = 15, 17$, and $n^* = 85$ for $m = 19$.

4 Main results

In this section, we will discuss, on simple examples, those properties of near-perfect matchings that hold for all the studied values of m. The generating functions $G_m^P(z)$ will be considered known, since they were found in [4] for $m \leqslant 30$.

Let's compare $G_m^B(z)$ and $G_m^P(z)$ for the simplest case $m = 3$

$$G_3^B(z) = \frac{1}{1-5\,z+z^2}, \qquad G_3^P(z) = \frac{1-z}{1-5\,z+z^2}.$$

The equality of the denominators $G_3^B(z)$ and $G_3^P(z)$ means that $\hat{K}_3^B(n)$ can be represented as a linear combination of $K_3^P(n)$. This property makes it much easier to obtain the asymptotic behavior of $\hat{K}_3^B(n)$ for large n

$$\hat{K}_3^B(n) = \frac{1}{3}\left(K_3^P(n+1) - K_3^P(n)\right), \qquad \lim_{n\to\infty} \hat{K}_3^B(n)/K_3^P(n) = \frac{\sqrt{3}+\sqrt{7}}{2\sqrt{3}}.$$

The quantity on the right-hand side of the last equality is closely related to the asymptotics of the number of perfect matchings in $G_{3,2n}$ graphs. This suggests that, for other odd m, the values of $\hat{K}_m^B(n)$ and $K_m^P(n)$ can also be calculated from the same formulas. As a result of simplifying expression (2) of [1], we conclude that to evaluate the $\hat{K}_m^B(n)$, we can substitute the odd values m and n in the formula (2) from [4], and then divide the obtained value by $\sqrt{m}$.

To compare with the results of Kong's numerical computations, it is necessary to clarify the properties of the functions $G_m^N(z)$. Their most important feature is that the denominators of $G_m^N(z)$ are the squares of the denominators of $G_m^P(z)$. In this case, as shown below, $\hat{K}_m^N(n)$ is also a linear combination of $K_m^P(n)$, but with coefficients linearly dependent on n

$$G_3^N(z) = 3\frac{1+2\,z-z^2}{(1-5\,z+z^2)^2}, \qquad \hat{K}_3^N(n) = \frac{27n+17}{21}K_3^P(n+1) - \frac{15n+5}{21}K_3^P(n).$$

For small m, we can even write out an explicit expression directly through the parameters of the graph

$$\hat{K}_3^N(n) = \frac{1}{7}\left((2+\sqrt{21})n + 2 + \frac{11}{\sqrt{21}}\right)\left(\frac{\sqrt{7}+\sqrt{3}}{2}\right)^{2n+2} + \frac{1}{7}\left((2-\sqrt{21})n + 2 - \frac{11}{\sqrt{21}}\right)\left(\frac{\sqrt{7}-\sqrt{3}}{2}\right)^{2n+2}.$$

An immediate consequence of the above formula is that the asymptotic expansions of the free energy per lattice site contain logarithmic corrections for any odd m.

With increasing m, the expressions for $G_m^N(z)$ become more complicated, but all the regularities formulated in this section remain valid. For example, for $m = 5$, the denominator of $G_5^N(z)$ is also the square of the denominator of $G_5^P(z)$

$$G_5^P(z) = \frac{(1-z)(1-7z+z^2)}{1-19z+41z^2-19z^3+z^4}, \qquad G_5^N(z) = 5\frac{1+10z-56z^2+84z^3-24z^4-10z^5+z^6}{(1-19z+41z^2-19z^3+z^4)^2}.$$

We have no reason to doubt the correctness of this property for *all* odd m. However, since verification was performed in a limited range of m, it has to be considered as a conjecture.

Conjecture. For *all* odd values of m the denominator of $G_m^N(z)$ is always the square of the denominator of $G_m^P(z)$.

In conclusion, it should be noted that numerous data that have been omitted due to a lack of space can be obtained from the author on request.

References

[1] F.Y. Wu, W.-J. Tzeng, and N. Sh. Izmailian, Physical Review **E83**, 011106 (2011)
[2] Y. Kong, Physical Review **E74**, 011102 (2006)
[3] H.S. Wilf, Journal of Combinatorial Theory **4**, 246 (1968)
[4] A.M. Karavaev and S.N. Perepechko, Matematicheskoe Modelirovanie **26**:11, 18 (2014)