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Note

The Merrifield-Simmons conjecture also holds for parity graphs

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Abstract The Merrifield-Simmons conjecture states a relation between the distance of vertices in a simple graph G and the number of independent sets, denoted as $\sigma(G)$, in vertex-deleted subgraphs. Namely, that the sign of the term $\sigma(G_{-u})\,\sigma(G_{-v}) - \sigma(G)\,\sigma(G_{-u-v})$ only depends on the parity of the distance of u and v in G. We prove this statement in the case of parity graphs, a generalization of bipartite graphs where for any two vertices u and v the lengths of all induced $u-v$-paths have to have the same parity. Additionally we give some evidence that this result may not be further generalized to other classes of graphs.

Keywords Independent sets; Merrifield-Simmons conjecture
AMS subject classifications 05C69

1 Introduction

Let $G = (V,E)$ be a simple graph and $\sigma(G)$ the number of independent (vertex) sets of G, that is the number of vertex subsets $W \subseteq V$ such that no two vertices of W are adjacent [5, 6]. In chemistry this number is also known as the Merrifield-Simmons index. For two

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vertices $u, v \in V$, the term $\Delta(G,u,v)$ is defined as

$$\Delta(G,u,v) = \sigma(G_{-u})\,\sigma(G_{-v}) - \sigma(G)\,\sigma(G_{-u-v}), \tag{1}$$

where G_{-w} is the graph with the vertex w and its incident edges removed. The *Merrifield-Simmons conjecture* (MSC) states that $\operatorname{sgn}(\Delta(G,u,v))$, the sign of $\Delta(G,u,v)$, only depends on the distance between the vertices u and v in G, denoted by $d(G,u,v)$.

Conjecture 1 (Merrifield-Simmons conjecture, MSC) *Let $G = (V,E)$ be a simple (bipartite) graph and $u, v \in V$ two vertices. Then*

$$\operatorname{sgn}(\Delta(G,u,v)) = (-1)^{d(G,u,v)+1}. \tag{2}$$

Merrifield and Simmons [6, page 144] noted the statement above as a property (without proof), but did not mention the class of graphs they were considering. Gutman [2] mentioned some counterexamples for arbitrary simple graphs and explicitly restated the conjecture for bipartite graphs. He also confirmed the statement for trees [3]. The present author proved the MSC in the case of bipartite graphs [10]. For more previous results see [2, 3, 4, 9, 10, 11].

This paper aims to show that the MSC also holds for parity graphs, a proper superclass of bipartite graphs – for example odd cycles of length 5 with two (crossing) chords can be subgraphs – but not for any of its familiar superclasses. To prove the MSC for parity graphs we basically go along the same line of arguments as in the bipartite case, however in a clarified and generalized version. Thus, in Section 2 we introduce generalizations of the terms used in the MSC to vertex subsets and some properties of them, on which the main theorem given in Section 3 is based. In Section 4 we conclude by presenting counterexamples which give some evidence that the result cannot be further generalized. In the remainder of this section we provide the necessary notation for graphs and the applied properties for the number of independent sets.

For a simple graph $G = (V,E)$ with a vertex $v \in V$ and a vertex subset $W \subseteq V$ we use the following notations: G_{-W} denotes the graph G where all vertices $v \in W$ are deleted, that is, these vertices and their incident edges are removed. The open neighborhood of W is denoted by $N_G(W)$, that is, the set of all vertices adjacent to a vertex $v \in W$. If $W = \{v\}$ then we write G_{-v} and $N_G(v)$ instead of $G_{-\{v\}}$ and $N_G(\{v\})$, respectively. $G_1 \mathbin{\dot\cup} G_2$ is the disjoint union of the graphs G_1 and G_2, that is, the union of disjoint copies of both graphs. For all other notations we refer to [1].

For the number of independent sets $\sigma(G)$ we use the following basic properties: First, it is multiplicative in components, that is

$$\sigma(G_1 \mathbin{\dot\cup} G_2) = \sigma(G_1)\,\sigma(G_2). \tag{3}$$

Second, it satisfies for each vertex $v \in V$ the recurrence relation

$$\sigma(G) = \sigma(G_{-v}) + \sigma(G_{-v-N_G(v)}). \tag{4}$$

Finally, this recurrence relation can be generalized to a vertex subset U via induction on the cardinality of U:

Theorem 2† *Let $G = (V,E)$ be a simple graph and $U \subseteq V$ a vertex subset. Then*

$$\sigma(G) = \sum_{\substack{W \subseteq U \\ W \text{ is independent in } G}} \sigma(G_{-U-N_G(W)}). \tag{5}$$

2 A generalization for vertex subsets

In the following, a generalization of $\Delta(G,u,v)$ is considered where vertex subsets instead of vertices are deleted.

Definition 3 Let $G = (V,E)$ be a simple graph and $A, B \subseteq V$ two vertex subsets. Then $\Delta(G,A,B)$ is defined as

$$\Delta(G,A,B) = \sigma(G_{-A})\,\sigma(G_{-B}) - \sigma(G)\,\sigma(G_{-A-B}). \tag{6}$$

This generalization has the advantage that a recurrence relation for $\Delta(G,A,B)$ can be derived which enables us to state the term for G as a sum over terms for proper subgraphs of G. In fact, in the case of bipartite graphs [10] this recurrence relation (and Proposition 6 as well) are "hidden" in the proof, here we state them explicitly.

Lemma 4 *Let $G = (V,E)$ be a simple graph and $A, B \subseteq V$ two disjoint vertex subsets. Then*

$$\Delta(G,A,B) = -\sum_{\substack{W \subseteq A \\ W \text{ is independent in } G}} \Delta(G_{-A}, N_G(W), B). \tag{7}$$

Proof. Applying the recurrence relation for vertex subsets (Theorem 2) we obtain

$$\begin{aligned}
\Delta(G,A,B) &= \sigma(G_{-A})\,\sigma(G_{-B}) - \sigma(G)\,\sigma(G_{-A-B}) \\
&= \sigma(G_{-A}) \sum_{\text{ind. } W \subseteq A} \sigma(G_{-B-A-N_{G_{-B}}(W)}) - \sum_{\text{ind. } W \subseteq A} \sigma(G_{-A-N_G(W)})\,\sigma(G_{-A-B}) \\
&= \sum_{\text{ind. } W \subseteq A} \left[\sigma(G_{-A})\,\sigma(G_{-B-A-N_{G_{-B}}(W)}) - \sigma(G_{-A-N_G(W)})\,\sigma(G_{-A-B})\right].
\end{aligned}$$

† In [10] the present author mentioned this theorem as Theorem 2, but gave a misleading reference. For a proof see Theorem 2 in [8].

As A and B are disjoint, for all $W \subseteq A$ we have $B \cup N_{G_{-B}}(W) = B \cup N_G(W)$ and consequently $G_{-B-A-N_{G_{-B}}(W)} = G_{-B-A-N_G(W)}$. Applying this, the statement follows:

$$\begin{aligned}\Delta(G,A,B) &= \sum_{\text{ind. } W\subseteq A} \left[\sigma(G_{-A})\,\sigma(G_{-B-A-N_G(W)}) - \sigma(G_{-A-N_G(W)})\,\sigma(G_{-A-B})\right] \\ &= -\sum_{\text{ind. } W\subseteq A} \left[\sigma(G_{-A-N_G(W)})\,\sigma(G_{-A-B}) - \sigma(G_{-A})\,\sigma(G_{-A-N_G(W)-B})\right] \\ &= -\sum_{\text{ind. } W\subseteq A} \Delta(G_{-A}, N_G(W), B).\end{aligned}$$

□

Let G^A, G^B, G^{AB} and G^* denote the unions of those connected components of G including vertices from A, from B, from A and B, and from neither of both, respectively. If there are no connected components which include vertices from both vertex subsets A and B, that means $G = G^A \mathbin{\dot\cup} G^B \mathbin{\dot\cup} G^*$ and $G^{AB} = \emptyset$, then the terms in $\Delta(G,A,B)$ cancel each other.

Proposition 5 (Corollary 5 in [10]) *Let $G = (V,E)$ be a simple graph and $A,B \subseteq V$ two vertex subsets, such that $G = G^A \mathbin{\dot\cup} G^B \mathbin{\dot\cup} G^*$. Then*

$$\Delta(G,A,B) = 0. \tag{8}$$

Proof. The vertices of A and B can only be deleted in G^A and G^B, respectively. Thus, the statement follows via

$$\begin{aligned}\Delta(G,A,B) &= \sigma(G_{-A})\,\sigma(G_{-B}) - \sigma(G)\,\sigma(G_{-A-B}) \\ &= \sigma((G^A \mathbin{\dot\cup} G^B \mathbin{\dot\cup} G^*)_{-A})\,\sigma((G^A \mathbin{\dot\cup} G^B \mathbin{\dot\cup} G^*)_{-B}) \\ &\quad - \sigma(G^A \mathbin{\dot\cup} G^B \mathbin{\dot\cup} G^*)\,\sigma((G^A \mathbin{\dot\cup} G^B \mathbin{\dot\cup} G^*)_{-A-B}) \\ &= \sigma(G^A_{-A} \mathbin{\dot\cup} G^B \mathbin{\dot\cup} G^*)\,\sigma(G^A \mathbin{\dot\cup} G^B_{-B} \mathbin{\dot\cup} G^*) \\ &\quad - \sigma(G^A \mathbin{\dot\cup} G^B \mathbin{\dot\cup} G^*)\,\sigma(G^A_{-A} \mathbin{\dot\cup} G^B_{-B} \mathbin{\dot\cup} G^*) \\ &= \sigma(G^A_{-A})\,\sigma(G^B)\,\sigma(G^*)\,\sigma(G^A)\,\sigma(G^B_{-B})\,\sigma(G^*) \\ &\quad - \sigma(G^A)\,\sigma(G^B)\,\sigma(G^*)\,\sigma(G^A_{-A})\,\sigma(G^B_{-B})\,\sigma(G^*) \\ &= 0.\end{aligned}$$

□

Proposition 6 *Let $G = (V,E)$ be a simple graph and $A,B \subseteq V$ two vertex subsets, such that $A \cap B = C \neq \emptyset$. Then*

$$\Delta(G,A,B) < \Delta(G_{-C}, A \setminus C, B \setminus C). \tag{9}$$

Proof. The statement follows by applying the recurrence relation for vertex subsets (Theorem 2):

$$\begin{aligned}
\Delta(G,A,B) &= \sigma(G_{-A})\,\sigma(G_{-B}) - \sigma(G)\,\sigma(G_{-A-B}) \\
&= \sigma(G_{-A})\,\sigma(G_{-B}) - \sum_{\text{ind. } W\subseteq C} \sigma(G_{-C-N_G(W)})\,\sigma(G_{-A-B}) \\
&= \sigma(G_{-A})\,\sigma(G_{-B}) - \sigma(G_{-C})\,\sigma(G_{-A-B}) \\
&\quad - \sum_{\text{ind. } \emptyset\neq W\subseteq C} \sigma(G_{-C-N_G(W)})\,\sigma(G_{-A-B}) \\
&< \sigma(G_{-A})\,\sigma(G_{-B}) - \sigma(G_{-C})\,\sigma(G_{-A-B}) \\
&= \sigma(G_{-C-(A\setminus C)})\,\sigma(G_{-C-(B\setminus C)}) - \sigma(G_{-C})\,\sigma(G_{-C-(A\setminus C)-(B\setminus C)}) \\
&= \Delta(G_{-C}, A\setminus C, B\setminus C).
\end{aligned}$$

□

In order to generalize the notion of distance between a pair of vertices to distance between two vertex subsets, the set of chord-free paths connecting vertices of the two vertex subsets is considered.

Definition 7 Let $G=(V,E)$ be a graph and $A,B\subseteq V$ two vertex subsets. A path $P=(v_1,\ldots,v_k)$ of G is an *induced $A-B$-path*, if $V(P)\cap A=\{v_1\}$ and $V(P)\cap B=\{v_k\}$, where $V(P)$ is the set of vertices of P, and $\{v_i,v_j\}\in E \Longleftrightarrow |i-j|=1$. By $P_i(G,A,B)$ we denote the *set of all induced $A-B$-paths* in G. The *length* of an induced $A-B$-path P is the number of edges in P, that means $|V(P)|-1$.

Definition 8 Let $G=(V,E)$ be a graph and $A,B\subseteq V$ two disjoint vertex subsets. We say $P_i(G,A,B)$ is *even* (*odd*) if the length of each path $P\in P_i(G,A,B)$ is even (odd) and $P_i(G,A,B)$ is *infinite*, if there is no induced $A-B$-path in G (the length of each $P\in P_i(G,A,B)$ is infinite).

Lemma 9 *Let $G=(V,E)$ be a graph, $A,B\subseteq V$ two disjoint vertex subsets and $W\subseteq A$ a subset of A. If $P_i(G,A,B)$ is even (odd), then $P_i(G_{-A},N_G(W),B)$ is odd (even) or infinite. There is at least one vertex subset $W\subseteq A$, such that $P_i(G_{-A},N_G(W),B)$ is not infinite and hence odd (even), namely $W=\{a\}$, where $a\in A$ is connected by an induced $A-B$-path in G to a vertex $b\in B$.*

Proof. The first part is shown by contradiction. Assume $P_i(G,A,B)$ is even (odd) and for a subset $W\subseteq A$ there is an even (odd) induced $N_G(W)-B$-path in G_{-A}, connecting a vertex $x\in N_G(W)$ with a vertex $b\in B$. Because $x\in N_G(W)$, there is a vertex $a\in W\subseteq A$, such that a and x are adjacent. As x is the only vertex of the path in $N_G(W)$ by definition, a is non-adjacent to all other of its vertices. Hence, the path from a to x to b in G is induced and has odd (even) length, which contradicts the assumption of the statement.

As $P_i(G,A,B)$ is even (odd), there is at least one induced $A-B$-path P in G. Thus, there is a vertex $a \in A$ connected by an induced $A-B$-path to a vertex $b \in B$. Consequently, there is an induced $N_G(a)-B$-path in G_{-A}, which proves the second part. $\square$

3 MSC for parity graphs

Theorem 10 *Let $G=(V,E)$ be a simple graph and $A,B \subseteq V$ two vertex subsets. Then*

$$\Delta(G,A,B) = \sigma(G_{-A})\,\sigma(G_{-B}) - \sigma(G)\,\sigma(G_{-A-B})$$
$$\begin{cases} <0 & \text{if } P_i(G,A,B) \text{ is even,} \\ =0 & \text{if } P_i(G,A,B) \text{ is infinite,} \\ >0 & \text{if } P_i(G,A,B) \text{ is odd.} \end{cases} \tag{10}$$

Proof. If $P_i(G,A,B)$ is infinite, then there are no connected components including vertices from both vertex subsets A and B. Thus, this case is stated in Proposition 5. Therefore, from now on we assume that $P_i(G,A,B)$ is not infinite, that means there is at least one vertex $a \in A$ and at least one vertex $b \in B$ connected by a path.

We prove the two cases $P_i(G,A,B)$ is even and $P_i(G,A,B)$ is odd by induction with respect to the number of vertices in G, denoted by $n(G)$.

For the basic step we assume a graph G with the minimal number of vertices, this is $n(G)=1$ if $P_i(G,A,B)$ is even and $n(G)=2$ if $P_i(G,A,B)$ is odd. For $P_i(G,A,B)$ is even and $n(G)=1$ we have $G=(\{a\},\emptyset)$ and $A=B=\{a\}$. Hence

$$\Delta(G,A,B) = \sigma(G_{-A})\,\sigma(G_{-B}) - \sigma(G)\,\sigma(G_{-A-B}) = -1 < 0.$$

For $P_i(G,A,B)$ is odd and $n(G)=2$ we have $G=(\{a,b\},\{\{a,b\}\})$ and $A=\{a\}$, $B=\{b\}$. Hence

$$\Delta(G,A,B) = \sigma(G_{-A})\,\sigma(G_{-B}) - \sigma(G)\,\sigma(G_{-A-B}) = 1 > 0.$$

We assume as induction hypothesis that the statement holds for any graph with at most k vertices and consider from now on a graph G with $n(G)=k+1$ vertices.

If A and B are not disjoint, that means $A \cap B = C \neq \emptyset$, which means that $P_i(G,A,B)$ is even, then by Proposition 6 we have

$$\Delta(G,A,B) < \Delta(G_{-C}, A \setminus C, B \setminus C).$$

As C is non-empty, G_{-C} has at most k vertices and hence we can use the induction hypothesis. Furthermore, as $P_i(G,A,B)$ is even, $P_i(G_{-C},A\setminus C,B\setminus C)$ is also even or infinite (by deleting C, no new paths occur, but some are destroyed), that means

$$\Delta(G,A,B) < \Delta(G_{-C},A\setminus C,B\setminus C) \leq 0.$$

Otherwise, if A and B are disjoint, we can apply Lemma 4:

$$\Delta(G,A,B) = -\sum_{\text{ind. } W\subseteq A} \Delta(G_{-A},N_G(W),B).$$

A is non-empty (otherwise $P_i(G,A,B)$ would be infinite), therefore G_{-A} has at most k vertices and the induction hypothesis can be applied: For all $W \subseteq A$ we have

$$\Delta(G_{-A},N_G(W),B) \begin{cases} \geq 0 & \text{if } P_i(G,A,B) \text{ is even,} \\ \leq 0 & \text{if } P_i(G,A,B) \text{ is odd,} \end{cases}$$

because if $P_i(G,A,B)$ is even (odd), then $P_i(G_{-A},N_G(W),B)$ is not even (odd) by Lemma 9. But at least for $W = \{a\} \subseteq A$ we have

$$\Delta(G_{-A},N_G(W),B) \begin{cases} > 0 & \text{if } P_i(G,A,B) \text{ is even,} \\ < 0 & \text{if } P_i(G,A,B) \text{ is odd,} \end{cases}$$

again by Lemma 9. Hence, we get the other two cases of the statement:

$$\Delta(G,A,B) \begin{cases} < 0 & \text{if } P_i(G,A,B) \text{ is even,} \\ > 0 & \text{if } P_i(G,A,B) \text{ is odd.} \end{cases}$$

□

Definition 11 A simple graph $G = (V,E)$ is a *parity graph*, if for any two vertices $u,v \in V$ the lengths of all induced $u-v$-paths in G have the same parity.

Parity graphs are a generalization of bipartite graphs, because only the lengths of all induced $u-v$-paths are claimed to have the same parity, instead of all $u-v$-paths as for bipartite graphs.

If two vertices have even (odd) distance in a parity graph, then all induced paths have even (odd) lengths and hence the previous theorem proves the MSC for parity graphs (and arbitrary vertices).

Corollary 12 *The Merrifield-Simmons conjecture holds for parity graphs.*

In relation to the corollary above, Theorem 10 is slightly more general, because there, only assumptions about the subgraph connecting the vertex subsets are made: The MSC holds in a graph $G = (V,E)$ for vertex subsets $A,B \subseteq V$, if the subgraph induced by all vertices in some $A-B$-path is a parity graph.

4 Counterexamples

Having shown in the preceding section that the MSC not only holds in bipartite graphs, but also holds in parity graphs, the question arises if it can be further generalized to larger graph classes.

It seems that this is not possible, because of the graphs displayed in Figure 1, where G_1 is the minimal counterexample for the MSC conjecture in arbitrary graphs.

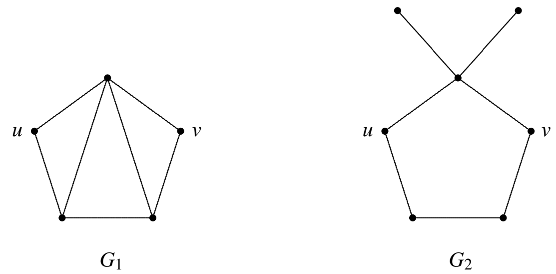

Figure 1. Graphs G_1 and G_2, which are counterexamples for the MSC in superclasses of parity graphs. It holds $\Delta(G_1,u,v) = 6\cdot 6 - 9\cdot 4 = 0$ and $\Delta(G_2,u,v) = 23\cdot 23 - 35\cdot 15 = 4$.

According to Ridder et al. [7], the following are the minimal superclasses of parity graphs: $(5,2)$-odd-chordal (equivalent to Meyniel, (odd building, odd-hole)-free, and very strongly perfect), P_4-bipartite, $(X_{38}, \text{gem}, \text{house})$-free, preperfect, and skeletal.

Remark 13 The graphs G_1 and G_2 in Figure 1 provide counterexamples for the MSC. G_1 is a $(5,2)$-odd-chordal, P_4-bipartite, preperfect and skeletal graph, and G_2 is a $(X_{38}, \text{gem}, \text{house})$-free graph. Consequently, the MSC cannot be generalized to any of the minimal superclasses of parity graphs listed by Ridder et al. [7].

Indeed, for general graphs, the value of $\Delta(G,u,v)$ may be arbitrarily different from what the MSC claims. In the following we present the construction of a simple graph G with non-adjacent vertices u and v of arbitrary distance (> 1) with arbitrarily small or big value of $\Delta(G,u,v)$. (For adjacent vertices the MSC is valid for general graphs [2, Corollary 5.1].)

First, for the case of distance 2, we observe the graph $G_{n,m}$ in Figure 2: starting with a cycle of length 5, where the vertices u and v have distance 2, we add n pendant vertices to one of the neighbors of u and m pendant vertices to the other one. It follows that

$$\begin{aligned}\Delta(G_{n,m},u,v) &= (3\cdot 2^{n+m} + 2\cdot 2^n + 2\cdot 2^m + 1)(4\cdot 2^{n+m} + 2^n + 2\cdot 2^m + 1)\\ &\quad - (6\cdot 2^{n+m} + 2\cdot 2^n + 2\cdot 2^m + 1)(2\cdot 2^{n+m} + 2^n + 2\cdot 2^m + 1)\\ &= 2^{n+m}(2^n - 2\cdot 2^m - 1). \end{aligned} \tag{11}$$

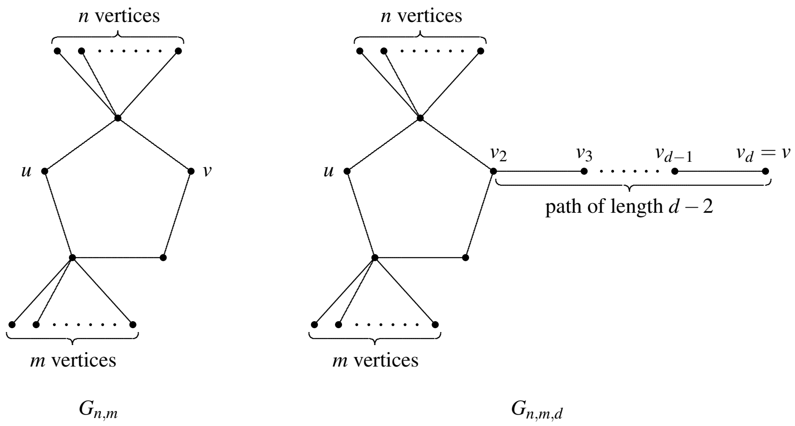

Figure 2. Graphs $G_{n,m}$ and $G_{n,m,d}$, which show that in general graphs the value of $\Delta(G,u,v)$ can be arbitrarily small or big.

Therefore $\Delta(G_{n,m},u,v)$ becomes arbitrarily small or big by choosing sufficiently large values of m and n, respectively. The construction of $G_{n,m}$ can be extended to arbitrary distances due to the fact that, by shifting the vertex v to a new pendant vertex attached to it, only the sign of Δ alternates. The following lemma states the case when v is a pendant vertex.

Lemma 14 *Let $G = (V,E)$ be a simple graph and $u,v,w \in V$ are vertices of G such that v is a pendant vertex and w is its only neighbor. Then*

$$\Delta(G,u,v) = -\Delta(G_{-v},u,w).$$

The statement can be seen as a corollary of Lemma 4, but a direct proof is quite easy.

Proof. Since w is the only neighbor of v, the recurrence relation for the number of independent sets has the form $\sigma(G) = \sigma(G_{-v}) + \sigma(G_{-v-w})$. Hence we have

$$\begin{aligned}
\Delta(G,u,v) &= \sigma(G_{-u})\,\sigma(G_{-v}) - \sigma(G)\,\sigma(G_{-u-v}) \\
&= (\sigma(G_{-u-v}) + \sigma(G_{-u-v-w}))\,\sigma(G_{-v}) \\
&\quad - (\sigma(G_{-v}) + \sigma(G_{-v-w}))\,\sigma(G_{-u-v}) \\
&= \sigma(G_{-u-v-w})\,\sigma(G_{-v}) - \sigma(G_{-v-w})\,\sigma(G_{-u-v}) \\
&= -\Delta(G_{-v},u,w).
\end{aligned}$$

□

Thus, for the case of arbitrary distance d, we obtain the graph $G_{n,m,d}$ in Figure 2 as follows: starting with the graph $G_{n,m}$ we attach a path of length $d-2$ to v and adjust the labels such that the other end-vertex of the path becomes v. Then for $G_{n,m,d}$ with $d \geq 2$, it follows that

$$-\Delta(G_{n,m,d+1},u,v) = \Delta(G_{n,m,d},u,v) = (-1)^d \Delta(G_{n,m},u,v), \tag{12}$$

where the vertices u and v are labeled accordingly (see Figure 2). Consequently, for sufficiently large values of n and m, the values of $\Delta(G_{n,m,d},u,v)$ become arbitrarily small or big.

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