Perfect matchings and ears in elementary bipartite graphs

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Abstract

We give lower and upper bounds for the number of reducible ears as well as upper bounds for the number of perfect matchings in an elementary bipartite graph. An application to chemical graphs is also discussed. In addition, a method to construct all minimal elementary bipartite graphs is described.

Keywords: Bipartite graph; Matching; Ear; Chemical graph

1. Introduction and terminology

All graphs considered in this paper are finite, connected, undirected and without loops or multiple edges. Let $G$ be a graph and $v(G)$, $e(G)$ the numbers of vertices and edges of $G$. A set of independent edges $M$ of $G$ is a perfect matching if these edges cover all vertices of $G$. An edge of $G$ is allowed if it lies in some perfect matching of $G$ and forbidden otherwise. We say $G$ is elementary if its allowed edges form a connected subgraph of $G$. Let $f(G)$ denote the number of perfect matchings of $G$. If $G$ is bipartite, we color its vertices in two colors such that adjacent vertices have different colors.

Let $G$ be an elementary bipartite graph. A path $P$ of odd length of $G$ (i.e., with an odd number of edges) is called a reducible ear if all its interior vertices are of degree 2, $G - P$ is elementary (where $G - P$ is the subgraph of $G$ obtained by deleting the edges and the interior vertices of $P$ from $G$). Let $er(G)$ denote the number of reducible ears of $G$, $v_3(G)$ the number of vertices of $G$ with degree larger than 2 and $\delta_3(G)$ the minimum degree of the vertices with degree larger than 2. A bipartite ear decomposition of $G$ is a representation of $G$ in the form $G = x + P_1 + P_2 + \cdots + P_r$ such that $x$ is an edge, $G_0 = x$, for $1 \leq i \leq r$, $P_i$ is a path of odd length, $G_i = x + P_1 + \cdots + P_i$.
and $P_i$ has no other vertices in common with $G_{i-1}$ than its two end vertices. Note that the $G_i$'s are also elementary.

An elementary bipartite graph $G$ is \textit{minimal} if $G - e$ is not elementary for any edge $e$ of $G$.

Lovász and Plummer [6] proved that a bipartite graph is elementary if and only if it is connected and each of its edges is allowed, and that a graph $G$ is elementary and bipartite if and only if $G$ has a bipartite ear decomposition. By these results, an elementary bipartite graph $G$ is connected and has at least one reducible ear, i.e., $\text{er}(G) \geq 1$. In Section 2, we present a lower and an upper bound for $\text{er}(G)$, which are tight.

Many papers are devoted to the study of $f(G)$. For surveys see [8, 9]. $f(G)$ is also of interest to chemists. The number of perfect matchings in a molecular graph (whose vertices are associated with atoms and edges with bonds between them) is related to the stability of the corresponding chemical compound (e.g. [5]). For an elementary bipartite graph $G$, the best-known lower bound on $f(G)$ is $e(G) - v(G) + 2$, which can be deduced from a result of [2]; few upper bounds for $f(G)$ are known.

We give upper bounds for $f(G)$ in Section 3, and discuss their application to mathematical chemistry in Section 4.

In Section 5, a method to construct all minimal elementary bipartite graphs is described.

\textbf{2. Reducible ears in an elementary bipartite graph}

Let $\mu(G) = e(G) - v(G) + 1$, i.e., the number of fundamental cycles of $G$. Let $K_2$ denote the complete graph with two vertices.

\textbf{Theorem 1.} For an elementary bipartite graph $G$ which is neither a cycle nor $K_2$, $\mu(G) + 1 \leq \text{er}(G) \leq 3(\mu(G) - 1)$.

\textbf{Proof.} We first prove the lower bound on $\text{er}(G)$, by induction on $\mu(G)$. When $\mu(G) = 2$, clearly $\mu(G) + 1 = \text{er}(G)$. Suppose that $\mu(G) + 1 \leq \text{er}(G)$ when $\mu(G) < n$. Let $\mu(G) = n$ and let $P$ be a reducible ear of $G$ with end vertices $x$ and $y$. By the induction hypothesis,

$$\text{er}(G - P) \geq \mu(G - P) + 1 = \mu(G) - 1 + 1 = \mu(G).$$

We assert that there is an injection from the reducible ears of $G - P$ to the reducible ears of $G$ which are not equal to $P$. Then

$$\text{er}(G) \geq 1 + \text{er}(G - P) \geq 1 + \mu(G).$$

Now we prove the assertion. Let $P'$ be a reducible ear of $G - P$ with end vertices $x'$ and $y'$. If $x$ and $y$ do not belong to $P'$, then $P'$ is a reducible ear of $G$. If both $x$ and
y belong to \( P' \), then the subpath of \( P' \) with end vertices \( x \) and \( y \) is a reducible ear of \( G \). The remaining case is that only one of \( x \) and \( y \) belongs to \( P' \). Without loss of generality, let \( x \) belong to \( P' \). Since the length of \( P' \) is odd, either the subpath of \( P' \) with end vertices \( x \) and \( x' \) or the subpath of \( P' \) with end vertices \( x \) and \( y' \) has odd length. Then we can check that such a subpath with odd length is a reducible ear of \( G \). The above discussion clearly indicates a mapping \( \mathcal{F} \) from the set of reducible ears of \( G - P \) to the set of reducible ears of \( G \) (which does not include \( P \)). The image \( \mathcal{F}(P') \) is contained in \( P' \). Thus the mapping is an injection.

Since \( G \) is 2-connected and neither a cycle nor \( K_2 \), each reducible ear of \( G \) is also a reducible chain of \( G \), and by Theorem 9 of [12], \( er(G) \leq 3(\mu(G) - 1) \). The proof is completed. \( \square \)

The graphs in Figs. 1 and 2 show that the lower and upper bounds on \( er(G) \) given by Theorem 1 are tight.

### 3. Upper bounds for \( f(G) \)

We first prove a lemma.

**Lemma 1.** Let \( G \) be an elementary bipartite graph which is neither a cycle nor \( K_2 \). Then \( G \) has \( \delta_3(G) - 1 \) reducible ears which have an end vertex in common.

![Fig. 1. A graph with \( \mu(G) + 1 \) reducible ears.](image1)

![Fig. 2. A graph with \( 3(\mu(G) - 1) \) reducible ears.](image2)
Proof. If the lemma is not true, each vertex of degree larger than 2 has at most \((\delta_3(G)-2)\) reducible ears incident to it. Then \((\delta_3(G)-2)v_3(G) \geq 2\varepsilon(G)\). By Theorem 1, \(2\varepsilon(G) \geq 2(\mu(G)+1) = 2\mu(G) + 2\). So \(\mu(G) \leq (\delta_3(G)-2)v_3(G)/2 - 1\). Let \(G'\) be the (multi-) graph obtained by replacing each reducible ear of \(G\) by an edge with the same end vertices. Then \(\mu(G) = \mu(G')\) and \(\mu(G') = e(G') - v(G') + 1 \geq \delta_3(G)v_3(G)/2 - v_3(G) + 1 = (\delta_3(G)-2)v_3(G)/2 + 1\). This is a contradiction. \(\square\)

Theorem 2. Let \(G\) be a bipartite graph. Then

1. \(f(G) \leq 2^{\mu(G)-1} + 1\) if \(G\) is elementary.
2. \(f(G) \leq 2^{\mu(G)}\) if \(G\) has forbidden edges.
3. \(f(G) \leq 2^{\mu(G)-1}\) if \(G\) has forbidden edges and does not have cut edges.

Proof. If \(G\) has no perfect matching, the theorem is clearly true. Assume that \(f(G) > 0\). By induction on the size of \(G\), we will prove the theorem. If \(G\) is a cycle or \(K_2\), the theorem is clearly true. First, let \(G\) be elementary. Suppose that \(G\) is neither a cycle nor \(K_2\). We say that a reducible ear \(P\) is contained in a perfect matching \(M\) if \(M \cap P\) is a perfect matching of \(P\). By Lemma 1, there are two reducible ears \(P\) and \(P'\) which have a common end vertex \(x\). Let \(M_P\) and \(M_{P'}\) be the set of perfect matchings which contain \(P\) or \(P'\), respectively. Let \(M_0\) be the set of perfect matchings which contain neither \(P\) nor \(P'\). Note that each perfect matching of \(G\) in \(M_0\) and \(M_P\) induces a unique perfect matching of \(G - P'\). Thus \(|M_P| \leq f(G - P') - |M_0|\). Similarly, \(|M_{P'}| \leq f(G - P) - |M_0|\). Without loss of generality, let \(f(G - P') \leq f(G - P)\). Then \(f(G) = |M_P| + |M_{P'}| + |M_0| \leq f(G - P) + f(G - P') - |M_0| \leq 2f(G - P) - |M_0|\). By the induction hypothesis, \(f(G - P) \leq 2^{\mu(G - P) - 1} + 1\). By noting that \(\mu(G) = \mu(G - P) + 1\) and \(|M_0| \geq 1\), \(f(G) \leq 2^{\mu(G) - 1} + 1\). Case (1) of the theorem is proved. Second, let \(G\) have forbidden edges. Let \(G'\) be the subgraph formed by all allowed edges of \(G\). Then \(G'\) is the union of disjoint elementary graphs \(G_1, G_2, \ldots, G_j\) (which are not \(K_2\)) and \(G_{j+1}, \ldots, G_k\) (which are \(K_2\)). Since \(f(G)\) is equal to the product of \(f(G_1), f(G_2), \ldots, f(G_j)\) and (1) holds for each \(G_i\), \(f(G) \leq \left(2^{\mu(G_1) - 1} + 1\right) \left(2^{\mu(G_2) - 1} + 1\right) \cdots \left(2^{\mu(G_j) - 1} + 1\right) = 2^{\mu(G_1) + \mu(G_2) + \cdots + \mu(G_j)}\). Note that \(\mu(G_1) + \mu(G_2) + \cdots + \mu(G_j) \leq \mu(G)\) and \(2^{\mu(G_1) + \mu(G_2) + \cdots + \mu(G_j)}\) is the largest term in the sum. There are in total \(2^j\) terms in the sum. Thus \(f(G) \leq \left(2^{\mu(G) - 1} \times 2^j\right)\). If \(G\) has no cut edges, \(\mu(G_1) + \mu(G_2) + \cdots + \mu(G_j) \leq \mu(G) - 1\). Then \(f(G) \leq 2^{\mu(G) - 1} \times 2^j = 2^{\mu(G)}\). The theorem is proved. \(\square\)

Theorem 3. Let \(G\) be an elementary bipartite graph and not a cycle. Then \(f(G) \leq (\delta_3(G) - 1)(2^{\mu(G) - \delta_3(G)} + 1)\).

Proof. By induction on the number of vertices of \(G\). If \(\delta_3(G) = 3\), by Theorem 2 the conclusion is true. Assume that \(\delta_3(G) > 3\). By Lemma 1, there are reducible ears \(P_1, P_2, \ldots, P_{\delta_3(G)-1}\) which have a vertex in common. We say a perfect matching \(M\) of \(G\) belongs to \(G - P_i\) if \(M \cap (G - P_i)\) is a perfect matching of \(G - P_i\). Then each perfect
matching of \( G \) belongs to at least \( \delta_3(G) - 2 \) of \( G - P_1, G - P_2, \ldots, G - P_{\delta_3(G) - 1} \). Thus, \( f(G) \leq (f(G - P_1) + f(G - P_2) + \cdots + f(G - P_{\delta_3(G) - 1}))/\delta_3(G) - 2 \). If \( \delta_3(G - P_i) \) is \( \delta_3(G) - 1 \), by the induction hypothesis \( f(G - P_i) \leq \delta_3(G) - 2(2^{\mu(G) - 1 - (\delta_3(G) - 1)} + 1) \).

If \( \delta_3(G - P_i) \) is \( \delta_3(G) \), by the induction hypothesis, \( f(G - P_i) \leq (\delta_3(G) - 1) (2^{\mu(G) - \delta_3(G) + 1} + 1) \).

4. An application to chemical graphs

We discuss an application of Theorem 2 in mathematical chemistry.

Many classes of graphs are of interest to chemists. One such class is that of benzenoid systems. A benzenoid system is a connected subgraph of the infinite hexagonal lattice which has no cut vertices or nonhexagonal interior forces. A benzenoid system is actually a geometric diagram. Benzenoid hydrocarbon molecules can be represented by benzenoid systems [1, 3, 11]. Here we restrict our discussion to benzenoid systems which have perfect matchings. The reason for this is that experimental evidence shows only benzenoid systems with perfect matchings correspond to benzenoid hydrocarbon molecules. There is a one-to-one correspondence between Kekulé structures of a benzenoid hydrocarbon and perfect matchings of the benzenoid system representing it. Kekulé structures play significant roles in many chemical theories, of which resonance theory and valence bond theory are the best known examples [1, 3]. A few upper or lower bounds on the number of Kekulé structures (or perfect matchings) for the cata-condensed benzenoid systems (a benzenoid system is cata-condensed if it has no interior vertices) are known [1]. We next give an upper bound for the number of perfect matchings of a benzenoid system.

**Theorem 4.** Let \( G \) be a benzenoid system with \( h \) hexagons. Then \( f(G) \leq 2^{h-1} + 1 \) if \( G \) has no forbidden edges else \( f(G) \leq 2^{h-1} \).

**Proof.** By Theorem 2. \( \square \)

5. Minimal elementary bipartite graphs

In this section, we present a method to construct all minimal elementary bipartite graphs.

Let \( G = (U, W, E) \) be a minimal elementary bipartite graph with more than 2 vertices and \( e = (u, v) \in E \) with \( u \in U \) and \( v \in W \). Since \( G - e \) has a perfect matching,
by the Dulmage-Mendelsohn decomposition theorem (see [7, pp. 138-139]), the
allowed edges of $G - e$ form a graph $G_e$ in which each connected component is an
elementary graph. Let $L_1, L_2, \ldots, L_k$ be the connected components of $G_e$. Since $G$
is minimal, $k > 1$. Let $S_i = U \cap L_i$ and $T_i = W \cap L_i$ ($i = 1, \ldots, k$). With the above nota-
tion, we have

**Lemma 2.** Let $G$ be a minimal elementary bipartite graph and $e = (u, v)$. Then the
connected components of $G_e$ can be labeled as $L_1, L_2, \ldots, L_k$ such that if $e' = (u_i, v_j) \in G$
with $u_i \in S_i$, $v_j \in T_j$ then $i \leq j$. Moreover, $u \in S_k$ and $v \in T_1$.

**Proof.** By Lemmas 4.3.1 and 4.3.2 of [7], the connected components of $G_e$ can be
labeled as $L_1, L_2, \ldots, L_k$ such that if $e' = (u_i, v_j) \in G$ with $u_i \in S_i$ and $v_j \in T_j$ then $i \leq j$.
Since $G$ is elementary and minimal, $u \in S_k$ and $v \in T_1$. Clearly $e$ is the only edge
between $S_k$ and $T_1$. The lemma is proved. ☐

Using the same notation as above, we define for $G$ the extremal components
(corresponding to $e$) to be $S_k$ and $T_1$. Let $u$ and $v$ be two vertices of $G$ with different
colors and $P$ be a path disjoint from $G$. Let $G_P = (G + P)_{uv}$ be the graph obtained by
identifying the two end vertices of $P$ with $u$ and $v$, respectively. We say $G_P$ is obtained
from $G$ and $P$ by an $e$-operation if $G$ is minimal and for any edge $e$ both $u$ and $v$ do not
respectively belong to the two extremal components which correspond to $e$.

We have the following lemma.

**Lemma 3.** Let $G = (U, W, E)$ be a minimal elementary bipartite graph, $u$ and $v$ be two
vertices of $G$ with different colors, and $P$ be an odd path disjoint from $G$. Then $(G + P)_{uv}$
is minimal elementary if and only if (i) the length of $P$ is larger than $1$ and (ii) $G_P$ is
obtained from $G$ and $P$ by an $e$-operation.

**Proof.** If $(G + P)_{uv}$ is minimal elementary, then (i) is clearly true. If (ii) is not true, let
$e = (x, y)$ be an edge such that $u$ and $v$ belong to the extremal components of $e$,
respectively. Let $L_1, L_2, \ldots, L_k$ be the decomposition of $G - e$ as in Lemma 2.
Clearly, all edges belonging to $L_i$ are allowed in $(G + P)_{uv} - e$. Let $e'$ be an edge of
$(G + P)_{uv} - e$ which is between $L_i$ and $L_j$ ($i < j$). Let $M$ be a perfect matching of
$G$ which contains $e'$. Extend $M$ to a perfect matching of $(G + P)_{uv}$ (using the same
notation to denote it) by choosing the disjoint edges of $P$ which cover all interior
vertices of $P$ but not its end vertices. Note there is only one edge of $M$, $e'$, between
$T_1$ and $S_k$. Thus there is only one edge $e_1$ ($e_1'$) of $M$ between $S_1$ ($T_k$) and $\bigcup_{j > 1} T_j$
($\bigcup_{j < k} S_j$). Let $v_1$ be the end vertex of $e_1$ in $S_1$ and $v_1'$ be the end vertex of $e_1'$ in $T_k$.
Assume that $u \in T_1$ and $v \in S_k$. Then since $L_1$ and $L_k$ are elementary, by Theorem 4.1.1
of [7], $L_1 - u - v_1$ ($L_k - v - v_1'$) has a perfect matching $M_1$ ($M_1'$). Let $M_2$ be a perfect
matching of $P$. Then $M' = M - (L_1 \cap M) - (L_k \cap M) - (P \cap M) + M_1 + M_1' + M_2$ is
a perfect matching of $(G + P)_{uv} - e$ which also contains $e'$. By the choice of $e'$, all edges
of $G - e$ are allowed in $(G + P)_{uv} - e$. Let $M''$ be a perfect matching of $G - e$. Then $M'' \cup (M \cap P)$ is a perfect matching of $(G + P)_{uv} - e$. Thus, all edges of $P$ are allowed in $(G + P)_{uv} - e$. Thus $(G + P)_{uv}$ is not minimal. The necessary condition is proved.

On the other hand, clearly $(G + P)_{uv}$ is elementary. We only need to prove it is also minimal. Let $e$ be an arbitrary edge of $(G + P)_{uv}$. If $e \in P$, clearly, $(G + P)_{uv} - e$ has pendant edge(s) and thus it is not elementary. Assume that $e \notin G$. Consider the decomposition $L_1, L_2, \ldots, L_k$ of $G - e$ as in Lemma 2. Since $u$ and $v$ do not respectively belong to the extremal components corresponding to $e$, then $u, v$ do not belong to $T_1$ or to $S_k$. In the first case, the edge(s) between $S_1$ and $\bigcup_{j>1} T_j$ are not allowed in $(G + P)_{uv} - e$. In the second case, the edge(s) between $T_k$ and $\bigcup_{j<k} S_j$ are not allowed in $(G + P)_{uv} - e$. Thus $(G + P)_{uv}$ is minimal. The proof is completed. 

Lemma 4. Let $G$ be a minimal elementary bipartite graph, $P$ be a reducible ear of $G$ and $u, v$ be the end vertices of $P$. Then $G - P$ is minimal elementary if it is not an edge, and $u$ and $v$ do not, respectively, belong to the extremal components corresponding to any edge of $G - P$.

Proof. By Theorem 4.2.1 of [7], $G - P$ is minimal. By the previous lemma, $u$ and $v$ do not respectively, belong to the extremal components corresponding to any edge of $G - P$.

By the above lemmas, we have the following theorem.

Theorem 5. $G$ is a minimal elementary bipartite graph if and only if it can be constructed from an even cycle with length greater than 4 through a series of $e$-operations.

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