# The Extremal Matching Energy of Graphs *

Shengjin Ji[1], Hongping Ma[2†]

[1] School of Science, Shangdong University of Technology
Zibo, Shandong 255049, China

Email: jishengjin2013@163.com

[2] School of Mathematics and Statistics, Jiangsu Normal University, Xuzhou, Jiangsu 221116, China
Email: hpma@163.com

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**Abstract**

Let G be a simple graph of order $n$ and $\mu_1, \mu_2, \ldots, \mu_n$ the roots of its matching polynomial. Recently, Gutman and Wagner defined the matching energy as the sum $\sum_{i=1}^{n} |\mu_i|$. In this paper, we first show that Turán graph $T_{r,n}$ is the $r$-partite graph of order $n$ with maximum matching energy. Then we characterize the connected graphs (and bipartite graph) of order $n$ having minimum matching energy with $m$ $(n+2 \leq m \leq 2n-4)$ $(n \leq m \leq 2n-5)$ edges.

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†Corresponding author.

# 1 Introduction

We use Bondy and Murty [2] for terminology and notations not defined in this paper and consider undirected and simple graphs only. A graph with order $n$ and size $m$ is called a $(n,m)$-graph. Let $G$ be a $(n,m)$-graph. Denote by $m(G,k)$ the number of $k$-matchings of $G$. Clearly, $m(G,1) = m$ and $m(G,k) = 0$ for $k > \lfloor n/2 \rfloor$. It is both consistent and convenient to define $m(G,0) = 1$.

The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of the adjacency matrix $A(G)$ of $G$ are said to be the eigenvalues of the graph $G$. The *energy* of $G$ is defined as

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{1.1}$$

The theory of graph energy is well developed nowadays, for details see [10, 12, 18]. The Coulson integral formula [15] plays an important role in the study on graph energy, its version for an acyclic graph $T$ is as follows:

$$E(T) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \Big[ \sum_{k \geq 0} m(T,k) x^{2k} \Big] dx. \tag{1.2}$$

Motivated by formula (1.2), Gutman and Wagner [16] defined the *matching energy* of a graph $G$ as

$$ME = ME(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \Big[ \sum_{k \geq 0} m(G,k) x^{2k} \Big] dx. \tag{1.3}$$

Energy and matching energy of graphs are closely related, and they are two quantities of relevance for chemical applications, for details see [1, 13, 14].

Recall that the matching polynomial of the graph $G$ is defined as

$$\alpha(G) = \alpha(G,\lambda) = \sum_{k\geq 0}(-1)^k m(G,\lambda)\lambda^{2k}.$$

The following result gives an equivalent definition of matching energy.

**Theorem 1.1** [16] *Let $G$ be a graph of order $n$, and let $\mu_1, \mu_2, \cdots, \mu_n$ be the roots of its matching polynomial. Then*

$$ME(G) = \sum_{i=1}^{n} |\mu_i|. \tag{1.4}$$

The formula (1.3) induces a quasi-order relation over the set of all graphs on $n$ vertices: if $G_1$ and $G_2$ are two graphs of order $n$, then

$$G_1 \succeq G_2 \Leftrightarrow m(G_1,k) \geq m(G_2,k) \text{ for all } k = 0,1,\ldots,\lfloor\frac{n}{2}\rfloor. \tag{1.5}$$

If $G_1 \succeq G_2$ and there exists some $i$ such that $m(G_1,i) > m(G_2,i)$, then we write $G_1 \succ G_2$. Clearly,

$$G_1 \succ G_2 \Rightarrow ME(G_1) > ME(G_2).$$

The following result gives two fundamental identities for the number of $k$-matchings of a graph [5, 9].

**Lemma 1.2** *Let $G$ be a graph, $e = uv$ an edge of $G$, and $N(u) = \{v_1(= v), v_2, \ldots, v_t\}$ the set of all neighbors of $u$ in $G$. Then we have*

$$m(G,k) = m(G-uv,k) + m(G-u-v,k-1), \tag{1.6}$$

$$m(G,k) = m(G-u,k) + \sum_{i=1}^{t} m(G-u-v_i,k-1). \tag{1.7}$$

From Lemma 1.2, it is easy to get the following result.

**Lemma 1.3** [16] *Let $G$ be a graph and $e$ one of its edges. Let $G-e$ be the subgraph obtained from $G$ by deleting the edge $e$. Then $G \succ G-e$ and $ME(G) > ME(G-e)$.*

Let $K_{t_1,t_2,\ldots,t_r}$ denote the complete $r(\geq 2)$-partite graph whose vertex set is partitioned into $r$ parts: $V_1, V_2, \ldots, V_r$ with $|V_1| = t_1, \ldots, |V_r| = t_r$, and $t_1 + \cdots + t_r = n$. A complete $r$-partite graph on $n$ vertices in which each part has either $\lfloor \frac{n}{r} \rfloor$ or $\lceil \frac{n}{r} \rceil$ vertices is called a Turán graph, and denoted by $T_{r,n}$. Suppose that $n \leq m \leq 2(n-2)$. Let $S_n^m$ and $B_n^m$ denote the two connected $(n,m)$-graphs as shown in Fig.1, respectively. Let $A_n$ be the $(n, n+2)$-graph obtained from $K_4$ by attaching $n-4$ pendent edges to one of the vertices of $K_4$.

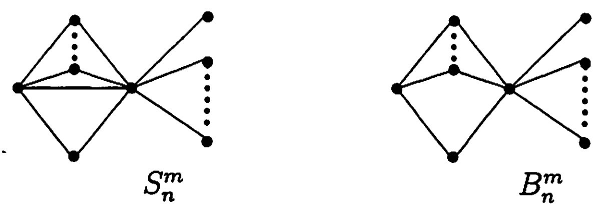

Fig.1 $(n,m)$-graphs: $S_n^m$ and $B_n^m$

Gutman and Wagner [16] proved that the bipartite graph with $n$ vertices having maximum matching energy is $T_{2,n}$. In Section 2, we will show that the $r$-partite graph with $n$ vertices having maximum matching energy is $T_{r,n}$.

In [16], the authors obtained that $ME(T) = E(T)$ for any tree $T$, and $ME(S_n^n) \leq ME(G) \leq ME(C_n)$ for any connected unicyclic graphs $G$ with $n$ vertices. The extremal graphs with respect to matching energy in connected bicyclic graphs were determined by [17], and $S_n^{n+1}$ is the connected bicyclic graph with minimum matching energy. In [7,8,11], the authors characterized the unicyclic, bicyclic, and tricyclic graphs with maximal matchings respectively, i.e., graphs that are extremal with regard to the quasi-ordering $\preceq$. By these results, finding unicyclic, bicyclic, and tricyclic graphs with maximum matching energy is an elementary task. In [19], Li and Zhang considered the minimal energy graph among connected bipartite $(n, m)$-graphs. With regard to skew energy, Gong et al. [6] determined the extremal graph in $(n, m)$-graphs. In Section 3, we will prove that $S_n^{n+2}$ and $A_n$ are the connected $(n, n+2)$-graphs with minimum matching energy, and $S_n^m$ $(n + 3 \leq m \leq 2(n - 2))$ is the connected $(n, m)$-graph with minimum matching energy, and $B_n^m$ $(n \leq m \leq 2n - 5)$ is the connected bipartite $(n, m)$-graph with minimum matching energy.

# 2 The r-partite graph with maximum matching energy

In this section, we will show that Turán graph $T_{r,n}$ is the r-partite graph with $n$ vertices having maximum matching energy. We begin with a key lemma.

**Lemma 2.1** *Let $K_{t_1,t_2,\ldots,t_r}$ be a complete r-partite graph with order $n$ and $1 \leq t_1 \leq \cdots \leq t_r$. If $t_j \geq t_i + 2$ for some $1 \leq i < j \leq r$, then we have*

$$K_{t_1,\ldots,t_{i-1},t_i+1,t_{i+1},\ldots,t_{j-1},t_j-1,t_{j+1}\ldots,t_r} \succ K_{t_1,\ldots,t_i,\ldots,t_j,\ldots,t_r}. \qquad (2.1)$$

*Proof.* We may assume, without loss of generality, that $t_i = t_1$ and $t_j = t_r$. By Lemma 1.2, we have

$$m(K_{t_1,t_2,\dots,t_r},k)=m(K_{t_1,\dots,t_{r-1},t_r-1},k)$$
$$+\sum_{l=1}^{r-1}t_l m(K_{t_1,\dots,t_{l-1},t_l-1,t_{l+1},\dots,t_{r-1},t_r-1},k-1),$$
$$(2.2)$$

$$m(K_{t_1+1,t_2,\dots,t_{r-1},t_r-1},k)=m(K_{t_1,t_2,\dots,t_{r-1},t_r-1},k)$$
$$+(t_r-1)m(K_{t_1,t_2,\dots,t_{r-1},t_r-2},k-1)$$
$$+\sum_{l=2}^{r-1}t_l m(K_{t_1,\dots,t_{l-1},t_l-1,t_{l+1},\dots,t_{r-1},t_r-1},k-1).$$
$$(2.3)$$

Since $m(K_{t_1,t_2,\dots,t_r},0)=m(K_{t_1+1,t_2,\dots,t_{r-1},t_r-1},0)=1$, we distinguish the following two cases.

**Case 1.** $1\le k\le t_1$.

Combining Eqs. (2.2) and (2.3), we obtain that

$$\begin{aligned}
&m(K_{t_1+1,t_2,\dots,t_{r-1},t_r-1},k)-m(K_{t_1,t_2,\dots,t_r},k)\\
&=(t_r-1)m(K_{t_1,t_2,\dots,t_{r-1},t_r-2},k-1)\\
&\qquad -t_1m(K_{t_1-1,t_2,\dots,t_{r-1},t_r-1},k-1)\\
&\ge t_1[m(K_{t_1,t_2,\dots,t_{r-1},t_r-2},k-1)\\
&\qquad -m(K_{t_1-1,t_2,\dots,t_{r-1},t_r-1},k-1)]\\
&\ge t_1(t_1-1)[m(K_{t_1-1,t_2,\dots,t_{r-1},t_r-3},k-2)\\
&\qquad -m(K_{t_1-2,t_2,\dots,t_{r-1},t_r-2},k-2)]\\
&\cdots\cdots\\
&\ge t_1(t_1-1)\cdots(t_1-k+2)[m(K_{t_1-k+2,t_2,\dots,t_{r-1},t_r-k},1)\\
&\qquad -m(K_{t_1-k+1,t_2,\dots,t_{r-1},t_r-k+1},1)]\\
&=t_1(t_1-1)\cdots(t_1-k+2)(t_r-t_1-1)>0
\end{aligned}$$

**Case 2.** $t_1<k\le\lfloor\frac{n}{2}\rfloor$.

Combining Lemma 1.3, Eqs. (2.2) and (2.3), we get that

$$
\begin{aligned}
&m(K_{t_1+1,t_2,\dots,t_{r-1},t_r-1},k) - m(K_{t_1,t_2,\dots,t_r},k)\\
&= (t_r-1)m(K_{t_1,t_2,\dots,t_{r-1},t_r-2},k-1)\\
&\qquad - t_1 m(K_{t_1-1,t_2,\dots,t_{r-1},t_r-1},k-1)\\
&\geq t_1[m(K_{t_1,t_2,\dots,t_{r-1},t_r-2},k-1) - m(K_{t_1-1,t_2,\dots,t_{r-1},t_r-1},k-1)]\\
&\geq t_1(t_1-1)[m(K_{t_1-1,t_2,\dots,t_{r-1},t_r-3},k-2)\\
&\qquad - m(K_{t_1-2,t_2,\dots,t_{r-1},t_r-2},k-2)]\\
&\cdots\cdots\\
&\geq t_1(t_1-1)\cdots 2[m(K_{2,t_2,\dots,t_{r-1},t_r-t_1},k-t_1+1)\\
&\qquad - m(K_{1,t_2,\dots,t_{r-1},t_r-t_1+1},k-t_1+1)]\\
&\geq t_1(t_1-1)\cdots 2\cdot 1[m(K_{1,t_2,\dots,t_{r-1},t_r-t_1-1},k-t_1)\\
&\qquad - m(K_{t_2,\dots,t_{r-1},t_r-t_1},k-t_1)]\\
&\geq 0.
\end{aligned}
$$

The proof is thus complete. ∎

**Theorem 2.2** *Let $G$ be a $r$-partite graph with $n$ vertices. Then $ME(G) \leq ME(T_{r,n})$, with equality if and only if $G \cong T_{r,n}$.*

*Proof.* Let $G \ncong T_{r,n}$ be a $r$-partite graph with $n$ vertices. If $G$ is not complete, then there is a complete r-partite graph $G'$ such that $G' \succ G$ by Lemma 1.3. Suppose $G' = K_{t_1,t_2,\dots,t_r}$ with $1 \leq t_1 \leq \cdots \leq t_r$. If $G' \ncong T_{r,n}$, then there exist some $i,j$ such that $1 \leq i < j \leq r$ and $t_j \geq t_i + 2$. Denote $G'' = K_{t_1,\dots,t_{i-1},t_i+1,t_{i+1},\dots,t_{j-1},t_j-1,t_{j+1}\dots,t_r}$. It follows from Lemma 2.1 that $G'' \succ G'$. If $G'' \ncong T_{r,n}$, then by repeatedly using Lemma 2.1, we can finally get that $T_{r,n} \succ G''$. Hence we have $T_{r,n} \succ G$ and the proof is complete. ∎

# 3 The $(n, m)$-graph with minimum matching energy

In this section, we will prove that $S_n^{n+2}$ and $A_n$ are the connected $(n, n+2)$-graphs with minimum matching energy, and $S_n^m$ $(n+3 \leq m \leq 2(n-2))$ is the connected $(n, m)$-graph with minimum matching energy, and $B_n^m$ $(n \leq m \leq 2n-5)$ is the connected bipartite $(n, m)$-graph with minimum matching energy.

Let $\mathbb{p} = (p_1, \ldots, p_n)$ and $\mathbb{q} = (q_1, \ldots, q_n)$ be two sequences of positive integers with $1 \leq p_l, q_l \leq n-1$ and $\sum_{l=1}^n p_l = \sum_{l=1}^n q_l = 2m$. Then we write $\mathbb{p} \preceq \mathbb{q}$ if $\sum_{l=1}^n \binom{p_l}{2} \leq \sum_{l=1}^n \binom{q_l}{2}$, and $\mathbb{p} \prec \mathbb{q}$ if $\sum_{l=1}^n \binom{p_l}{2} < \sum_{l=1}^n \binom{q_l}{2}$.

**Lemma 3.1** *Let $G$ be a connected $(n, m)$-graph with $n+2 \leq m \leq 2(n-2)$. If $G$ has no pendent vertices, then*

$$\sum_{v \in V(G)} \binom{d_G(v)}{2} < \sum_{v \in V(S_n^m)} \binom{d_{S_n^m}(v)}{2}.$$

*Proof.* let $\mathbb{d}_G = (d_1, d_2, \ldots, d_n)$ be the degree sequence of the connected graph $G$ with $d_1 \geq d_2 \geq \cdots \geq d_n$. Since $G$ has no pendent vertices, we have $d_1 \leq n-1$ and $d_n \geq 2$. It is easy to obtain that the degree sequence of graph $S_n^m$ is $\mathbb{d}_{S_n^m} = (n-1, m-n+2, \underbrace{2, 2, \ldots, 2}_{m-n+1}, \underbrace{1, 1, \ldots, 1}_{2n-m-3})$. So it suffices to prove that $\mathbb{d}_G \prec \mathbb{d}_{S_n^m}$.

**Claim 1.** $\mathbb{d}_G \prec (d_1, \ldots, d_{i-1}, d_i + 1, d_{i+1}, \ldots, d_{j-1}, d_j - 1, d_{j+1}, \ldots, d_n)$ *for any $1 \leq i < j \leq n$ with $d_i < n-1$ and $d_j > 1$.*

*Proof.* Denote $\mathbb{d}' = (d'_1, d'_2, \ldots, d'_n) \triangleq (d_1, \ldots, d_{i-1}, d_i + 1, d_{i+1}, \ldots, d_{j-1}, d_j - 1, d_{j+1}, \ldots, d_n)$. Then we have $1 \leq d'_l \leq n-1$,

$\sum_{l=1}^{n} d'_l = 2m$, and

$$\sum_{l=1}^{n} \binom{d_l}{2} - \sum_{l=1}^{n} \binom{d'_l}{2} = \binom{d_i}{2} + \binom{d_j}{2} - \binom{d_i+1}{2} - \binom{d_j-1}{2}$$
$$= d_j - d_i - 1 < 0.$$

Hence $\mathbb{d}_G \prec \mathbb{d}'$. ∎

By Claim 1, we get that

$$\begin{aligned} &(d_1, d_2, \ldots, d_n) \\ &\prec \begin{cases} (d_1+1, d_2, \ldots, d_{n-1}, d_n - 1), & \text{if } d_1 < n-1 \\ (n-1, d_2+1, \ldots, d_{n-1}, d_n - 1), & \text{if } d_1 = n-1 \end{cases} \\ &\prec \cdots \\ &\prec (d''_1, d''_2, d_3, \ldots, d_{m-n+3}, \underbrace{1, 1, \ldots, 1}_{2n-m-3}), \end{aligned}$$

where $d''_1 < n-1, d''_2 = d_2$ or $d''_1 = n-1, d''_2 \geq d_2$. Since $d''_1 \geq d''_2 \geq d_3 \geq \cdots \geq d_{m-n+3} \geq 2$, by applying the above procedure repeatedly, we can finally obtain that $(d''_1, d''_2, d_3, \ldots, d_{m-n+3}, \underbrace{1, 1, \ldots, 1}_{2n-m-3}) \preceq (n-1, m-n+2, \underbrace{2, 2, \ldots, 2}_{m-n+1}, \underbrace{1, 1, \ldots, 1}_{2n-m-3})$. Hence $\mathbb{d}_G \prec \mathbb{d}_{S_n^m}$ and the proof is thus complete. ∎

Let $H$ be a connected bipartite $(n, m)$-graph with $n \leq m \leq 2n-5$. Then the maximum degree of $H$ is at most $n-2$. By an argument similar to the proof of Lemma 3.1, we get immediately the following result.

**Lemma 3.2** *Let $H$ be a connected bipartite $(n, m)$-graph with $n \leq m \leq 2n-5$. If $H$ has no pendent vertices, then*

$$\sum_{v \in V(H)} \binom{d_H(v)}{2} < \sum_{v \in V(B_n^m)} \binom{d_{B_n^m}(v)}{2}.$$

**Theorem 3.3** *Let $G$ be a connected $(n, m)$-graph with $n + 2 \leq m \leq 2(n-2)$. Then $ME(G) \geq ME(S_n^m)$, with equality if and only if $G \cong S_n^m$ and $G \cong A_n$ when $m = n+2$, and $G \cong S_n^m$ when $n + 3 \leq m \leq 2(n-2)$.*

*Proof.* Let $G \ncong S_n^m$ and $G \ncong A_n$ when $m = n+2$ be a connected $(n, m)$-graph. Notice that $m(A_n, k) = m(S_n^m, k) = m(G, k)$ for $k = 0, 1$. It is easy to check that $m(A_n, k) = m(S_n^m, k) = 0$ for $k \geq 3$, and $m(A_n, 2) = m(S_n^{n+2}, 2)$. Therefore, it suffices to prove that $m(G, 2) > m(S_n^m, 2)$. We apply induction on $n$ to prove it. By the tables of [4] and [3], it is not difficult to check that the result is true for $n = 6$ and $n = 7$. Hence we suppose $n \geq 8$ and the result is true for smaller $n$.

**Case 1.** $G$ contains no pendent vertex.

Notice that $m(G, 2) = \binom{m}{2} - \sum_{v \in V(G)} \binom{d_G(v)}{2}$ and $m(S_n^m, 2) = \binom{m}{2} - \sum_{v \in V(S_n^m)} \binom{d_{S_n^m}(v)}{2}$. It follows from Lemma 3.1 that $m(G, 2) > m(S_n^m, 2)$.

**Case 2.** There is a pendent edge $uv$ in $G$ with pendent vertex $v$. By Lemma 1.2, we have

$$m(G, 2) = m(G - v, 2) + m(G - u - v, 1),$$
$$m(S_n^m, 2) = m(S_{n-1}^{m-1}, 2) + m(S_{m-n+2}, 1).$$

Suppose that $n + 2 \leq m \leq 2n - 5$. Then $(n-1) + 2 \leq m - 1 \leq 2(n-1) - 4$. Notice that $m(G - u - v, 1) = e(G - u - v) = m - d_G(u) \geq m - n + 1 = m(S_{m-n+2}, 1)$. If $d_G(u) \neq n - 1$, then we have $m(G - u - v, 1) > m(S_{m-n+2}, 1)$ and $m(G - v, 2) \geq m(S_{n-1}^{m-1}, 2)$ by induction hypothesis. So $m(G, 2) > m(S_n^m, 2)$. Otherwise, it is easy to see that $G - v \ncong S_{n-1}^{m-1}$ and $G - v \ncong A_{n-1}$ when $m = n + 2$. Hence we have $m(G - v, 2) > m(S_{n-1}^{m-1}, 2)$ by induction hypothesis, and so $m(G, 2) > m(S_n^m, 2)$.

Suppose that $m = 2n - 4$. Let $\mathbb{d}_G = (d_1, d_2, \ldots, d_n)$ and $\mathbb{d}_{S_n^{2n-4}}$ be the non-increasing degree sequences of $G$ and $S_n^{2n-4}$, respectively. Denote by $p$ the number of pendent vertices of $G$. If $p = 1$, then by a proof similar to Lemma 3.1, we have $\mathbb{d}_G \prec \mathbb{d}_{S_n^{2n-4}}$ and so $m(G,2) > m(S_n^{2n-4},2)$. If $p = 2$, then by a proof similar to Lemma 3.1, we get that $\mathbb{d}_G \preceq (n-1, n-3, 4, \underbrace{2, 2, \dots, 2}_{n-5}, 1, 1) \prec \mathbb{d}_{S_n^{2n-4}}$ and so $m(G,2) > m(S_n^{2n-4},2)$. Now we suppose $p \geq 3$ and we show that there exist an edge $e_1 = xy$ in $G$ such that $e_1$ is not a cut edge and $d_G(x) + d_G(y) \leq n$. If not, we may assume, without loss of generality, that each cut edge of $G$ is a pendent edge. Hence we get $4n - 8 - p = d_1 + \cdots + d_{n-p} \leq (n-p)(n-p-1) + p$ and thus $p \leq n - 5$. On the other hand, when $p \leq n/2$, we obtain that $4n - 8 = d_1 + \cdots + d_n \geq (n-p)(n+1)/2 + p > 4n - 8$, which is a contradiction. When $n/2 + 1 \leq p \leq n - 5$, we have $4n - 8 = d_1 + \cdots + d_n \geq (n-p)(n+1)/2 + p > (n-p)(n-p-1) + 2p \geq 4n - 8$, which is again a contradiction.

Since $p(G) \geq 3$ and $n \geq 8$, we have $G - xy \ncong S_n^{2n-5}, A_n$ and so $m(G - xy, 2) > m(S_n^{2n-5}, 2) = (n-4)(n-3)$ by induction hypothesis. Notice that $m(G - x - y, 1) = e(G - x - y) = m + 1 - d_G(x) - d_G(y) \geq n - 3$. Hence $m(G,2) = m(G - xy, 2) + m(G - x - y, 1) > (n-3)^2 = m(S_n^{2n-4}, 2)$.

Combining the above two cases, the proof is complete. ∎

By an argument similar to the proof of Theorem 3.3, we can get the following result.

**Theorem 3.4** *Let $n \leq m \leq 2n - 5$. Then $B_n^m$ is the unique graph having minimum matching energy among all connected bipartite $(n, m)$-graphs.*

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