

Darko Dimitrov, B. I., Riste Škrekovski. Maximum external Wiener index of graphs. *Discrete Appl. Math.* **257**, 331–337 (2019).

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$$\mathcal{W}(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

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$$\mathcal{W}(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

• [Wiener, 1947]

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$$\mathcal{W}(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

- [Wiener, 1947]
- correlation with paraffin boiling points

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$$\mathcal{W}(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

- [Wiener, 1947]
- correlation with paraffin boiling points
- quantitative structure-activity relationships (QSAR) and quantitative property-activity relationships (QPAR) modelling

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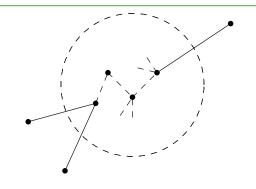
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$$W(G) = \sum_{\substack{u,v \in V(G) \\ \min\{d(u),d(v)\} \ge 2}} d(u,v) + \sum_{\substack{u,v \in V(G) \\ \min\{d(u),d(v)\} = 1}} d(u,v)$$

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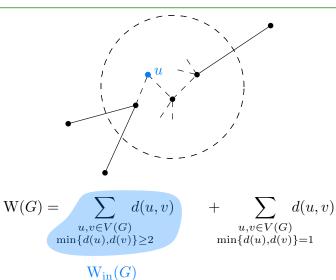
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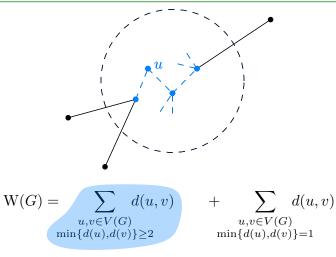
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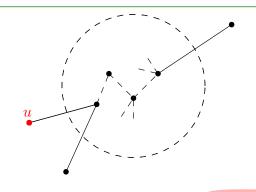
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$$\mathbf{W}(G) = \sum_{\substack{u,v \in V(G) \\ \min\{d(u),d(v)\} \ge 2}} d(u,v)$$

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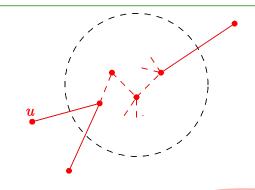
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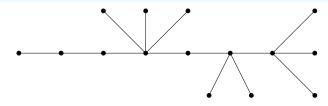
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A **caterpillar** is a tree with a central path in which vertices located outside this path are directly connected to it by an edge.



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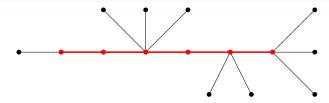
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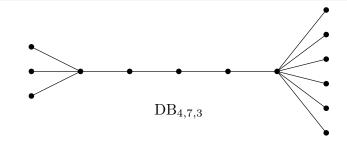
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A double broom $DB_{a,b,c}$ is a caterpillar obtained from P_{c+2} by attaching a - 1 pendant vertices to one of its endpoints and b - 1 pendant vertices to its other endpoint. A double broom is **balanced** if $|a - b| \leq 1$.



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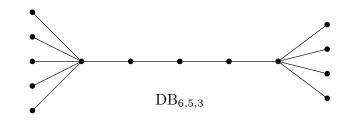
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Conjecture [Gutman et al., 2016]

Among all trees of a fixed order, double brooms have the greatest $W_{e {\boldsymbol{\mathrm{x}}}}.$

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Conjecture [Gutman et al., 2016]

Among all trees of a fixed order, double brooms have the greatest $\ensuremath{W_{ex}}\xspace.$

The double broom that attains the maximal W_{ex} is the balanced double broom $DB_{a.b.c.}$

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Conjecture [Gutman et al., 2016]

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The double broom that attains the maximal W_{ex} is the balanced double broom $\mathrm{DB}_{a,b,c}.$

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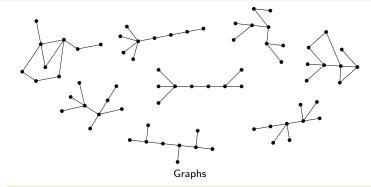
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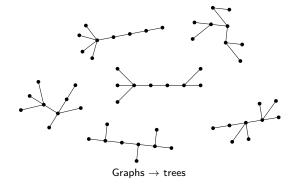
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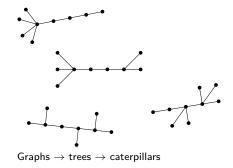
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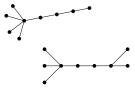
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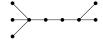
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$$\mathsf{Graphs} o \mathsf{trees} o \mathsf{caterpillars} o \mathrm{DB}_{a,b,c} o \mathsf{balanced} \ \mathrm{DB}_{a,b,c}$$

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A vertex is a **branching point** if at least three of its neighbours are non-leaf vertices.

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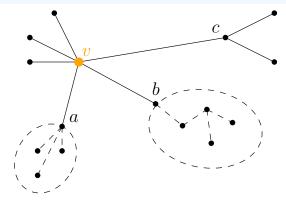
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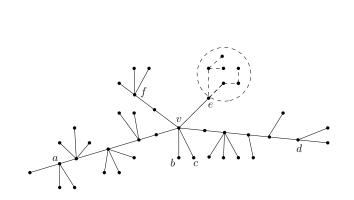
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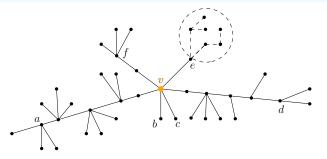
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A branching point v is **peripheral** if all connected components of G - v, except at most one, are caterpillars with an endpoint adjacent to v.



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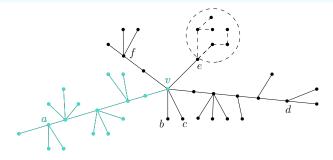
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A (peripheral) branching point together with such a caterpillar component is called a **brush**.



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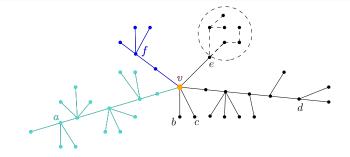
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Two brushes are **adjacent** if they share the same attachment point.



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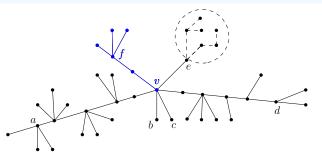
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A **broom** is a brush in which every vertex of the central path, except for the attachment point and (possibly) the other endpoint of this path, has degree two.



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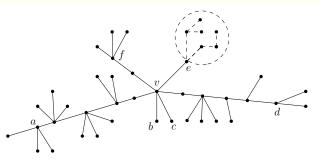
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Observation

Every pair of brushes either has disjoint vertex sets or shares precisely one vertex, the attaching vertex. Additionally, $d_B(v) = 1$ holds for every brush B and its attaching vertex v.



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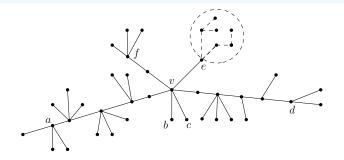
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Definition

The internal degree $d_i(v)$ of v is the number of its non-leaf neighbours. The branching sum of $G\!:$

$$BS(G) = \sum_{v \text{ is a branching}} d_i(v).$$

point in G



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Theorem [main result]

The graphs on n vertices with the maximum W_{ex} are balanced double brooms $DB_{a,b,c}$ with suitably chosen a, b and c, n = a + b + c.

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Theorem [main result]

The graphs on n vertices with the maximum W_{ex} are balanced double brooms $DB_{a,b,c}$ with suitably chosen a, b and c, n = a + b + c.

Claim 1

The maximum W_ex is attained by a tree.

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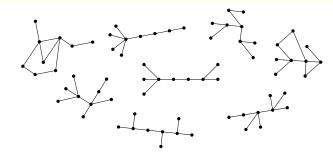
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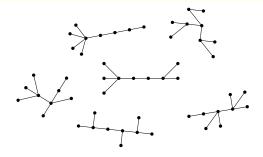
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Theorem [main result]

The graphs on n vertices with the maximum W_{ex} are balanced double brooms $DB_{a,b,c}$ with suitably chosen a, b and c, n = a + b + c.

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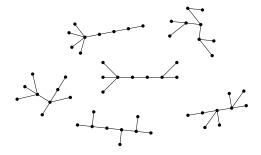
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Assume BS(G) > 0.

Claim 2

Let ${\cal B}$ be a brush of the extremal graph. Then there exist two other non-trivial brushes that are adjacent to each other.



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Claim 3

All brushes of the extremal graph except for at most one are brooms.

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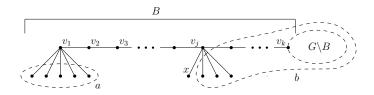
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Claim 3

All brushes of the extremal graph except for at most one are brooms.

Lemma

Let B be a non-trivial brush. If b>a, moving a pendant vertex x from v_j to v_1 strictly increases $W_{\rm ex}$. If b< a, this move strictly decreases $W_{\rm ex}$, and if b = a, $W_{\rm ex}$ remains the same.



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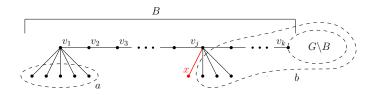
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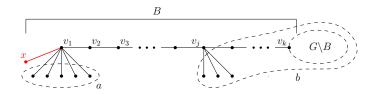
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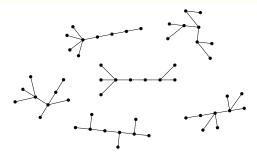
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The extremal graph is a tree with at most one non-broom brush; for every brush there exist two brooms that are adjacent to each other.

Claim 4

The maximum external Wiener index is attained by a caterpillar tree.



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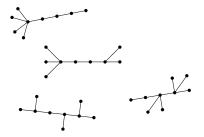
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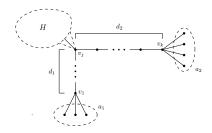
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The maximum external Wiener index is attained by a caterpillar tree.

The Sliding Lemma

If G consists of a double broom D with a subgraph H attached to v_j , then the maximum W_{ex} is attained for j = 1 or j = k.



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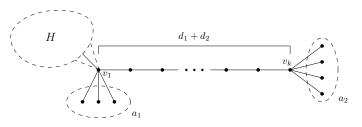
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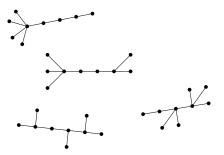
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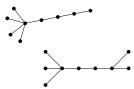
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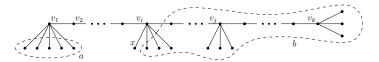
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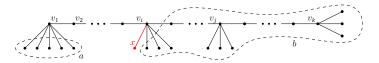
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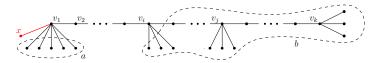
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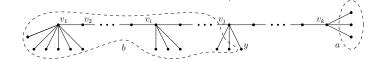
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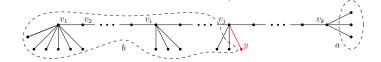
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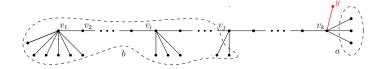
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[Stevanović, 2008]

Problem

Determine the graphs of a given order n and maximum degree Δ that attain the maximum value of the external Wiener index.

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[Plesník, 1984]

Problem

Determine the graphs of a given order \boldsymbol{n} and diameter that attain the maximum value of the external Wiener index.

References (1)

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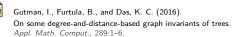
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