GRAPHS WITH MAXIMAL ENERGY

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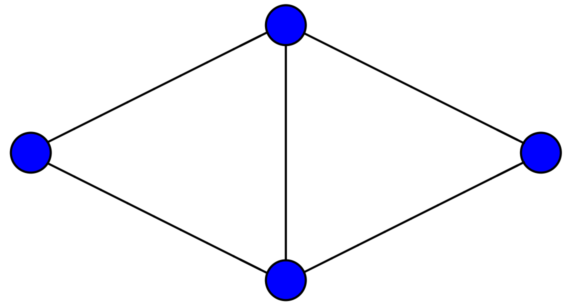
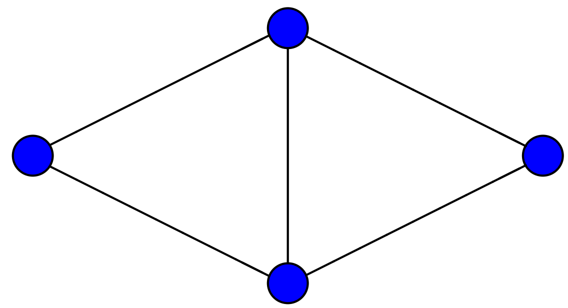
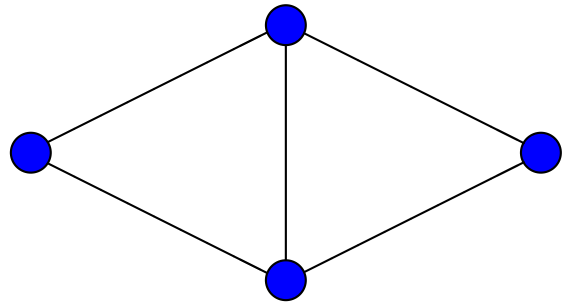
$\Gamma =$ 

$\Gamma =$ 

$$A_\Gamma = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

$\Gamma =$ 

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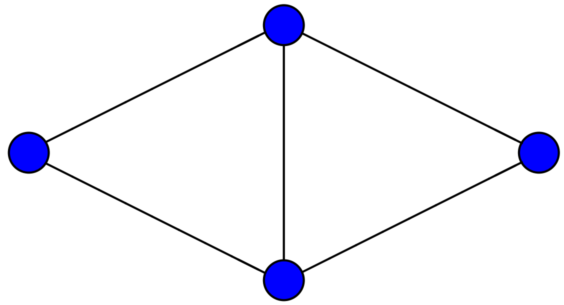
Eigenvalues: $0,\ -1,\ \frac{1}{2}(1 \pm \sqrt{17})$

$\Gamma =$ 

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Energy: $\mathcal{E}(\Gamma) = 0 + 1 + \frac{1}{2}(1 + \sqrt{17}) - \frac{1}{2}(1 - \sqrt{17}) = 1 + \sqrt{17}$

(Gutman 1978)

PROPOSITION

$$\mathcal{E}(K_n) = 2n - 2,\ \mathcal{E}(K_{k,k}) = n$$

$$\mathcal{E}(\Gamma + \Delta) = \mathcal{E}(\Gamma) + \mathcal{E}(\Delta),\ \ \mathcal{E}(\Gamma \times \Delta) = \mathcal{E}(\Gamma)\mathcal{E}(\Delta)$$

$$\mathcal{E}(\Delta) \leq \mathcal{E}(\Gamma) \text{ if } \Delta \text{ is an induced subgraph of } \Gamma$$

THEOREM (Koolen and Moulton 2001)

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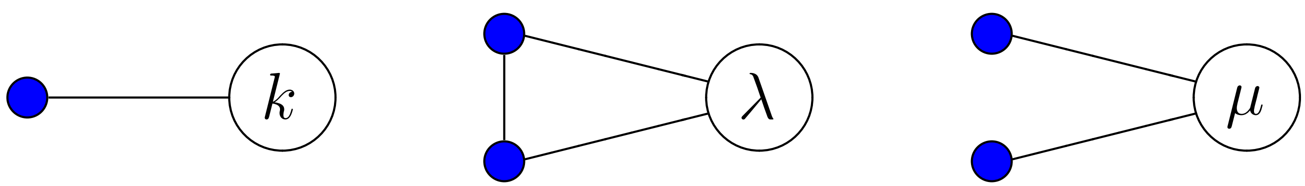

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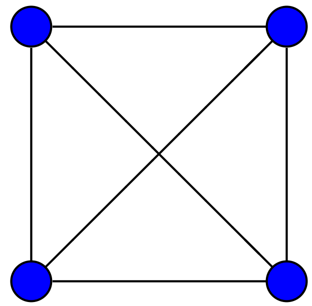
Max energy graph

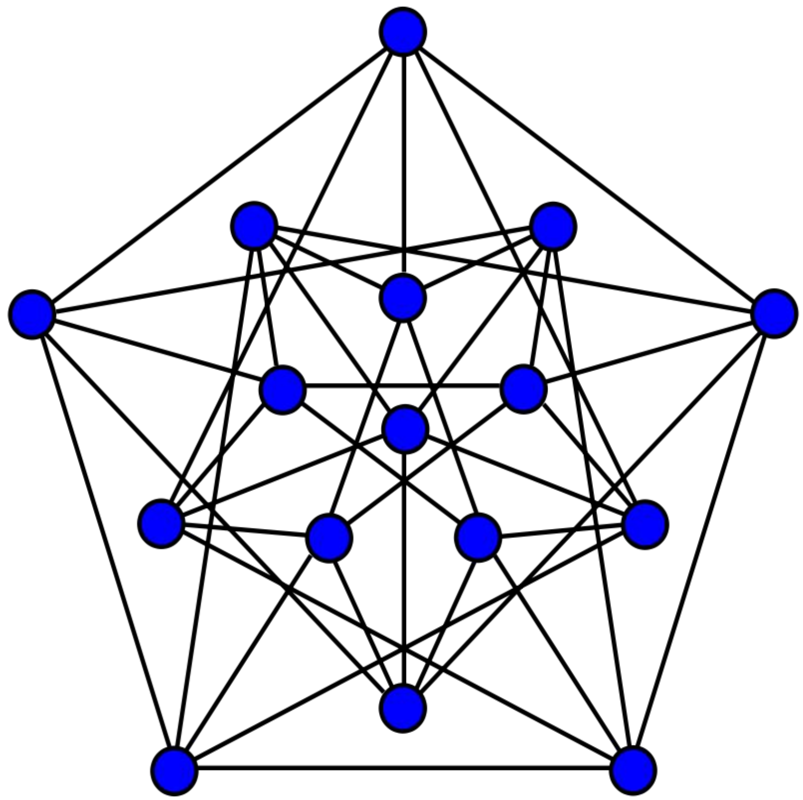
Max energy graph for $n = 4$



$$k = 3,\ \lambda = 2$$

$$\mathcal{E}(K_4) = 6$$

Max energy graph for $n = 16$



$$k = 5,\ \lambda = 0,\ \mu = 2$$

Complement $k = 10,\ \lambda = \mu = 6$ (Clebsch graph)

$$\mathcal{E}(\text{Clebsch}) = 40$$

Max energy graph for $n = 36$

THEOREM (McKay and Spence 2001)

There exist exactly 180 nonisomorphic max energy graphs with $n = 36$

$$k = 21,\ \lambda = \mu = 12,\ \mathcal{E}(\Gamma) = 126$$

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J: all-one matrix; H: $(+1,-1)$-matrix, $HH^\top = nI$,

$(H)_{i,i} = 1$, $H = H^\top$, $HJ = \ell J$, $\ell = -\sqrt{n}$.

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EXISTENCE

Necessary: $n = 4m^2$. **Sufficient:** $n = 4m^4$ (H and Xiang 2010),

$n = 4m^2$ and $m < 11$. Several construction for even m.

THEOREM (Nikiforov 2007)

Suppose Γ has maximum energy over all graphs on n vertices, then

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PROOF: Take a smallest max energy graph with $m \geq n$ vertices and delete $m{-}n$ vertices (arbitrarily)

AIM, Palo Alto, October 2006

Energy per vertex $\overline{\mathcal{E}}(\Gamma) = \mathcal{E}(\Gamma)/n$

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CONJECTURE (AIM group 2006)

If Γ is regular of degree k, then

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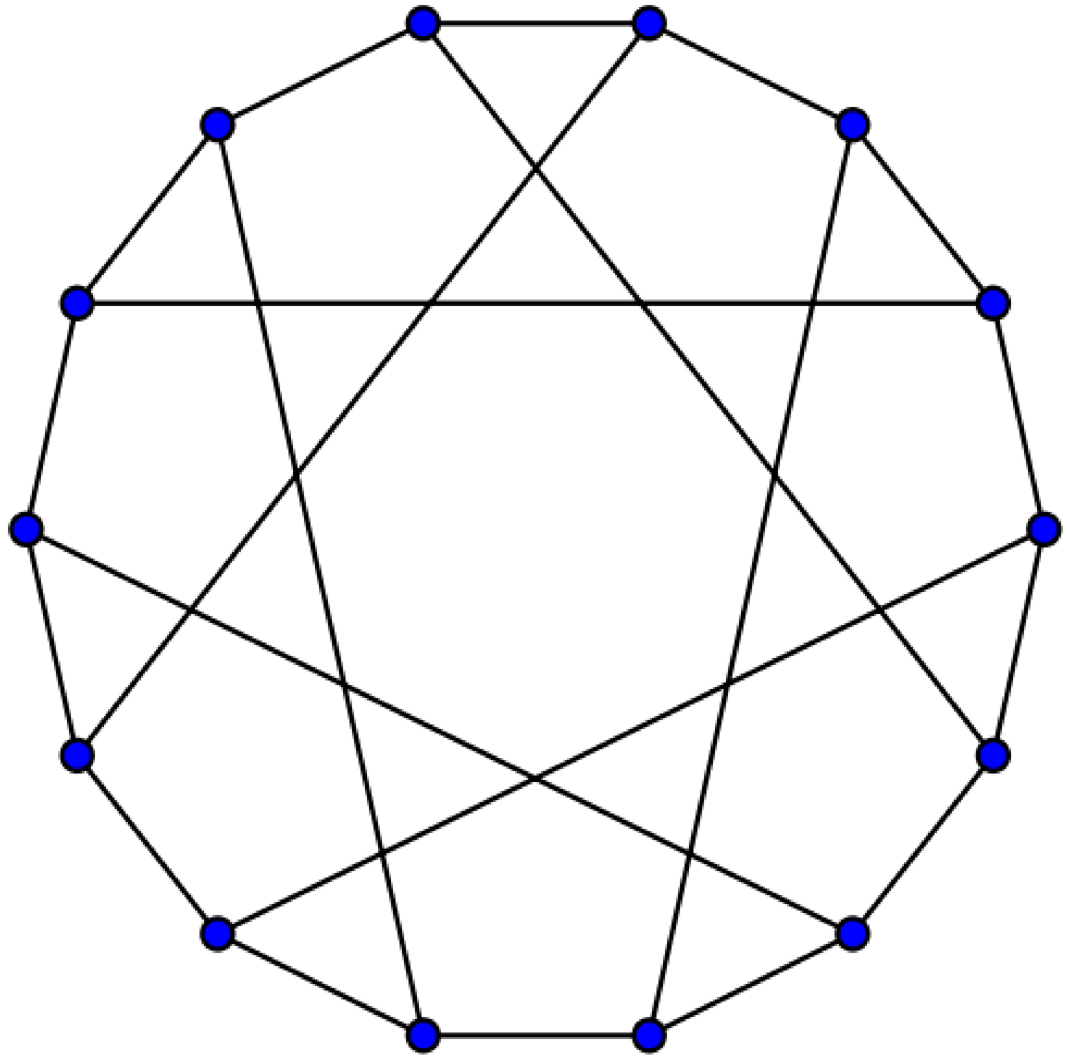
CONJECTURE (AIM group 2006)

If Γ is connected and regular of degree k, then

$$\overline{\mathcal{E}}(\Gamma) \ \leq \ \frac{k + (k^2 - k)\sqrt{k-1}}{k^2 - k + 1}$$

Equality holds **if and only if** Γ is the incidence graph of a projective plane of order $k-1$ or, when $k=2$, a hexagon or a triangle

$k = 3$



Incidence graph of the Fano plane (Heawood graph)

$$\overline{\mathcal{E}}(\Gamma) = (3 + 6\sqrt{2})/7 \approx 1.64$$

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PROOF: $\overline{\mathcal{E}}(\Gamma) = \overline{\mathcal{E}}(\Gamma \times K_2)$, so we can assume Γ is bipartite

Eigenvalues of A_Γ: $k = \lambda_1 \geq \cdots \geq \lambda_n$

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Apply Karush-Kuhn-Tucker to maximize $\Sigma\,|\lambda_i|$, subject to

$$\lambda_i = -\lambda_{n+1-i},\ |\lambda_i| \leq k,\ \Sigma\,\lambda_i^2 = kn,\ \Sigma\,\lambda_i^4 \geq nk(2k-1)$$

EXISTENCE

Necessary: If $k \equiv 2$ or $3 \pmod 4$, then $k-1$ is the sum of two squares; $k \neq 11$. **Sufficient:** $k-1$ is a prime power

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If Γ is k-regular with maximal $\overline{\mathcal{E}}(\Gamma)$, then $\overline{\mathcal{E}}(\Gamma) = \sqrt{k}(1+o(1))$

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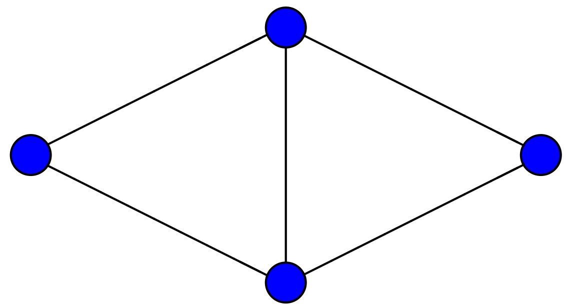
If Γ is k-regular with maximal $\overline{\mathcal{E}}(\Gamma)$, then $\overline{\mathcal{E}}(\Gamma) = \sqrt{k}(1+o(1))$

PROOF: Take a projective plane of smallest order $\ell > k$. Delete a flag. The remaining geometry is an elliptic semi-plane with point and line parallel classes. Delete $\ell - k + 1$ point and line classes. The incidence graph Γ is k-regular and $\overline{\mathcal{E}}(\Gamma) \approx \sqrt{k}$.

$\Gamma =$ 

$$S_\Gamma = \begin{bmatrix} 0 & -1 & -1 & 1 \\ -1 & 0 & -1 & -1 \\ -1 & -1 & 0 & -1 \\ 1 & -1 & -1 & 0 \end{bmatrix}$$

Eigenvalues: $\pm 1, \ \pm\sqrt{5}$

Seidel Energy: $\mathcal{E}_s(\Gamma) = 2 + 2\sqrt{5}$

PROPOSITION

$$\mathcal{E}_s(K_n) = 2n - 2, \;\; \mathcal{E}_s(K_{k,n-k}) = 2n - 2$$

$\mathcal{E}_s(\Gamma)$ is invariant under complementation and Seidel switching

$\mathcal{E}_s(\Delta) \leq \mathcal{E}_s(\Gamma)$ if Δ is an induced subgraph of Γ

THEOREM

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$$S_\Gamma^2 = (n-1)I$$

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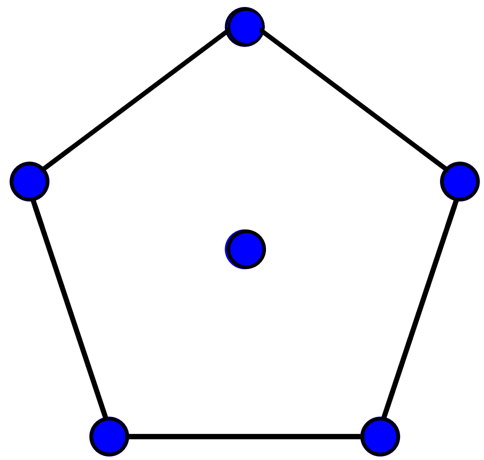
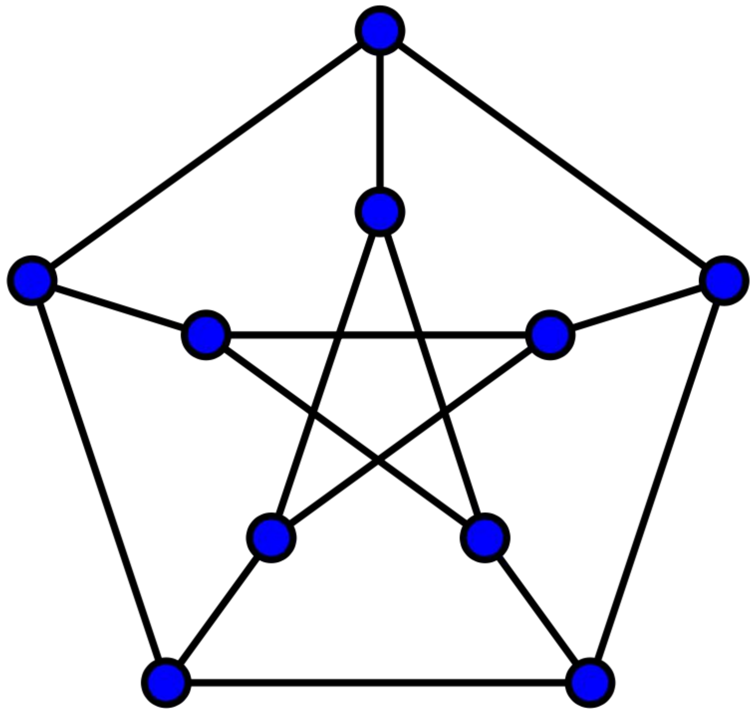
Max S-energy graph

Max S-energy graph for $n = 6$



$$\mathcal{E}_s(\text{Pentagon} + K_1) = 6\sqrt{5}$$

Max S-energy graph for $n = 10$



$\mathcal{E}_s(\text{Petersen}) = 30$

EXISTENCE

Necessary: $n \equiv 2 (\mathrm{mod}\ 4)$, $n-1$ is sum of two squares

Sufficient: $n \equiv 2 (\mathrm{mod}\ 4)$ and $n-1$ is a prime power

THEOREM

Suppose Γ has maximal $\mathcal{E}_s(\Gamma)$ over all graphs on n vertices, then

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PROOF: Take a smallest max S-energy graph with $m \geq n$ vertices

and add $m - n$ vertices (arbitrarily)

MINIMUM ENERGY

$\mathcal{E}(\Gamma) \geq 0$, equality **iff** Γ has no edges

Γ is k-regular, then $\overline{\mathcal{E}}(\Gamma) \geq 1$, equality **iff** $\Gamma = mK_{k,k}$

$\mathcal{E}_s(\Gamma) \geq \sqrt{2n(n-1)}$, equality impossible if $n > 2$

CONJECTURE

$$\mathcal{E}_s(\Gamma) \geq 2(n-1)$$

True if $n \leq 10$ (Swinkels 2010)

True if $|\det S_\Gamma| \geq n-1$ (Ghorbani 2013)

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- **W.H. Haemers**, Strongly regular graphs with maximal energy, *Linear Algebra and its Applications* 429 (2008), 2719–2723.
- **W.H. Haemers**, Seidel switching and graph energy, *MATCH Commun. Math. Comput. Chem.* 68 (2012), 653–659.
- **W.H. Haemers** and **Q. Xiang**, Strongly regular graphs with parameters $(4m^4, 2m^4+m^2, m^4+m^2, m^4+m^2)$ exist for all $m > 1$, *European Journal of Combinatorics* 31 (2010), 1553–1559.
- **J.H. Koolen** and **V. Moulton**, Maximal energy graphs, *Adv. in Appl. Math.* 26 (2001), 47-52.
- **X.Li, Y.Shi** and **I.Gutman**, *Graph Energy*, Springer, 2012.