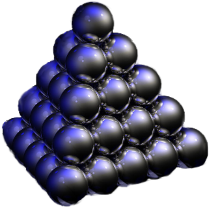
Moment methods in energy minimization

David de Laat

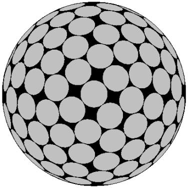
CWI Amsterdam

Andrejewski-Tage
Moment problems in theoretical physics
Konstanz, 9 April 2016

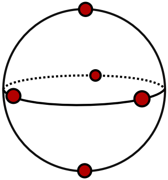
Packing and energy minimization



Sphere packing
Kepler conjecture (1611)



Spherical cap packing
Tammes problem (1930)



Energy minimization
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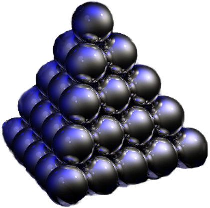

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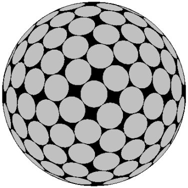

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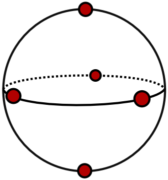

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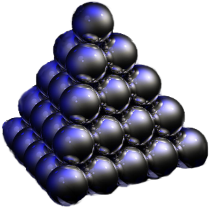

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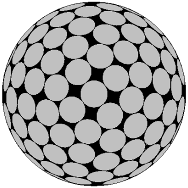

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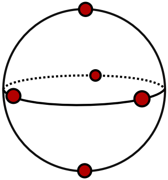

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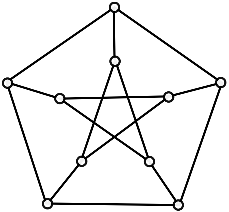
- This talk: Methods to find obstructions

The maximum independent set problem



Example: the Petersen graph

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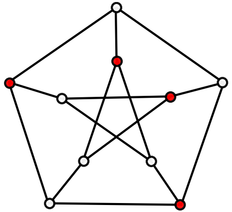

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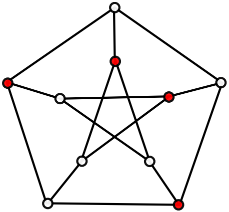

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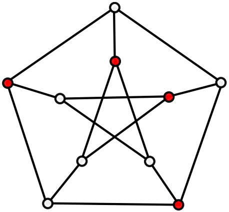

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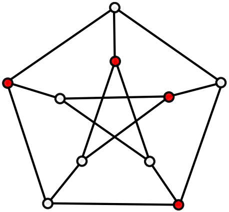

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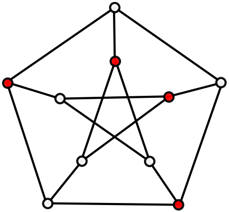

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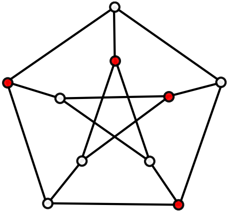

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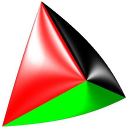
3×3 positive semidefinite matrices with unit diagonal:



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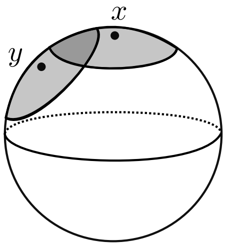

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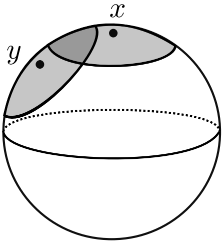

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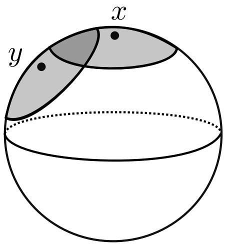

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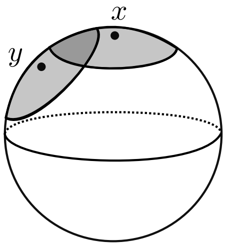

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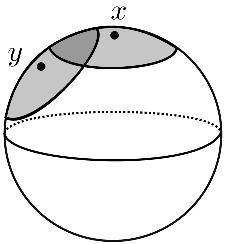

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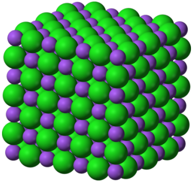
- Using symmetry reduction this reduces to a linear program known as the Delsarte LP bound

Bounds for binary packings [L–Oliveira–Vallentin 2014]



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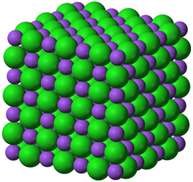

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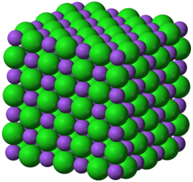

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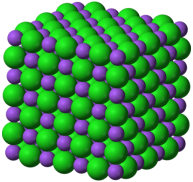

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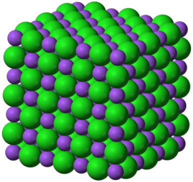

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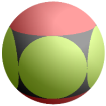

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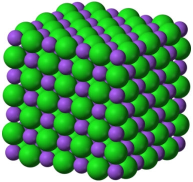

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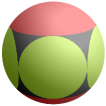

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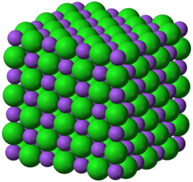

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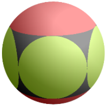

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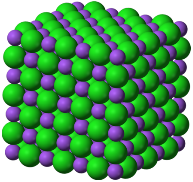

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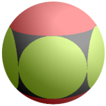

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- Question 2: Can we obtain arbitrarily good bounds?

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- Here $V = S^2$, $d(x, y) = \|x_i - x_j\|_2$, and $h(w) = 1/w$

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- Minimal energy:

$$E = \min_{S \in I_{=N}} \sum_{P \subseteq S} f(P)$$

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- E_t is a $\min\{2t, N\}$-point bound

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- E_t is a $\min\{2t, N\}$-point bound

$$E_1 \leq E_2 \leq \cdots \leq E_N$$

Moment methods in energy minimization

- For $S \in I_{=N}$, define the measure $\chi_S = \sum_{R \subseteq S} \delta_R$
- We can use this measure to compute the energy of S
- The energy of S is given by

$$\chi_S(f) = \int f(P)\, d\chi_S(P) = \sum_{R \subseteq S} f(R)$$

- This measure satisfies the following 3 properties:
  - χ_S is a positive measure
  - χ_S satisfies $\lambda(I_{=i}) = \binom{N}{i}$ for all i
  - χ_S is a *measure of positive type* (see next slide)
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Measures of positive type [L–Vallentin 2015]

- Operator:

$$A_t \colon \mathcal{C}(I_t \times I_t)_{\mathrm{sym}} \to \mathcal{C}(I_{2t}),\; A_t K(S) = \sum_{J,J' \in I_t : J \cup J' = S} K(J, J')$$

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- A measure $\lambda \in \mathcal{M}(I_{2t})$ is of *positive type* if

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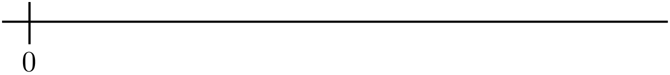
Computations using the dual hierarchy



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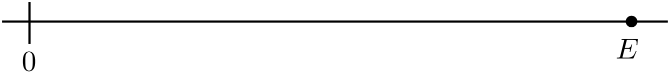

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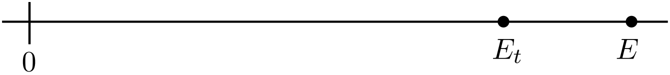

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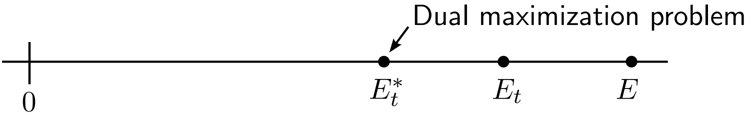

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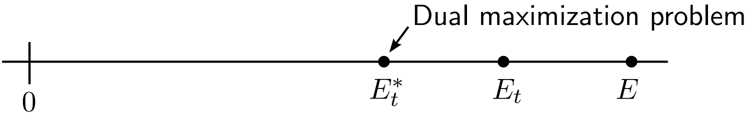

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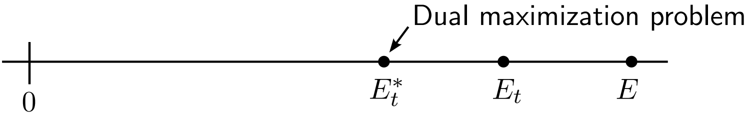

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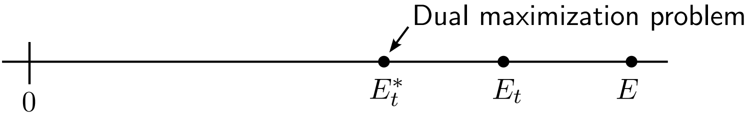

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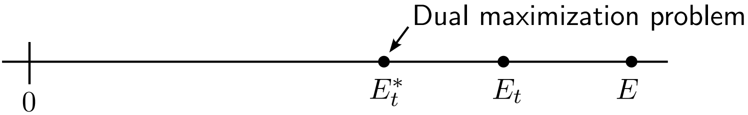

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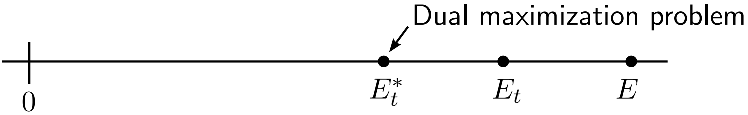

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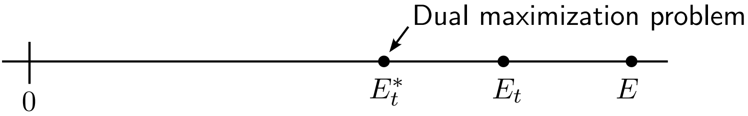

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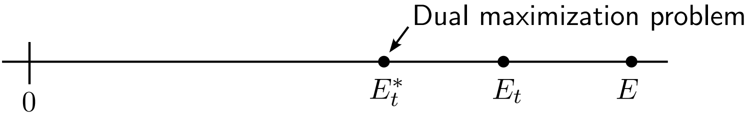

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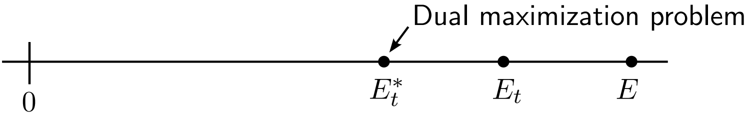

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- In principle this can be the trivial group, but for symmetry reduction a bigger group is better

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- By an "averaging argument" we may assume
  $K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}$ to be Γ-invariant:
  $K(\gamma J, \gamma J') = K(J, J')$ for all $\gamma \in \Gamma$ and $J, J' \in I_t$

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- To construct the matrices $Z_\pi(x, y)$ we need to "perform the harmonic analysis of I_t with respect to Γ"

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- We use this to lower bound E_2^* by maximization problems that have finitely many positive semidefinite matrix variables (but still infinitely many constraints)

Invariant theory

- These constraints are of the form

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- Now we have constraints of the form

$$q(u_1, \ldots, u_l) \geq 0 \quad \text{for} \quad (u_1, \ldots, u_l) \in \text{some semialgebraic set}$$

Sums of squares characterizations

- Putinar: Every positive polynomial on a compact set $S = \{x \in \mathbb{R}^n : g_1(x) \geq 0, \ldots, g_m(x) \geq 0\}$, where the set $\{g_1, \ldots, g_m\}$ has the Archimedean property, is of the form

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- This translates into interesting symmetries of the $q(u_1, \ldots, u_l)$ polynomials

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- This gives significant computational savings for our problems

Computational results for the Thomson problem

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$$V = S^2, \quad d(x,y) = \|x-y\|_2, \quad \text{and} \quad h(w) = \frac{1}{w}$$

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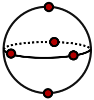
- We compute E_2^* using a semidefinite programming solver
- This is the first time a four 4-bound has been computed for a continuous problem
- We show E_2^* is sharp for 5 particles on S^2 (up to solver precision), which suggests we can use E_2^* to derive a small proof of optimality for this problem



Phase transitions

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- It would be very interesting if E_2^* is sharp for all s
  - Lower bound that stays sharp throughout a phase transition
  - Local-to-global behaviour in confined geometries

Thank you!

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