Moment methods in energy minimization

David de Laat Delft University of Technology (Joint with Fernando Oliveira and Frank Vallentin)

> László Fejes Tóth Centennial 26 June 2015, Budapest

Packing and energy minimization



Sphere packing Kepler conjecture (1611)





Energy minimization Thomson problem (1904)

Spherical cap packing Tammes problem (1930)

Packing and energy minimization



Sphere packing Kepler conjecture (1611)





Energy minimization Thomson problem (1904)

Spherical cap packing Tammes problem (1930)

Typically difficult to prove optimality of constructions

Packing and energy minimization



Sphere packing Kepler conjecture (1611)





Energy minimization Thomson problem (1904)

Spherical cap packing Tammes problem (1930)

- Typically difficult to prove optimality of constructions
- This talk: Methods to find obstructions







Example: the Petersen graph

In general difficult to solve to optimality (NP-hard)



- In general difficult to solve to optimality (NP-hard)
- The Lovász ϑ -number upper bounds the independence number



- In general difficult to solve to optimality (NP-hard)
- The Lovász ϑ -number upper bounds the independence number
- Efficiently computable through semidefinite programming



- In general difficult to solve to optimality (NP-hard)
- The Lovász ϑ -number upper bounds the independence number
- Efficiently computable through semidefinite programming
- Semidefinite program: optimize a linear functional over the intersection of an affine space with the cone of $n \times n$ positive semidefinite matrices



- In general difficult to solve to optimality (NP-hard)
- The Lovász ϑ -number upper bounds the independence number
- Efficiently computable through semidefinite programming
- Semidefinite program: optimize a linear functional over the intersection of an affine space with the cone of $n \times n$ positive semidefinite matrices
 - 3×3 positive semidefinite matrices with unit diagonal:



- Example: the spherical cap packing problem
 - As vertex set we take the unit sphere

- As vertex set we take the unit sphere
- Two distinct vertices x and y are adjacent if the spherical caps centered about x and y intersect in their interiors:



Example: the spherical cap packing problem

- As vertex set we take the unit sphere
- Two distinct vertices x and y are adjacent if the spherical caps centered about x and y intersect in their interiors:



Optimal density is proportional to the independence number

- As vertex set we take the unit sphere
- Two distinct vertices x and y are adjacent if the spherical caps centered about x and y intersect in their interiors:



- Optimal density is proportional to the independence number
- \blacktriangleright ϑ generalizes to an infinite dimensional maximization problem

- As vertex set we take the unit sphere
- Two distinct vertices x and y are adjacent if the spherical caps centered about x and y intersect in their interiors:



- Optimal density is proportional to the independence number
- ϑ generalizes to an infinite dimensional maximization problem
- ► Use optimization duality, harmonic analysis, and real algebraic geometry to approximate ϑ by a semidefinite program

- As vertex set we take the unit sphere
- ► Two distinct vertices x and y are adjacent if the spherical caps centered about x and y intersect in their interiors:



- Optimal density is proportional to the independence number
- ϑ generalizes to an infinite dimensional maximization problem
- ► Use optimization duality, harmonic analysis, and real algebraic geometry to approximate ϑ by a semidefinite program
- For this problem this reduces to the Delsarte LP bound





Density: $79.3 \dots \%$



Density: 79.3...%Our upper bound: 81.3...%

Sodium Chloride



Density: 79.3...%Our upper bound: 81.3...%

Sodium Chloride

Question 1: Can we use this method for optimality proofs?



Density: $79.3 \dots \%$ Our upper bound: $81.3 \dots \%$

Sodium Chloride

- Question 1: Can we use this method for optimality proofs?
- Florian and Heppes prove optimality of the following packing:





Density: $79.3 \dots \%$ Our upper bound: $81.3 \dots \%$

Sodium Chloride

- Question 1: Can we use this method for optimality proofs?
- Florian and Heppes prove optimality of the following packing:



► We prove ϑ is sharp for this problem, which gives a simple optimality proof



Density: 79.3...%Our upper bound: 81.3...%

Sodium Chloride

- Question 1: Can we use this method for optimality proofs?
- Florian and Heppes prove optimality of the following packing:



- ► We prove ϑ is sharp for this problem, which gives a simple optimality proof
- ► We slightly improve the Cohn-Elkies bound to give the best known bounds for sphere packing in dimensions 4 - 7 and 9



Density: 79.3...%Our upper bound: 81.3...%

Sodium Chloride

- Question 1: Can we use this method for optimality proofs?
- Florian and Heppes prove optimality of the following packing:



- ► We prove ϑ is sharp for this problem, which gives a simple optimality proof
- ► We slightly improve the Cohn-Elkies bound to give the best known bounds for sphere packing in dimensions 4 - 7 and 9
- Question 2: Can we obtain arbitrarily good bounds?

▶ Goal: Find the ground state energy of a system of N particles in a compact container V with pair potential h

- ▶ Goal: Find the ground state energy of a system of N particles in a compact container V with pair potential h
- Assume $h(\{x, y\}) \to \infty$ as x and y converge

- ▶ Goal: Find the ground state energy of a system of N particles in a compact container V with pair potential h
- Assume $h(\{x,y\}) \to \infty$ as x and y converge
- ▶ Define a graph with vertex set V where two distinct vertices x and y are adjacent if h({x, y}) is large

- ▶ Goal: Find the ground state energy of a system of N particles in a compact container V with pair potential h
- Assume $h(\{x, y\}) \to \infty$ as x and y converge
- ▶ Define a graph with vertex set V where two distinct vertices x and y are adjacent if h({x, y}) is large
- Let I_t be the set of independent sets with $\leq t$ elements

- ▶ Goal: Find the ground state energy of a system of N particles in a compact container V with pair potential h
- Assume $h(\{x, y\}) \to \infty$ as x and y converge
- ▶ Define a graph with vertex set V where two distinct vertices x and y are adjacent if h({x, y}) is large
- Let I_t be the set of independent sets with $\leq t$ elements
- Let $I_{=t}$ be the set of independent sets with t elements

- ▶ Goal: Find the ground state energy of a system of N particles in a compact container V with pair potential h
- Assume $h(\{x,y\}) \to \infty$ as x and y converge
- ▶ Define a graph with vertex set V where two distinct vertices x and y are adjacent if h({x, y}) is large
- Let I_t be the set of independent sets with $\leq t$ elements
- Let $I_{=t}$ be the set of independent sets with t elements
- These sets are compact topological spaces

- ▶ Goal: Find the ground state energy of a system of N particles in a compact container V with pair potential h
- Assume $h(\{x,y\}) \to \infty$ as x and y converge
- ▶ Define a graph with vertex set V where two distinct vertices x and y are adjacent if h({x, y}) is large
- Let I_t be the set of independent sets with $\leq t$ elements
- Let $I_{=t}$ be the set of independent sets with t elements
- These sets are compact topological spaces
- We can view h as a function in $C(I_N)$ supported on $I_{=2}$

- ▶ Goal: Find the ground state energy of a system of N particles in a compact container V with pair potential h
- Assume $h(\{x, y\}) \to \infty$ as x and y converge
- ▶ Define a graph with vertex set V where two distinct vertices x and y are adjacent if h({x, y}) is large
- Let I_t be the set of independent sets with $\leq t$ elements
- Let $I_{=t}$ be the set of independent sets with t elements
- These sets are compact topological spaces
- We can view h as a function in $C(I_N)$ supported on $I_{=2}$
- Minimal energy:

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

Moment methods in energy minimization

▶ For $S \in I_{=N}$, define the measure $\chi_S = \sum_{R \subseteq S} \delta_R$
• For $S \in I_{=N}$, define the measure $\chi_S = \sum_{R \subseteq S} \delta_R$

• The energy of S is given by $\chi_S(h)$

- For $S \in I_{=N}$, define the measure $\chi_S = \sum_{R \subseteq S} \delta_R$
- The energy of S is given by $\chi_S(h)$
- This measure
 - is positive
 - ► is a moment measure
 - \blacktriangleright satisfies $\lambda(I_{=i}) = \binom{N}{i}$ for all i

- ▶ For $S \in I_{=N}$, define the measure $\chi_S = \sum_{R \subseteq S} \delta_R$
- The energy of S is given by $\chi_S(h)$
- This measure
 - is positive
 - is a moment measure
 - satisfies $\lambda(I_{=i}) = \binom{N}{i}$ for all i
- Relaxations: For $t = 1, \ldots, N$,

$$E_t = \min\left\{\lambda(h) : \lambda \in \mathcal{M}(I_{2t}) \text{ positive moment measure}, \\ \lambda(I_{=i}) = \binom{N}{i} \text{ for all } 0 \le i \le 2t\right\}$$

- ▶ For $S \in I_{=N}$, define the measure $\chi_S = \sum_{R \subseteq S} \delta_R$
- The energy of S is given by $\chi_S(h)$
- This measure
 - is positive
 - is a moment measure
 - \blacktriangleright satisfies $\lambda(I_{=i}) = \binom{N}{i}$ for all i
- Relaxations: For $t = 1, \ldots, N$,

$$E_t = \min\left\{\lambda(h) : \lambda \in \mathcal{M}(I_{2t}) \text{ positive moment measure}, \\ \lambda(I_{=i}) = \binom{N}{i} \text{ for all } 0 \le i \le 2t\right\}$$

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

- ▶ For $S \in I_{=N}$, define the measure $\chi_S = \sum_{R \subseteq S} \delta_R$
- The energy of S is given by $\chi_S(h)$
- This measure
 - is positive
 - is a moment measure
 - satisfies $\lambda(I_{=i}) = \binom{N}{i}$ for all i
- Relaxations: For $t = 1, \ldots, N$,

$$E_t = \min\left\{\lambda(h) : \lambda \in \mathcal{M}(I_{2t}) \text{ positive moment measure}, \\ \lambda(I_{=i}) = \binom{N}{i} \text{ for all } 0 \le i \le 2t\right\}$$

$$E_1 \le E_2 \le \dots \le E_N = E$$

► Operator:

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

► Operator:

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

Dual operator

$$A_t^* \colon \mathcal{M}(I_{2t}) \to \mathcal{M}(I_t \times I_t)$$

Operator:

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

Dual operator

$$A_t^* \colon \mathcal{M}(I_{2t}) \to \mathcal{M}(I_t \times I_t)$$

• Cone of positive definite kernels: $C(I_t \times I_t)_{\succeq 0}$

Operator:

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

Dual operator

$$A_t^* \colon \mathcal{M}(I_{2t}) \to \mathcal{M}(I_t \times I_t)$$

- Cone of positive definite kernels: $C(I_t \times I_t)_{\succeq 0}$
- Dual cone:

 $\mathcal{M}(I_t \times I_t)_{\succeq 0} = \{ \mu \in \mathcal{M}(I_t \times I_t)_{\text{sym}} : \mu(K) \ge 0 \text{ for all } K \in \mathcal{C}(I_t \times I_t)_{\succeq 0} \}$

Operator:

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

Dual operator

$$A_t^* \colon \mathcal{M}(I_{2t}) \to \mathcal{M}(I_t \times I_t)$$

- Cone of positive definite kernels: $C(I_t \times I_t)_{\succeq 0}$
- Dual cone:

 $\mathcal{M}(I_t \times I_t)_{\succeq 0} = \{ \mu \in \mathcal{M}(I_t \times I_t)_{\text{sym}} : \mu(K) \ge 0 \text{ for all } K \in \mathcal{C}(I_t \times I_t)_{\succeq 0} \}$

• A measure $\lambda \in \mathcal{M}(I_{2t})$ is a *moment measure* if

$$A_t^* \lambda \in \mathcal{M}(I_t \times I_t)_{\succeq 0}$$

• Recall:
$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

- Recall: $E_1 \leq E_2 \leq \cdots \leq E_N = E$
- Positive semidefinite form $\langle f,g\rangle = A_t^*\lambda(f\otimes g)$ on $\mathcal{C}(I_t)$

• Recall:
$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

- Positive semidefinite form $\langle f,g\rangle = A_t^*\lambda(f\otimes g)$ on $\mathcal{C}(I_t)$
- Define $\mathcal{N}_t(\lambda) = \{f \in \mathcal{C}(I_t) : \langle f, f \rangle = 0\}$

• Recall:
$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

- Positive semidefinite form $\langle f,g\rangle = A_t^*\lambda(f\otimes g)$ on $\mathcal{C}(I_t)$
- Define $\mathcal{N}_t(\lambda) = \{f \in \mathcal{C}(I_t) : \langle f, f \rangle = 0\}$

• Recall:
$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

- Positive semidefinite form $\langle f,g\rangle = A_t^*\lambda(f\otimes g)$ on $\mathcal{C}(I_t)$
- Define $\mathcal{N}_t(\lambda) = \{f \in \mathcal{C}(I_t) : \langle f, f \rangle = 0\}$
- If $\lambda \in \mathcal{M}(I_{2t})$ is a moment measure and

$$\mathcal{C}(I_t) = \mathcal{C}(I_{t-1}) + \mathcal{N}_t(\lambda),$$

then for every $l\geq t,$ we can extend λ to a moment measure $\bar{\lambda}\in\mathcal{M}(I_{2l})$

• Recall:
$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

- Positive semidefinite form $\langle f,g\rangle = A_t^*\lambda(f\otimes g)$ on $\mathcal{C}(I_t)$
- Define $\mathcal{N}_t(\lambda) = \{f \in \mathcal{C}(I_t) : \langle f, f \rangle = 0\}$
- If $\lambda \in \mathcal{M}(I_{2t})$ is a moment measure and

$$\mathcal{C}(I_t) = \mathcal{C}(I_{t-1}) + \mathcal{N}_t(\lambda),$$

then for every $l \geq t$, we can extend λ to a moment measure $\bar{\lambda} \in \mathcal{M}(I_{2l})$

► $\lambda(I_{=i}) = {N \choose i}$ for $0 \le i \le 2t \Rightarrow \overline{\lambda}(I_{=i}) = {N \choose i}$ for $0 \le i \le 2l$

• Recall:
$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

- Positive semidefinite form $\langle f,g\rangle = A_t^*\lambda(f\otimes g)$ on $\mathcal{C}(I_t)$
- Define $\mathcal{N}_t(\lambda) = \{f \in \mathcal{C}(I_t) : \langle f, f \rangle = 0\}$
- If $\lambda \in \mathcal{M}(I_{2t})$ is a moment measure and

$$\mathcal{C}(I_t) = \mathcal{C}(I_{t-1}) + \mathcal{N}_t(\lambda),$$

then for every $l\geq t,$ we can extend λ to a moment measure $\bar{\lambda}\in\mathcal{M}(I_{2l})$

► $\lambda(I_{=i}) = {N \choose i}$ for $0 \le i \le 2t \Rightarrow \overline{\lambda}(I_{=i}) = {N \choose i}$ for $0 \le i \le 2l$

If an optimal solution λ of E_t satisfies $C(I_t) = C(I_{t-1}) + \mathcal{N}_t(\lambda)$, then $E_t = E_N = E$













▶ In E_t^* we optimize over kernels $K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}$



- ▶ In E_t^* we optimize over kernels $K \in C(I_t \times I_t)_{\succeq 0}$
- Idea: Optimize over truncated Fourier series of K

• A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$

- A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Let Γ be a group such that h is Γ -invariant

- A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Let Γ be a group such that h is Γ -invariant
- We may assume K to be Γ -invariant

- A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Let Γ be a group such that h is Γ -invariant
- We may assume K to be Γ-invariant

$$\blacktriangleright$$
 We have $K(x,y) = \sum_{\pi \in \hat{\Gamma}} \langle \hat{K}(\pi), Z_{\pi}(x,y) \rangle$

- A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Let Γ be a group such that h is Γ -invariant
- We may assume K to be Γ-invariant
- We have $K(x,y) = \sum_{\pi \in \hat{\Gamma}} \langle \hat{K}(\pi), Z_{\pi}(x,y) \rangle$
- To construct Z_{π} we need a symmetry adapted basis of $\mathcal{C}(I_t)$

- A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Let Γ be a group such that h is Γ -invariant
- We may assume K to be Γ-invariant
- We have $K(x,y) = \sum_{\pi \in \hat{\Gamma}} \langle \hat{K}(\pi), Z_{\pi}(x,y) \rangle$
- To construct Z_{π} we need a symmetry adapted basis of $\mathcal{C}(I_t)$
- We can construct such a basis if we know how to

- A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Let Γ be a group such that h is Γ -invariant
- We may assume K to be Γ-invariant
- We have $K(x,y) = \sum_{\pi \in \hat{\Gamma}} \langle \hat{K}(\pi), Z_{\pi}(x,y) \rangle$
- To construct Z_{π} we need a symmetry adapted basis of $\mathcal{C}(I_t)$
- We can construct such a basis if we know how to
 - 1. explicitly decompose $\mathcal{C}(V)$ into irreducibles

- A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Let Γ be a group such that h is Γ -invariant
- We may assume K to be Γ-invariant
- We have $K(x,y) = \sum_{\pi \in \hat{\Gamma}} \langle \hat{K}(\pi), Z_{\pi}(x,y) \rangle$
- To construct Z_{π} we need a symmetry adapted basis of $\mathcal{C}(I_t)$
- We can construct such a basis if we know how to
 - 1. explicitly decompose $\mathcal{C}(V)$ into irreducibles
 - 2. explicitly decompose tensor products of these into irreducibles

- A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Let Γ be a group such that h is Γ -invariant
- We may assume K to be Γ-invariant

• We have
$$K(x,y) = \sum_{\pi \in \hat{\Gamma}} \langle \hat{K}(\pi), Z_{\pi}(x,y) \rangle$$

- To construct Z_{π} we need a symmetry adapted basis of $\mathcal{C}(I_t)$
- We can construct such a basis if we know how to
 - 1. explicitly decompose $\mathcal{C}(V)$ into irreducibles
 - 2. explicitly decompose tensor products of these into irreducibles
- Let $V = S^2$, $\Gamma = O(3)$, and t = 2

- A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Let Γ be a group such that h is Γ -invariant
- We may assume K to be Γ-invariant

• We have
$$K(x,y) = \sum_{\pi \in \hat{\Gamma}} \langle \hat{K}(\pi), Z_{\pi}(x,y) \rangle$$

- To construct Z_{π} we need a symmetry adapted basis of $\mathcal{C}(I_t)$
- We can construct such a basis if we know how to
 - 1. explicitly decompose $\mathcal{C}(V)$ into irreducibles
 - 2. explicitly decompose tensor products of these into irreducibles
- Let $V = S^2$, $\Gamma = O(3)$, and t = 2
- Decompose $\mathcal{C}(S^2)$ into irreducibles: Spherical harmonics

- A group action of Γ on V extends to an action on I_t by $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Let Γ be a group such that h is Γ -invariant
- We may assume K to be Γ-invariant

• We have
$$K(x,y) = \sum_{\pi \in \hat{\Gamma}} \langle \hat{K}(\pi), Z_{\pi}(x,y) \rangle$$

- To construct Z_{π} we need a symmetry adapted basis of $\mathcal{C}(I_t)$
- We can construct such a basis if we know how to
 - 1. explicitly decompose $\mathcal{C}(V)$ into irreducibles
 - 2. explicitly decompose tensor products of these into irreducibles
- Let $V = S^2$, $\Gamma = O(3)$, and t = 2
- Decompose $\mathcal{C}(S^2)$ into irreducibles: Spherical harmonics
- Decompose the tensor products: Clebsch-Gordan coefficients

Invariant theory and real algebraic geometry

• In E_2^* we have the constraints

 $A_t K(S) \ge \ldots$ for $S \in I_4$
• In E_2^* we have the constraints

 $A_t K(S) \ge \ldots$ for $S \in I_4$

▶ We can view
$$A_t K(S)$$
 as a polynomial
 $p: \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ with
 $p(\gamma x_1, \dots, \gamma x_4) = p(x_1, \dots, x_4)$ for all $\gamma \in O(3)$

• In E_2^* we have the constraints

 $A_t K(S) \ge \ldots$ for $S \in I_4$

- ► We can view $A_t K(S)$ as a polynomial $p: \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ with $p(\gamma x_1, \dots, \gamma x_4) = p(x_1, \dots, x_4)$ for all $\gamma \in O(3)$
- Invariant theory: we can write A_tK(S) as a polynomial in 6 inner products

• In E_2^* we have the constraints

 $A_t K(S) \ge \ldots$ for $S \in I_4$

- ► We can view $A_t K(S)$ as a polynomial $p: \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ with $p(\gamma x_1, \dots, \gamma x_4) = p(x_1, \dots, x_4)$ for all $\gamma \in O(3)$
- ► Invariant theory: we can write A_tK(S) as a polynomial in 6 inner products
- To compute these polynomials we need to solve large sparse linear systems

• In E_2^* we have the constraints

$$A_t K(S) \ge \dots$$
 for $S \in I_4$

- ► We can view $A_t K(S)$ as a polynomial $p: \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ with $p(\gamma x_1, \dots, \gamma x_4) = p(x_1, \dots, x_4)$ for all $\gamma \in O(3)$
- ► Invariant theory: we can write A_tK(S) as a polynomial in 6 inner products
- To compute these polynomials we need to solve large sparse linear systems
- Use sum of squares techniques from real algebraic geometry to model the inequality constraints using semidefinite constraints

• In E_2^* we have the constraints

$$A_t K(S) \ge \dots$$
 for $S \in I_4$

- ► We can view $A_t K(S)$ as a polynomial $p: \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ with $p(\gamma x_1, \dots, \gamma x_4) = p(x_1, \dots, x_4)$ for all $\gamma \in O(3)$
- ► Invariant theory: we can write A_tK(S) as a polynomial in 6 inner products
- To compute these polynomials we need to solve large sparse linear systems
- Use sum of squares techniques from real algebraic geometry to model the inequality constraints using semidefinite constraints
- ▶ We give a symmetrized version of Putinar's theorem to exploit the S_N symmetry in the particles

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

In the Thomson problem we take

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

The Thomson problem has been solved for:
 3 (1912), 4, 6 (1992), 12 (1996), and 5 (2010) particles

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

- The Thomson problem has been solved for:
 3 (1912), 4, 6 (1992), 12 (1996), and 5 (2010) particles
- E_1^* is sharp for 3, 4, 6, and 12 particles (Yudin's LP bound)

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

- The Thomson problem has been solved for:
 3 (1912), 4, 6 (1992), 12 (1996), and 5 (2010) particles
- E_1^* is sharp for 3, 4, 6, and 12 particles (Yudin's LP bound)
- \blacktriangleright Compute E_2^* numerically using semidefinite programming

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

- The Thomson problem has been solved for:
 3 (1912), 4, 6 (1992), 12 (1996), and 5 (2010) particles
- E_1^* is sharp for 3, 4, 6, and 12 particles (Yudin's LP bound)
- Compute E_2^* numerically using semidefinite programming
- E_2^* appears to be sharp for 5 particles (6 digits of precision)



Thank you!

- D. de Laat, Moment methods in energy minimization, In preparation.
- D. de Laat, F. Vallentin, A semidefinite programming hierarchy for packing problems in discrete geometry, Math. Program., Ser. B 151 (2015), 529-553.
- D. de Laat, F.M. Oliveira, F. Vallentin, Upper bounds for packings of spheres of several radii, Forum Math. Sigma 2 (2014), e23 (42 pages).

Image credits: Sphere packing: Grek L Elliptope: Philipp Rostalski Sodium Chloride: Ben Mills