# Energy minimization via moment hierarchies 

## David de Laat (TU Delft)

ESI Workshop on Optimal Point Configurations and Applications
16 October 2014

## Energy minimization

- What is the minimal potential energy $E$ when we put $N$ particles with pair potential $h$ in a container $V$ ?


## Energy minimization

- What is the minimal potential energy $E$ when we put $N$ particles with pair potential $h$ in a container $V$ ?
- Example: For the Thomson problem we take

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

## Energy minimization

- What is the minimal potential energy $E$ when we put $N$ particles with pair potential $h$ in a container $V$ ?
- Example: For the Thomson problem we take

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

- As an optimization problem:

$$
E=\min _{S \in\binom{V}{N}} \sum_{P \in\binom{S}{2}} h(P)
$$

## Approach

- Configurations provide upper bounds on the optimal energy $E$


## Approach

- Configurations provide upper bounds on the optimal energy $E$
- To prove a configuration is good (or optimal) we need good lower bounds for $E$


## Approach

- Configurations provide upper bounds on the optimal energy $E$
- To prove a configuration is good (or optimal) we need good lower bounds for $E$

Some systematic approaches for obtaining bounds:

- Linear programming bounds using the pair correlation function [Delsarte 1973, Delsarte-Goethals-Seidel 1977, Yudin 1992]


## Approach

- Configurations provide upper bounds on the optimal energy $E$
- To prove a configuration is good (or optimal) we need good lower bounds for $E$

Some systematic approaches for obtaining bounds:

- Linear programming bounds using the pair correlation function [Delsarte 1973, Delsarte-Goethals-Seidel 1977, Yudin 1992]
- 3-point bounds using 3-point correlation functions and constraints arising from the stabilizer subgroup of 1 point [Schrijver 2005, Bachoc-Vallentin 2008, Cohn-Woo 2012]


## Approach

- Configurations provide upper bounds on the optimal energy $E$
- To prove a configuration is good (or optimal) we need good lower bounds for $E$

Some systematic approaches for obtaining bounds:

- Linear programming bounds using the pair correlation function [Delsarte 1973, Delsarte-Goethals-Seidel 1977, Yudin 1992]
- 3-point bounds using 3-point correlation functions and constraints arising from the stabilizer subgroup of 1 point [Schrijver 2005, Bachoc-Vallentin 2008, Cohn-Woo 2012]
- $k$-point bounds using stabilizer subgroup of $k-2$ points [Musin 2007]


## Approach

- Configurations provide upper bounds on the optimal energy $E$
- To prove a configuration is good (or optimal) we need good lower bounds for $E$

Some systematic approaches for obtaining bounds:

- Linear programming bounds using the pair correlation function [Delsarte 1973, Delsarte-Goethals-Seidel 1977, Yudin 1992]
- 3-point bounds using 3-point correlation functions and constraints arising from the stabilizer subgroup of 1 point [Schrijver 2005, Bachoc-Vallentin 2008, Cohn-Woo 2012]
- $k$-point bounds using stabilizer subgroup of $k-2$ points [Musin 2007]
- Hierarchy for packing problems [L.-Vallentin 2014]


## This talk

- Hierarchy obtained by generalizing Lasserre's hierarchy from combinatorial optimization to the continuous setting


## This talk

- Hierarchy obtained by generalizing Lasserre's hierarchy from combinatorial optimization to the continuous setting
- Finite convergence to the optimal energy


## This talk

- Hierarchy obtained by generalizing Lasserre's hierarchy from combinatorial optimization to the continuous setting
- Finite convergence to the optimal energy
- A duality theory


## This talk

- Hierarchy obtained by generalizing Lasserre's hierarchy from combinatorial optimization to the continuous setting
- Finite convergence to the optimal energy
- A duality theory
- Reduction to a converging sequence of semidefinite programs


## This talk

- Hierarchy obtained by generalizing Lasserre's hierarchy from combinatorial optimization to the continuous setting
- Finite convergence to the optimal energy
- A duality theory
- Reduction to a converging sequence of semidefinite programs
- Towards computations using several types of symmetry reduction

Approach


## Approach



## Approach



## Approach



## Approach



## Approach

Conic dual:
Infinite dimensional maximization problem


## Approach

Conic dual:
Infinite dimensional maximization problem


## Approach

Conic dual:
Infinite dimensional maximization problem


Semi-infinite semidefinite program

## The minimization problem

- $I_{=t}\left(I_{t}\right)$ is the set of subsets of $V$ which
- have cardinality $t(\leq t)$
- contain no points which are too close


## The minimization problem

- $I_{=t}\left(I_{t}\right)$ is the set of subsets of $V$ which
- have cardinality $t(\leq t)$
- contain no points which are too close
- Assuming $h(\{x, y\}) \rightarrow \infty$ when $x$ and $y$ converge, we have

$$
E=\min _{S \in I_{=N}} \sum_{P \in\binom{S}{2}} h(P)
$$

## The minimization problem

- $I_{=t}\left(I_{t}\right)$ is the set of subsets of $V$ which
- have cardinality $t(\leq t)$
- contain no points which are too close
- Assuming $h(\{x, y\}) \rightarrow \infty$ when $x$ and $y$ converge, we have

$$
E=\min _{S \in I=N} \sum_{P \in\binom{S}{2}} h(P)
$$

- We will also assume that $V$ is compact and $h$ continuous


## The minimization problem

- $I_{=t}\left(I_{t}\right)$ is the set of subsets of $V$ which
- have cardinality $t(\leq t)$
- contain no points which are too close
- Assuming $h(\{x, y\}) \rightarrow \infty$ when $x$ and $y$ converge, we have

$$
E=\min _{S \in I=N} \sum_{P \in\binom{S}{2}} h(P)
$$

- We will also assume that $V$ is compact and $h$ continuous
- $I_{=t}$ gets its topology as a subset of a quotient of $V^{t}$


## Moment hierarchy of relaxations

- In the relaxation $E_{t}$ we minimize over measures $\lambda$ on the space $I_{s}$, where $s=\min \{2 t, N\}$


## Moment hierarchy of relaxations

- In the relaxation $E_{t}$ we minimize over measures $\lambda$ on the space $I_{s}$, where $s=\min \{2 t, N\}$


## Lemma

When $t=N$, the feasible measures $\lambda$ are (generalized) convex combinations of measures

$$
\chi_{S}=\sum_{R \subseteq S} \delta_{R} \quad \text { where } \quad S \in I_{=N}
$$

## Moment hierarchy of relaxations

- In the relaxation $E_{t}$ we minimize over measures $\lambda$ on the space $I_{s}$, where $s=\min \{2 t, N\}$


## Lemma

When $t=N$, the feasible measures $\lambda$ are (generalized) convex combinations of measures

$$
\chi_{S}=\sum_{R \subseteq S} \delta_{R} \quad \text { where } \quad S \in I_{=N}
$$

- Objective function: $\lambda(h)=\int_{I_{=N}} h(S) d \lambda(S)$


## Moment hierarchy of relaxations

- In the relaxation $E_{t}$ we minimize over measures $\lambda$ on the space $I_{s}$, where $s=\min \{2 t, N\}$


## Lemma

When $t=N$, the feasible measures $\lambda$ are (generalized) convex combinations of measures

$$
\chi_{S}=\sum_{R \subseteq S} \delta_{R} \quad \text { where } \quad S \in I_{=N}
$$

- Objective function: $\lambda(h)=\int_{I_{=N}} h(S) d \lambda(S)$
- Moment constraints: $A_{t}^{*} \lambda \in \mathcal{M}\left(I_{t} \times I_{t}\right)_{\succeq 0}$


## Moment hierarchy of relaxations

- In the relaxation $E_{t}$ we minimize over measures $\lambda$ on the space $I_{s}$, where $s=\min \{2 t, N\}$


## Lemma

When $t=N$, the feasible measures $\lambda$ are (generalized) convex combinations of measures

$$
\chi_{S}=\sum_{R \subseteq S} \delta_{R} \quad \text { where } \quad S \in I_{=N}
$$

- Objective function: $\lambda(h)=\int_{I_{=N}} h(S) d \lambda(S)$
- Moment constraints: $A_{t}^{*} \lambda \in \mathcal{M}\left(I_{t} \times I_{t}\right)_{\succeq 0}$
- Here $A_{t}^{*}$ is an operator $\mathcal{M}\left(I_{s}\right) \rightarrow \mathcal{M}\left(I_{t} \times I_{t}\right)$


## Moment hierarchy of relaxations

- In the relaxation $E_{t}$ we minimize over measures $\lambda$ on the space $I_{s}$, where $s=\min \{2 t, N\}$


## Lemma

When $t=N$, the feasible measures $\lambda$ are (generalized) convex combinations of measures

$$
\chi_{S}=\sum_{R \subseteq S} \delta_{R} \quad \text { where } \quad S \in I_{=N}
$$

- Objective function: $\lambda(h)=\int_{I_{=N}} h(S) d \lambda(S)$
- Moment constraints: $A_{t}^{*} \lambda \in \mathcal{M}\left(I_{t} \times I_{t}\right)_{\succeq 0}$
- Here $A_{t}^{*}$ is an operator $\mathcal{M}\left(I_{s}\right) \rightarrow \mathcal{M}\left(I_{t} \times I_{t}\right)$
- $\mathcal{M}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ is the cone dual to the cone $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ of positive kernels


## Moment hierarchy of relaxations

- In the relaxation $E_{t}$ we minimize over measures $\lambda$ on the space $I_{s}$, where $s=\min \{2 t, N\}$


## Lemma

When $t=N$, the feasible measures $\lambda$ are (generalized) convex combinations of measures

$$
\chi_{S}=\sum_{R \subseteq S} \delta_{R} \quad \text { where } \quad S \in I_{=N}
$$

- Objective function: $\lambda(h)=\int_{I_{=N}} h(S) d \lambda(S)$
- Moment constraints: $A_{t}^{*} \lambda \in \mathcal{M}\left(I_{t} \times I_{t}\right)_{\succeq 0}$
- Here $A_{t}^{*}$ is an operator $\mathcal{M}\left(I_{s}\right) \rightarrow \mathcal{M}\left(I_{t} \times I_{t}\right)$
- $\mathcal{M}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ is the cone dual to the cone $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ of positive kernels: $\mu(K) \geq 0$ for all $K \succeq 0$


## Moment hierarchy of relaxations

- In the relaxation $E_{t}$ we minimize over measures $\lambda$ on the space $I_{s}$, where $s=\min \{2 t, N\}$


## Lemma

When $t=N$, the feasible measures $\lambda$ are (generalized) convex combinations of measures

$$
\chi_{S}=\sum_{R \subseteq S} \delta_{R} \quad \text { where } \quad S \in I_{=N}
$$

- Objective function: $\lambda(h)=\int_{I_{=N}} h(S) d \lambda(S)$
- Moment constraints: $A_{t}^{*} \lambda \in \mathcal{M}\left(I_{t} \times I_{t}\right)_{\succeq 0}$
- Here $A_{t}^{*}$ is an operator $\mathcal{M}\left(I_{s}\right) \rightarrow \mathcal{M}\left(I_{t} \times I_{t}\right)$
- $\mathcal{M}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ is the cone dual to the cone $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ of positive kernels: $\mu(K) \geq 0$ for all $K \succeq 0$
- We have $\chi_{S}(h)=\sum_{P \in\binom{S}{2}} h(P)$


## Moment hierarchy of relaxations

- In the relaxation $E_{t}$ we minimize over measures $\lambda$ on the space $I_{s}$, where $s=\min \{2 t, N\}$


## Lemma

When $t=N$, the feasible measures $\lambda$ are (generalized) convex combinations of measures

$$
\chi_{S}=\sum_{R \subseteq S} \delta_{R} \quad \text { where } \quad S \in I_{=N}
$$

- Objective function: $\lambda(h)=\int_{I_{=N}} h(S) d \lambda(S)$
- Moment constraints: $A_{t}^{*} \lambda \in \mathcal{M}\left(I_{t} \times I_{t}\right)_{\succeq 0}$
- Here $A_{t}^{*}$ is an operator $\mathcal{M}\left(I_{s}\right) \rightarrow \mathcal{M}\left(I_{t} \times I_{t}\right)$
- $\mathcal{M}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ is the cone dual to the cone $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ of positive kernels: $\mu(K) \geq 0$ for all $K \succeq 0$
- We have $\chi_{S}(h)=\sum_{P \in\binom{S}{2}} h(P)$


## Theorem (Finite convergence)

We have $E_{1} \leq \cdots \leq E_{N}=E$

## Dual hierarchy

- $E_{t}$ is a minimization problem, so we need an optimal solution to find a lower bound


## Dual hierarchy

- $E_{t}$ is a minimization problem, so we need an optimal solution to find a lower bound
- The conic dual $E_{t}^{*}$ is a maximization problem where any feasible solution provides an upper bound


## Dual hierarchy

- $E_{t}$ is a minimization problem, so we need an optimal solution to find a lower bound
- The conic dual $E_{t}^{*}$ is a maximization problem where any feasible solution provides an upper bound
- In $E_{t}^{*}$ optimization is over scalars $a_{i} \in \mathbb{R}$ and positive definite kernels $K \in \mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$


## Dual hierarchy

- $E_{t}$ is a minimization problem, so we need an optimal solution to find a lower bound
- The conic dual $E_{t}^{*}$ is a maximization problem where any feasible solution provides an upper bound
- In $E_{t}^{*}$ optimization is over scalars $a_{i} \in \mathbb{R}$ and positive definite kernels $K \in \mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$
- The dual program:

$$
\begin{aligned}
E_{t}^{*}=\sup \left\{\sum_{i=0}^{s}\binom{N}{i} a_{i}: a_{0}, \ldots, a_{s}\right. & \in \mathbb{R}, K \in \mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0} \\
& \left.a_{i}+A_{t} K \leq h \text { on } I_{=i} \text { for } i=0, \ldots, s\right\}
\end{aligned}
$$

## Dual hierarchy

- $E_{t}$ is a minimization problem, so we need an optimal solution to find a lower bound
- The conic dual $E_{t}^{*}$ is a maximization problem where any feasible solution provides an upper bound
- In $E_{t}^{*}$ optimization is over scalars $a_{i} \in \mathbb{R}$ and positive definite kernels $K \in \mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$
- The dual program:

$$
\begin{aligned}
E_{t}^{*}=\sup \left\{\sum_{i=0}^{s}\binom{N}{i} a_{i}: a_{0}, \ldots, a_{s}\right. & \in \mathbb{R}, K \in \mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}, \\
& \left.a_{i}+A_{t} K \leq h \text { on } I_{=i} \text { for } i=0, \ldots, s\right\}
\end{aligned}
$$

- Here $A_{t}$ is the linear operator $\mathcal{C}\left(I_{t} \times I_{t}\right) \rightarrow \mathcal{C}\left(I_{t}\right)$ given by $A_{t} K(S)=\sum_{J, J^{\prime} \in I_{t}: J \cup J^{\prime}=S} K\left(J, J^{\prime}\right)$


## Dual hierarchy

- $E_{t}$ is a minimization problem, so we need an optimal solution to find a lower bound
- The conic dual $E_{t}^{*}$ is a maximization problem where any feasible solution provides an upper bound
- In $E_{t}^{*}$ optimization is over scalars $a_{i} \in \mathbb{R}$ and positive definite kernels $K \in \mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$
- The dual program:

$$
\begin{aligned}
E_{t}^{*}=\sup \left\{\sum_{i=0}^{s}\binom{N}{i} a_{i}: a_{0}, \ldots, a_{s}\right. & \in \mathbb{R}, K \in \mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0} \\
& \left.a_{i}+A_{t} K \leq h \text { on } I_{=i} \text { for } i=0, \ldots, s\right\}
\end{aligned}
$$

- Here $A_{t}$ is the linear operator $\mathcal{C}\left(I_{t} \times I_{t}\right) \rightarrow \mathcal{C}\left(I_{t}\right)$ given by $A_{t} K(S)=\sum_{J, J^{\prime} \in I_{t}: J \cup J^{\prime}=S} K\left(J, J^{\prime}\right)$


## Theorem

Strong duality holds: $E_{t}=E_{t}^{*}$ for each $t$

## Closing the gaps

Conic dual:
Infinite dimensional maximization problem


Semi-infinite semidefinite program

## Finite dimensional approximations to $E_{t}^{*}$

- Define $E_{t, d}^{*}$ by replacing the cone $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ in $E_{t}^{*}$ by a finite dimensional inner approximating cone $C_{d}$


## Finite dimensional approximations to $E_{t}^{*}$

- Define $E_{t, d}^{*}$ by replacing the cone $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ in $E_{t}^{*}$ by a finite dimensional inner approximating cone $C_{d}$
- Let $e_{1}, e_{2}, \ldots$ be a dense sequence in $\mathcal{C}\left(I_{t}\right)$ and define

$$
C_{d}=\left\{\sum_{i, j=1}^{d} F_{i, j} e_{i} \otimes e_{j}: F \in \mathbb{R}^{d \times d} \text { positive semidefinite }\right\}
$$

## Finite dimensional approximations to $E_{t}^{*}$

- Define $E_{t, d}^{*}$ by replacing the cone $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ in $E_{t}^{*}$ by a finite dimensional inner approximating cone $C_{d}$
- Let $e_{1}, e_{2}, \ldots$ be a dense sequence in $\mathcal{C}\left(I_{t}\right)$ and define

$$
C_{d}=\left\{\sum_{i, j=1}^{d} F_{i, j} e_{i} \otimes e_{j}: F \in \mathbb{R}^{d \times d} \text { positive semidefinite }\right\}
$$

## Lemma

Suppose $X$ is a compact metric space. Then the extreme rays of the cone $\mathcal{C}(X \times X)_{\succeq 0}$ are precisely the kernels $f \otimes f$ with $f \in \mathcal{C}(X)$

## Finite dimensional approximations to $E_{t}^{*}$

- Define $E_{t, d}^{*}$ by replacing the cone $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ in $E_{t}^{*}$ by a finite dimensional inner approximating cone $C_{d}$
- Let $e_{1}, e_{2}, \ldots$ be a dense sequence in $\mathcal{C}\left(I_{t}\right)$ and define

$$
C_{d}=\left\{\sum_{i, j=1}^{d} F_{i, j} e_{i} \otimes e_{j}: F \in \mathbb{R}^{d \times d} \text { positive semidefinite }\right\}
$$

## Lemma

Suppose $X$ is a compact metric space. Then the extreme rays of the cone $\mathcal{C}(X \times X)_{\succeq 0}$ are precisely the kernels $f \otimes f$ with $f \in \mathcal{C}(X)$

- This implies $\cup_{d=0}^{\infty} C_{d}$ is uniformly dense in $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$


## Finite dimensional approximations to $E_{t}^{*}$

- Define $E_{t, d}^{*}$ by replacing the cone $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$ in $E_{t}^{*}$ by a finite dimensional inner approximating cone $C_{d}$
- Let $e_{1}, e_{2}, \ldots$ be a dense sequence in $\mathcal{C}\left(I_{t}\right)$ and define

$$
C_{d}=\left\{\sum_{i, j=1}^{d} F_{i, j} e_{i} \otimes e_{j}: F \in \mathbb{R}^{d \times d} \text { positive semidefinite }\right\}
$$

## Lemma

Suppose $X$ is a compact metric space. Then the extreme rays of the cone $\mathcal{C}(X \times X)_{\succeq 0}$ are precisely the kernels $f \otimes f$ with $f \in \mathcal{C}(X)$

- This implies $\cup_{d=0}^{\infty} C_{d}$ is uniformly dense in $\mathcal{C}\left(I_{t} \times I_{t}\right)_{\succeq 0}$


## Theorem

If $V$ is a compact metric space, then $E_{t, d}^{*} \rightarrow E_{t}^{*}$ as $d \rightarrow \infty$ for all $t$

## Block diagonalization

- For computations use the symmetry of $V$ and $h$, expressed by the action of a group $\Gamma$, and Bochner's theorem to block diagonalize the matrix $F$


## Block diagonalization

- For computations use the symmetry of $V$ and $h$, expressed by the action of a group $\Gamma$, and Bochner's theorem to block diagonalize the matrix $F$
- For this we need a symmetry adapted basis of $\mathcal{C}\left(I_{t}\right)$


## Block diagonalization

- For computations use the symmetry of $V$ and $h$, expressed by the action of a group $\Gamma$, and Bochner's theorem to block diagonalize the matrix $F$
- For this we need a symmetry adapted basis of $\mathcal{C}\left(I_{t}\right)$
- If $t=1$ and $V=S^{2}$, then

$$
\mathcal{C}\left(I_{t}\right) \simeq \mathbb{R} \oplus \mathcal{C}\left(S^{2}\right)
$$

## Block diagonalization

- For computations use the symmetry of $V$ and $h$, expressed by the action of a group $\Gamma$, and Bochner's theorem to block diagonalize the matrix $F$
- For this we need a symmetry adapted basis of $\mathcal{C}\left(I_{t}\right)$
- If $t=1$ and $V=S^{2}$, then

$$
\mathcal{C}\left(I_{t}\right) \simeq \mathbb{R} \oplus \mathcal{C}\left(S^{2}\right)=\mathbb{R} \oplus \bigoplus_{k=0}^{\infty} H_{k}
$$

## Block diagonalization

- For computations use the symmetry of $V$ and $h$, expressed by the action of a group $\Gamma$, and Bochner's theorem to block diagonalize the matrix $F$
- For this we need a symmetry adapted basis of $\mathcal{C}\left(I_{t}\right)$
- If $t=1$ and $V=S^{2}$, then

$$
\mathcal{C}\left(I_{t}\right) \simeq \mathbb{R} \oplus \mathcal{C}\left(S^{2}\right)=\mathbb{R} \oplus \bigoplus_{k=0}^{\infty} H_{k}
$$

- This will block diagonalize to a diagonal matrix and we get (something close to) Yudin's LP bound


## Block diagonalization

- For computations use the symmetry of $V$ and $h$, expressed by the action of a group $\Gamma$, and Bochner's theorem to block diagonalize the matrix $F$
- For this we need a symmetry adapted basis of $\mathcal{C}\left(I_{t}\right)$
- If $t=1$ and $V=S^{2}$, then

$$
\mathcal{C}\left(I_{t}\right) \simeq \mathbb{R} \oplus \mathcal{C}\left(S^{2}\right)=\mathbb{R} \oplus \bigoplus_{k=0}^{\infty} H_{k}
$$

- This will block diagonalize to a diagonal matrix and we get (something close to) Yudin's LP bound
- In general $\mathcal{C}\left(I_{t}\right)$ injects into $\mathcal{C}(V)^{\odot t}$


## Block diagonalization

- For computations use the symmetry of $V$ and $h$, expressed by the action of a group $\Gamma$, and Bochner's theorem to block diagonalize the matrix $F$
- For this we need a symmetry adapted basis of $\mathcal{C}\left(I_{t}\right)$
- If $t=1$ and $V=S^{2}$, then

$$
\mathcal{C}\left(I_{t}\right) \simeq \mathbb{R} \oplus \mathcal{C}\left(S^{2}\right)=\mathbb{R} \oplus \bigoplus_{k=0}^{\infty} H_{k}
$$

- This will block diagonalize to a diagonal matrix and we get (something close to) Yudin's LP bound
- In general $\mathcal{C}\left(I_{t}\right)$ injects into $\mathcal{C}(V)^{\odot t}$
- $\mathcal{C}(V)^{\odot t}$ can be written in terms of tensor products of the irreducible subspaces of $\mathcal{C}(V)$


## Block diagonalization

- For computations use the symmetry of $V$ and $h$, expressed by the action of a group $\Gamma$, and Bochner's theorem to block diagonalize the matrix $F$
- For this we need a symmetry adapted basis of $\mathcal{C}\left(I_{t}\right)$
- If $t=1$ and $V=S^{2}$, then

$$
\mathcal{C}\left(I_{t}\right) \simeq \mathbb{R} \oplus \mathcal{C}\left(S^{2}\right)=\mathbb{R} \oplus \bigoplus_{k=0}^{\infty} H_{k}
$$

- This will block diagonalize to a diagonal matrix and we get (something close to) Yudin's LP bound
- In general $\mathcal{C}\left(I_{t}\right)$ injects into $\mathcal{C}(V)^{\odot t}$
- $\mathcal{C}(V)^{\odot t}$ can be written in terms of tensor products of the irreducible subspaces of $\mathcal{C}(V)$
- If we know how to decompose $\mathcal{C}(V)$ into irreducibles, and how to decompose tensor products of those irreducibles into irreducibles, then we have a symmerty adapted basis of $V_{t}$


## The case $t=2$ and $V=S^{2}$

- We know how to these decompositions from the quantum mechanics literature (angular momentum coupling): use Clebsch-Gordan coefficients


## The case $t=2$ and $V=S^{2}$

- We know how to these decompositions from the quantum mechanics literature (angular momentum coupling): use Clebsch-Gordan coefficients
- The affine constraints in $E_{t, d}^{*}$ are nonnegativity constraints of a polynomial $p \in \mathbb{R}\left[x_{1}, \ldots, x_{4}\right]$, where each $x_{i}$ is a vector of 3 variables (the coefficients of these polynomials depend on the entries in the block diagonalization of $F$ )


## The case $t=2$ and $V=S^{2}$

- We know how to these decompositions from the quantum mechanics literature (angular momentum coupling): use Clebsch-Gordan coefficients
- The affine constraints in $E_{t, d}^{*}$ are nonnegativity constraints of a polynomial $p \in \mathbb{R}\left[x_{1}, \ldots, x_{4}\right]$, where each $x_{i}$ is a vector of 3 variables (the coefficients of these polynomials depend on the entries in the block diagonalization of $F$ )
- We have $p\left(\gamma x_{1}, \ldots, \gamma x_{4}\right)=p\left(x_{1}, \ldots, x_{4}\right)$ for all $\gamma \in O(3)$


## The case $t=2$ and $V=S^{2}$

- We know how to these decompositions from the quantum mechanics literature (angular momentum coupling): use Clebsch-Gordan coefficients
- The affine constraints in $E_{t, d}^{*}$ are nonnegativity constraints of a polynomial $p \in \mathbb{R}\left[x_{1}, \ldots, x_{4}\right]$, where each $x_{i}$ is a vector of 3 variables (the coefficients of these polynomials depend on the entries in the block diagonalization of $F$ )
- We have $p\left(\gamma x_{1}, \ldots, \gamma x_{4}\right)=p\left(x_{1}, \ldots, x_{4}\right)$ for all $\gamma \in O(3)$
- Invariant theory: there is a polynomial $q$ such that $p\left(x_{1}, \ldots, x_{4}\right)=q\left(x_{1} \cdot x_{2}, \ldots, x_{3} \cdot x_{4}\right)$


## The case $t=2$ and $V=S^{2}$

- We know how to these decompositions from the quantum mechanics literature (angular momentum coupling): use Clebsch-Gordan coefficients
- The affine constraints in $E_{t, d}^{*}$ are nonnegativity constraints of a polynomial $p \in \mathbb{R}\left[x_{1}, \ldots, x_{4}\right]$, where each $x_{i}$ is a vector of 3 variables (the coefficients of these polynomials depend on the entries in the block diagonalization of $F$ )
- We have $p\left(\gamma x_{1}, \ldots, \gamma x_{4}\right)=p\left(x_{1}, \ldots, x_{4}\right)$ for all $\gamma \in O(3)$
- Invariant theory: there is a polynomial $q$ such that $p\left(x_{1}, \ldots, x_{4}\right)=q\left(x_{1} \cdot x_{2}, \ldots, x_{3} \cdot x_{4}\right)$
- Model nonnegativity constraints as sum of squares constraints using Putinar's theorem from real algebraic geometry


## The case $t=2$ and $V=S^{2}$

- We know how to these decompositions from the quantum mechanics literature (angular momentum coupling): use Clebsch-Gordan coefficients
- The affine constraints in $E_{t, d}^{*}$ are nonnegativity constraints of a polynomial $p \in \mathbb{R}\left[x_{1}, \ldots, x_{4}\right]$, where each $x_{i}$ is a vector of 3 variables (the coefficients of these polynomials depend on the entries in the block diagonalization of $F$ )
- We have $p\left(\gamma x_{1}, \ldots, \gamma x_{4}\right)=p\left(x_{1}, \ldots, x_{4}\right)$ for all $\gamma \in O(3)$
- Invariant theory: there is a polynomial $q$ such that $p\left(x_{1}, \ldots, x_{4}\right)=q\left(x_{1} \cdot x_{2}, \ldots, x_{3} \cdot x_{4}\right)$
- Model nonnegativity constraints as sum of squares constraints using Putinar's theorem from real algebraic geometry
- A sum of squares polynomial $s$ can be written as $s(x)=v(x)^{\top} Q v(x)$, where $Q$ is a positive semidefinite matrix and $v(x)$ a vector containing all monomials up to some degree


## More symmetry

- More symmetry: $p\left(x_{1}, \ldots, x_{4}\right)=p\left(x_{\sigma(1)}, \ldots, x_{\sigma(4)}\right)$ for all permutations $\sigma \in S_{4}$


## More symmetry

- More symmetry: $p\left(x_{1}, \ldots, x_{4}\right)=p\left(x_{\sigma(1)}, \ldots, x_{\sigma(4)}\right)$ for all permutations $\sigma \in S_{4}$
- This means that $q$ is symmetric under a subgroup of $S_{6}$


## More symmetry

- More symmetry: $p\left(x_{1}, \ldots, x_{4}\right)=p\left(x_{\sigma(1)}, \ldots, x_{\sigma(4)}\right)$ for all permutations $\sigma \in S_{4}$
- This means that $q$ is symmetric under a subgroup of $S_{6}$
- Use this to block diagonalize the positive semidefinite matrices showing up in the sums of squares characterizations


## More symmetry

- More symmetry: $p\left(x_{1}, \ldots, x_{4}\right)=p\left(x_{\sigma(1)}, \ldots, x_{\sigma(4)}\right)$ for all permutations $\sigma \in S_{4}$
- This means that $q$ is symmetric under a subgroup of $S_{6}$
- Use this to block diagonalize the positive semidefinite matrices showing up in the sums of squares characterizations
- We give a symmetrized version of Putinar's theorem using the method of Gatermann and Parillo for symmetry reduction in sums of squares characterizations


## More symmetry

- More symmetry: $p\left(x_{1}, \ldots, x_{4}\right)=p\left(x_{\sigma(1)}, \ldots, x_{\sigma(4)}\right)$ for all permutations $\sigma \in S_{4}$
- This means that $q$ is symmetric under a subgroup of $S_{6}$
- Use this to block diagonalize the positive semidefinite matrices showing up in the sums of squares characterizations
- We give a symmetrized version of Putinar's theorem using the method of Gatermann and Parillo for symmetry reduction in sums of squares characterizations
- Significant simplifications in the semidefinite programs


## More symmetry

- More symmetry: $p\left(x_{1}, \ldots, x_{4}\right)=p\left(x_{\sigma(1)}, \ldots, x_{\sigma(4)}\right)$ for all permutations $\sigma \in S_{4}$
- This means that $q$ is symmetric under a subgroup of $S_{6}$
- Use this to block diagonalize the positive semidefinite matrices showing up in the sums of squares characterizations
- We give a symmetrized version of Putinar's theorem using the method of Gatermann and Parillo for symmetry reduction in sums of squares characterizations
- Significant simplifications in the semidefinite programs
- Not clear yet whether we can compute $E_{2, d}^{*}$ for large enough $d$ (with current SDP solvers) to get improved bounds for $S^{2}$


## More symmetry

- More symmetry: $p\left(x_{1}, \ldots, x_{4}\right)=p\left(x_{\sigma(1)}, \ldots, x_{\sigma(4)}\right)$ for all permutations $\sigma \in S_{4}$
- This means that $q$ is symmetric under a subgroup of $S_{6}$
- Use this to block diagonalize the positive semidefinite matrices showing up in the sums of squares characterizations
- We give a symmetrized version of Putinar's theorem using the method of Gatermann and Parillo for symmetry reduction in sums of squares characterizations
- Significant simplifications in the semidefinite programs
- Not clear yet whether we can compute $E_{2, d}^{*}$ for large enough $d$ (with current SDP solvers) to get improved bounds for $S^{2}$
- Toy example: $E_{1}$ is not sharp for 3 points on $S^{1}$ with the Lennard-Jones potential


## More symmetry

- More symmetry: $p\left(x_{1}, \ldots, x_{4}\right)=p\left(x_{\sigma(1)}, \ldots, x_{\sigma(4)}\right)$ for all permutations $\sigma \in S_{4}$
- This means that $q$ is symmetric under a subgroup of $S_{6}$
- Use this to block diagonalize the positive semidefinite matrices showing up in the sums of squares characterizations
- We give a symmetrized version of Putinar's theorem using the method of Gatermann and Parillo for symmetry reduction in sums of squares characterizations
- Significant simplifications in the semidefinite programs
- Not clear yet whether we can compute $E_{2, d}^{*}$ for large enough $d$ (with current SDP solvers) to get improved bounds for $S^{2}$
- Toy example: $E_{1}$ is not sharp for 3 points on $S^{1}$ with the Lennard-Jones potential
- Using a reduction to 3 variables using trigonometric polynomials we compute that $E_{2}=E$ (up to solver precision)

Thank you!

