Title: Bounding the purification rank of mixed states

Date: Feb 25, 2013 04:00 PM

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Abstract: A mixed state can be expressed as a sum of D tensor product matrices, where D is its operator Schmidt rank, or as the result of a purification with a purifying state of Schmidt rank D', where D' is its purification rank. The question whether D' can be upper bounded by D is important theoretically (to establish a description of mixed states with tensor networks), as well as numerically (as the first decomposition is more efficient, but the second one guarantees positive-semidefiniteness after truncation). Here we show that no upper bounds of the purification rank that depend only on operator Schmidt rank exist, but provide upper bounds that also depend on the number of eigenvalues. In addition, we formulate the approximation problem as a Semidefinite Program.
Joint work with N. Schuch, D. Perez-Garcia, and J. I. Cirac.

Bounding the purification rank of mixed states

Gemma De las Cuevas
Max Planck Institut für Quantenoptik, Garching, Germany

Joint work with Norbert Schuch,
David Perez-Garcia, and
Ignacio Cirac

(to appear soon in the arXiv)

Mixed states

Used to describe

- Thermal states of quantum many-body systems
- Systems out of equilibirium, e.g. experiments
- Dissipative dynamics
- Lack of knowledge of a system

Appear in
- condensed matter
- atomic physics
- chemistry
- high energy physics

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→ **Develop good theoretical description of mixed states**

Tensor networks

Goal: develop an alternative description of quantum many-body systems

establish neat relations between

Physics of the system ⟷ Mathematical properties of the tensors

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Tensor networks

in 1D

Matrix Product States (MPS)

- Canonical form:
  - injective/non-injective
  - parent Hamiltonian
  - symmetries
  - topological order
  - classification of phases
  - link to CP maps
- Numerical algorithms

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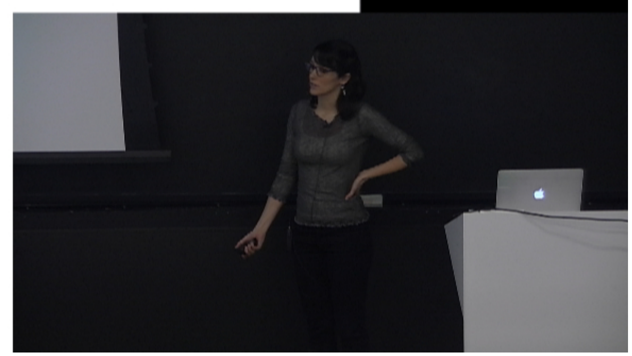
Matrix Product Density Operators (MPDOs)

Canonical form ?



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Unique decomposition of MPDOs?

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Outline

- The setting — Can one upper bound the purification rank as a function of the operator Schmidt rank?
- A counterexample — No.
- Upper bounds
- Approximate solutions
- Conclusions & Outlook

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- The setting — Can one upper bound the purification rank as a function of the operator Schmidt rank?
- A counterexample — No.
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The setting

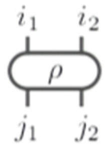
Can one upper bound the purification rank
as a function of the operator Schmidt rank?

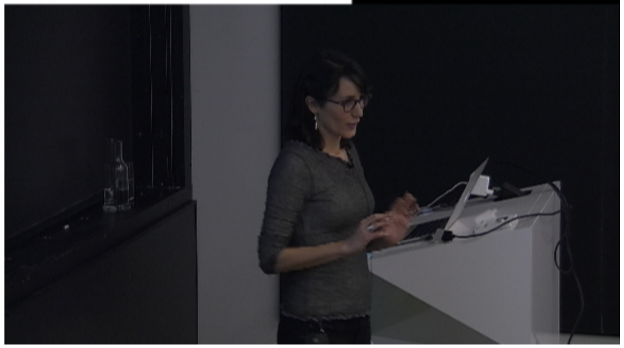
Prelude

- **Mixed state**

  It is described by a positive semidefinite tensor of trace 1.

$$\rho = \sum \rho_{i_1 i_2, j_1 j_2} |i_1 i_2\rangle\langle j_1 j_2|$$





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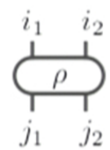
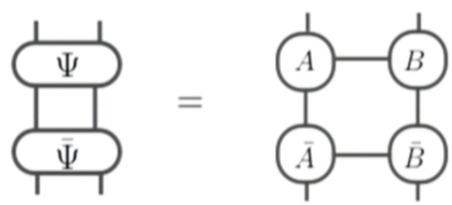


- **Purification**

  Every mixed state can be seen as a subsystem of a larger pure state.

$$\rho = \mathrm{tr}_{\mathrm{anc}} |\Psi\rangle\ \langle\Psi| \ =$$



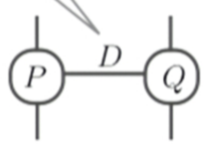
The setting

Given a positive semidefinite matrix ρ, consider these 2 decompositions:

Operator Schmidt decomposition

$$\rho = \sum_{\alpha=1}^{D} P_\alpha \otimes Q_\alpha$$

operator Schmidt rank



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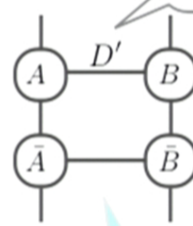
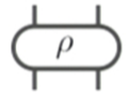


Choose the purifying state with minimal bond dimension

The setting

Given a positive semidefinite matrix  , consider these 2 decompositions:

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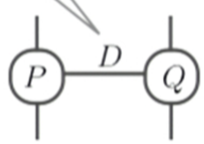

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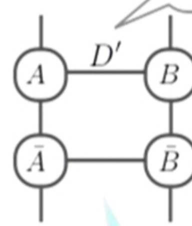

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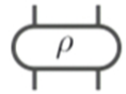
Given a positive semidefinite matrix 

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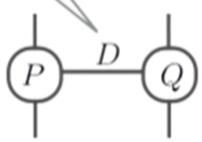

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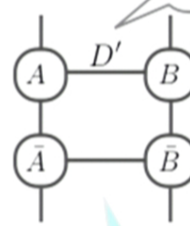

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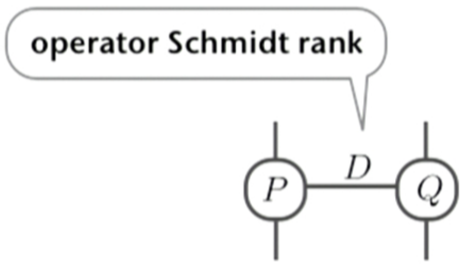

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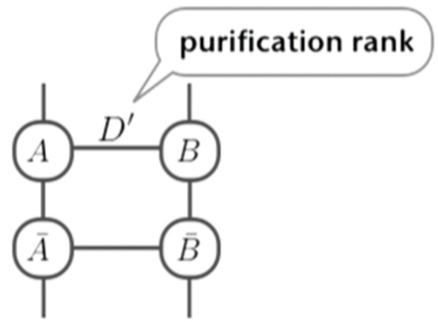

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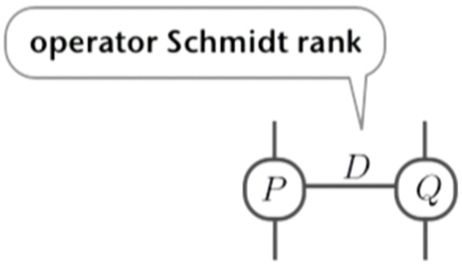
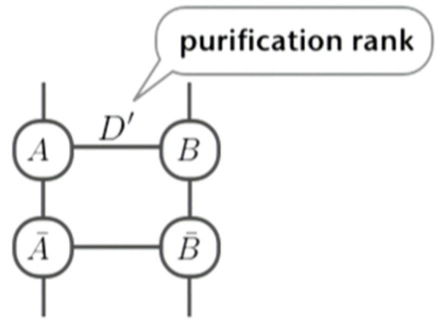


✓ minimal bond dimension

✗ not positive semidef. locally

Local Purification



✓ positive semidefinite locally

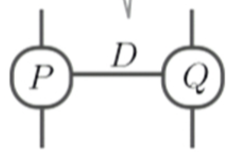
✗ bond dimension of purifying state?

The setting

Operator Schmidt decomposition

Local Purification

operator Schmidt rank



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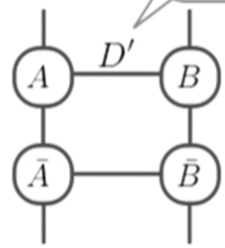

Important numerically

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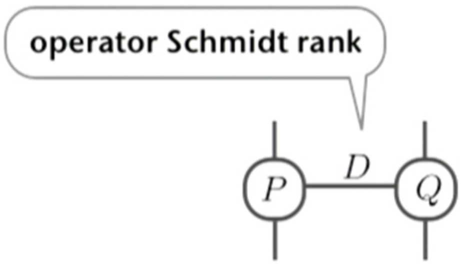

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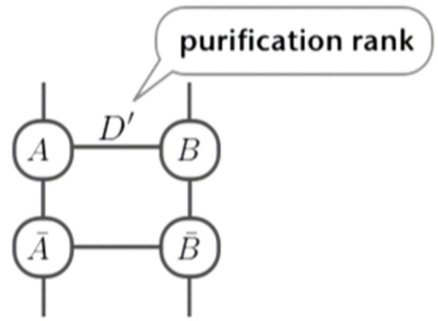

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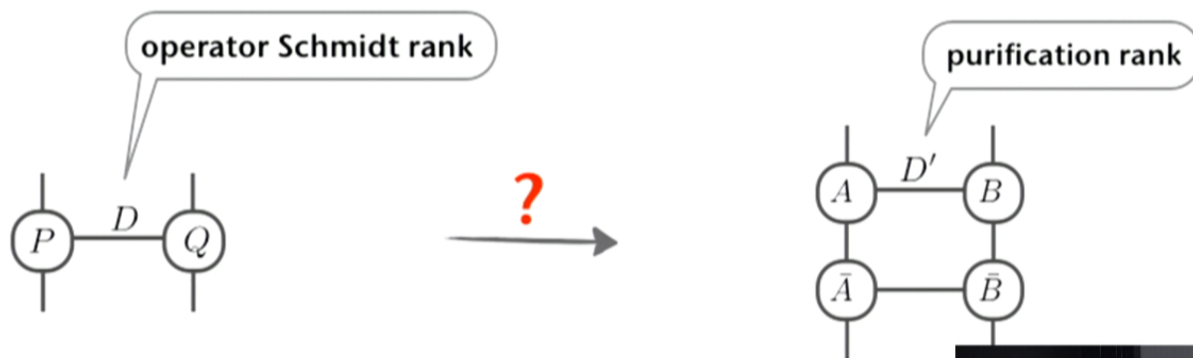
Operator Schmidt decomposition | **Local Purification**



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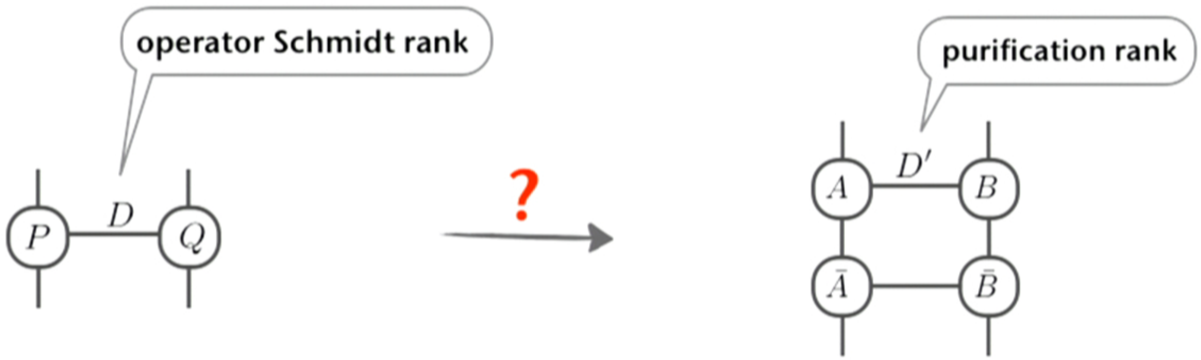
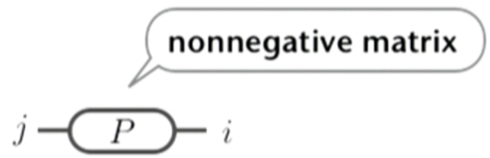


Can D' be upper bounded by a function of D ?

Classical states

- **Diagonal in the computational basis:**

$$\rho = \sum_{i,j=1}^{d} p_{ij} |i\rangle\langle i| \otimes |j\rangle\langle j|$$



In how many ways can P be decomposed?

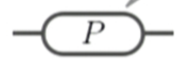
Classical states

Arbitrary matrices	Nonnegative matrices
	
Rank $\mathrm{rank}(P)$	**Nonnegative rank** $\mathrm{rank}_+(P)$
min r s.t. P can be written as a sum of r rank-1 matrices.	min r s.t. P can be written as a sum of r non-negative rank-1 matrices.

Cohen & Israel, Lin. Alg. and its Appl. 190, 149 (1993).

Classical states

Nonnegative matrix



Arbitrary matrices	Nonnegative matrices	Positive semidef. matrices

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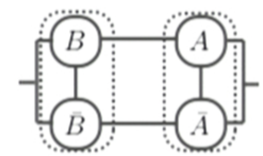


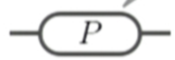
Positive semidefinite rank
$\mathrm{rank}_{\mathrm{psd}}(P)$

min r s.t. there exist positive semidef. matrices E_i and F_j of size r x r such that $P_{ij} = \mathrm{tr}(E_i F_j)$

Fiorini, Massar, Pokutta, Tiwary & de Wolf, arXiv:1111.0837.

Classical states

Nonnegative matrix



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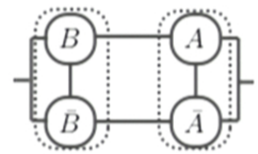

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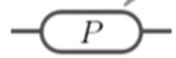
Classical states

via the states-maps duality

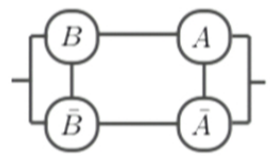
stochastic map



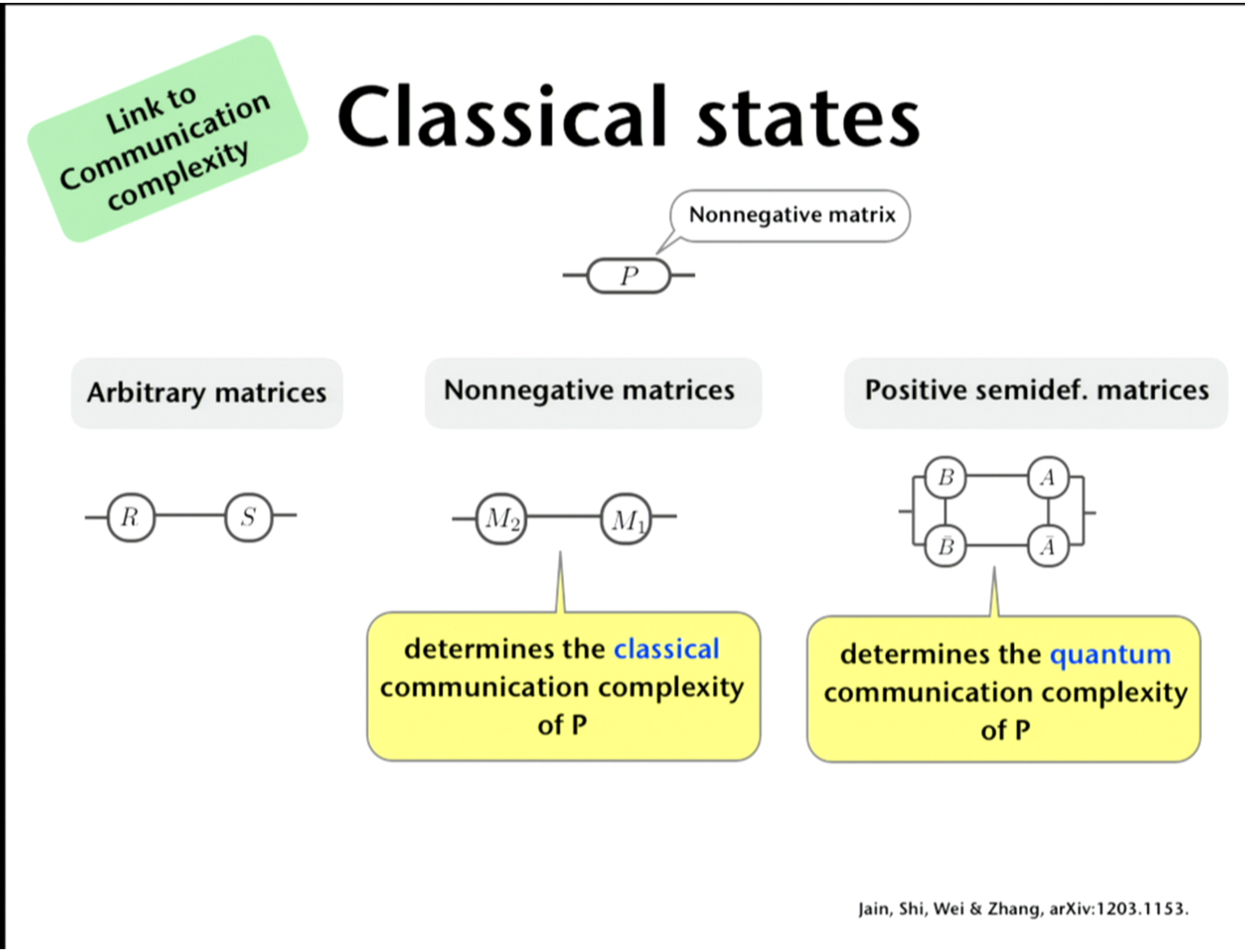
Arbitrary matrices	Nonnegative matrices	Positive semidef. matrices

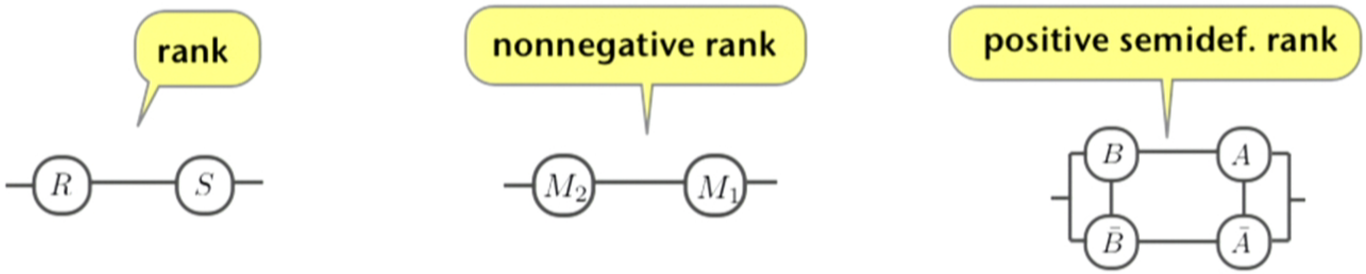
rank of the map

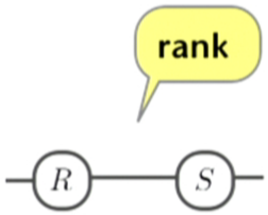
minimal middle dimension needed to decompose P as a sequence of two stochastic maps

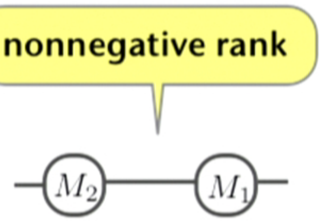


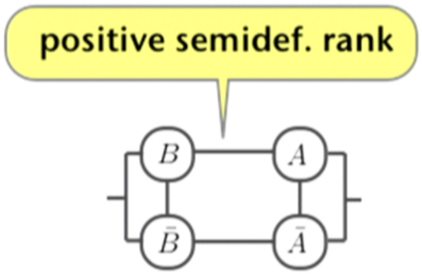
minimal middle dimension needed to decompose P as a sequence of two completely positive maps

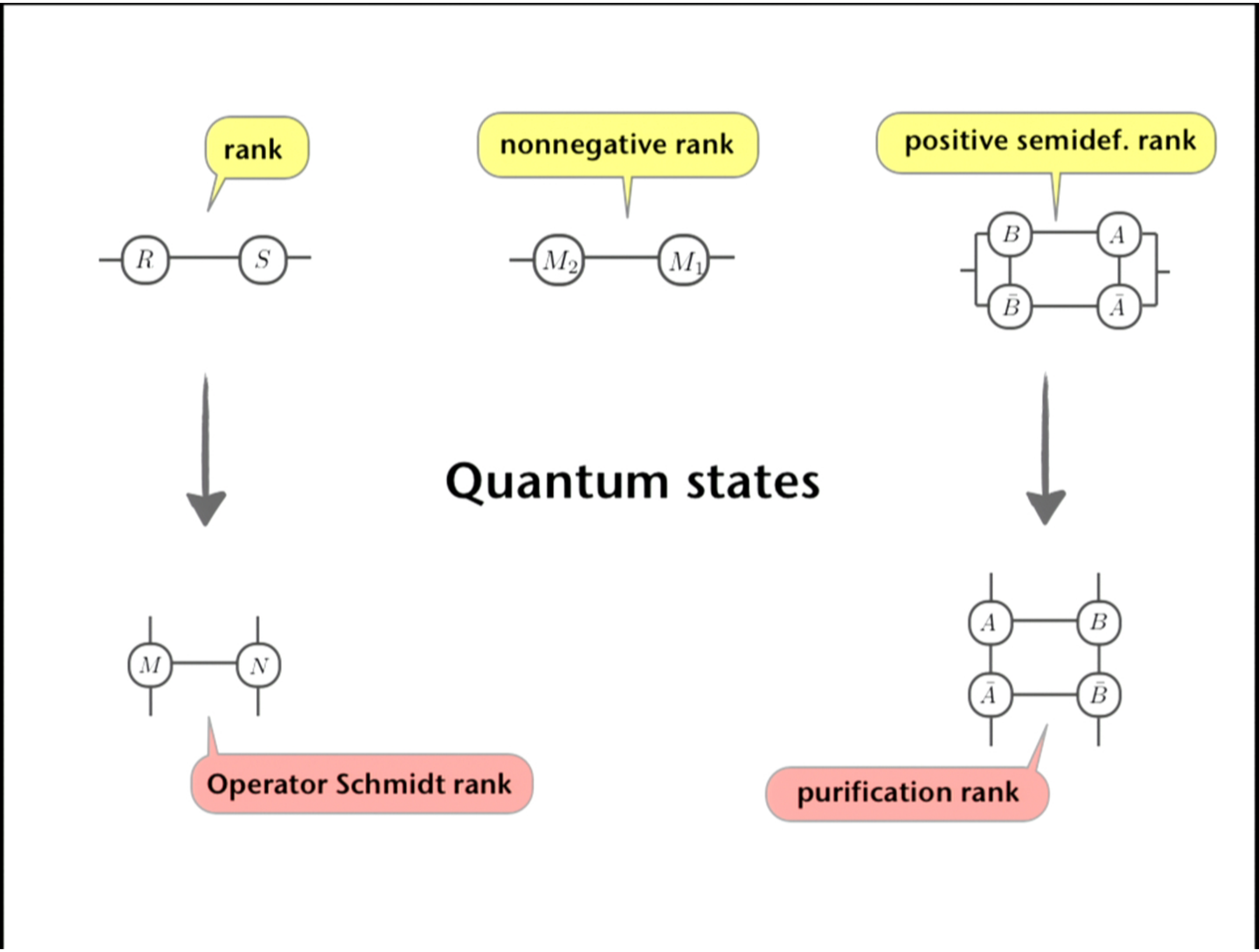

Link to Communication complexity
Classical states
Nonnegative matrix
P
Arbitrary matrices
Nonnegative matrices
Positive semidef. matrices
R
S
M2
M1
B
A
determines the classical communication complexity of P
determines the quantum communication complexity of P
Jain, Shi, Wei & Zhang, arXiv:1203.1153.


rank
R
S
nonnegative rank
M_2
M_1
positive semidef. rank
B
A
$\bar{B}$
$\bar{A}$


rank
R
S

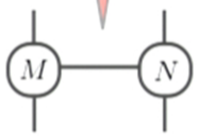

nonnegative rank
M_2
M_1


positive semidef. rank
B
A
$\bar{B}$
$\bar{A}$


rank
nonnegative rank
positive semidef. rank
Quantum states
Operator Schmidt rank
purification rank

Quantum states

Operator Schmidt rank



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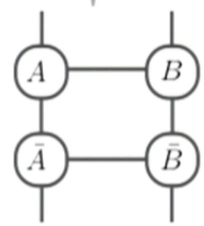

minimal middle dimension needed to decompose ρ as a sequence of two completely positive maps

via the states-maps duality

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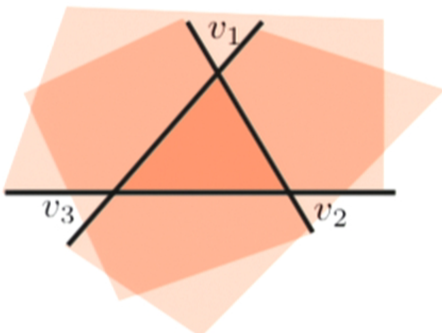
Link to Communication complexity

Jain, Shi, Wei & Zhang, arXiv:1203.1153.

The counterexample

- **Polytopes:**



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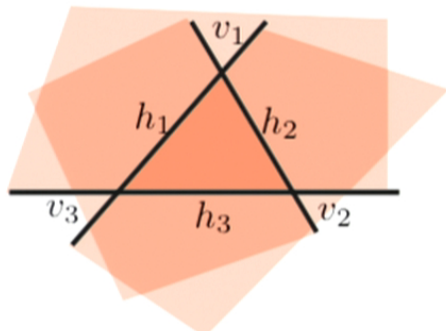

P is the convex hull of its vertices $v_1, \ldots, v_n$

P is the finite intersection of the halfspaces defined by the facets $h_1(x) \leq b_1$

$$\vdots$$

$$h_f(x) \leq b_f$$

nonnegative matrix

Slack matrix S $S_{ij} = b_j - h_j(v_i)$

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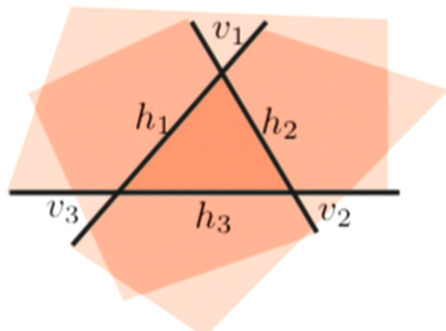

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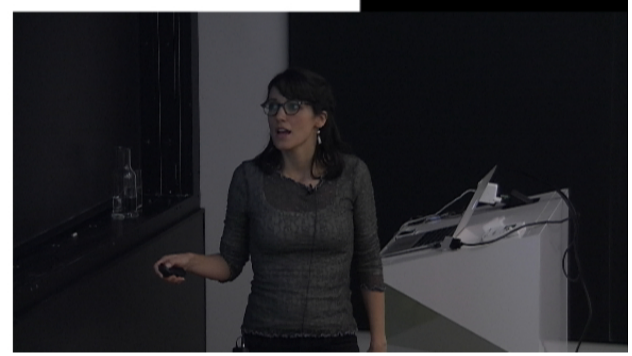

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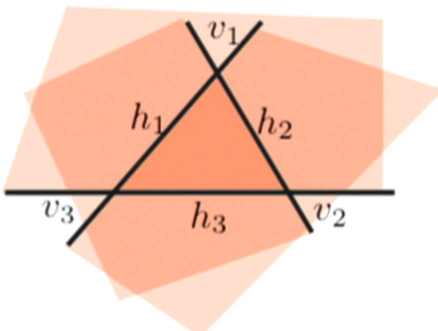

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nonnegative matrix

Slack matrix S $S_{ij} = b_j - h_j(v_i)$

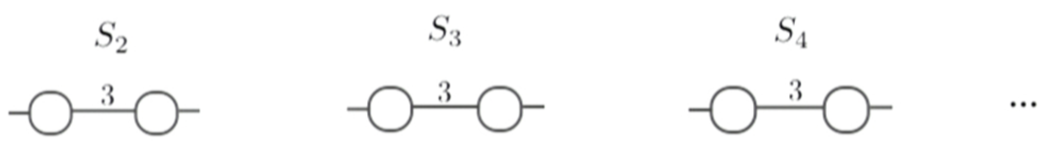
- **Regular t-gon in 2 dimensions:** with slack matrix S_t

t = 3 t = 4 t = 5 t = 6 t = 7 ...

The counterexample

The slack matrix of the regular t-gon in 2 dimensions satisfies:

The rank is constant: $\mathrm{rank}(S_t) = 3$



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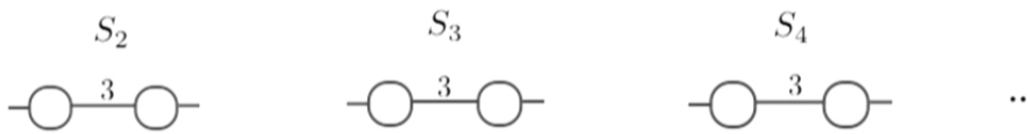
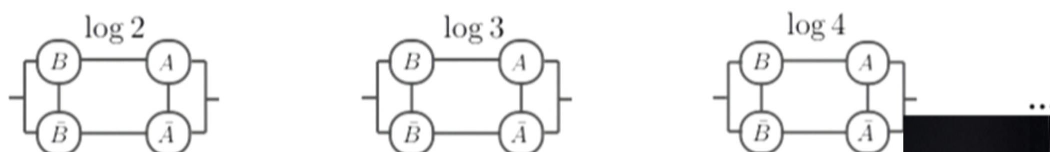


The positive semidef. rank grows unboundedly with t: $\mathrm{rank}_{\mathrm{psd}}(S_t) \sim \log t$



Gouveia, Parrilo, Thomas, arXiv:1111.3164

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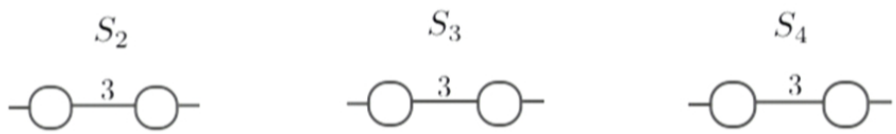

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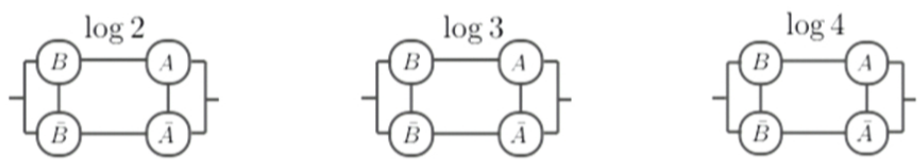

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Hence, there does not exist an upper bound of the rank that depends only on the positive semidefinite rank

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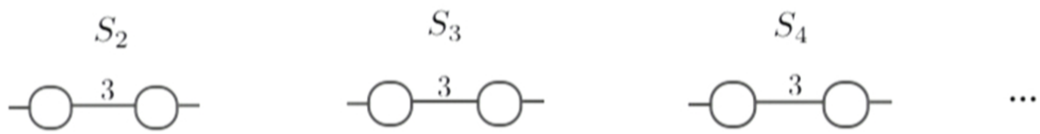

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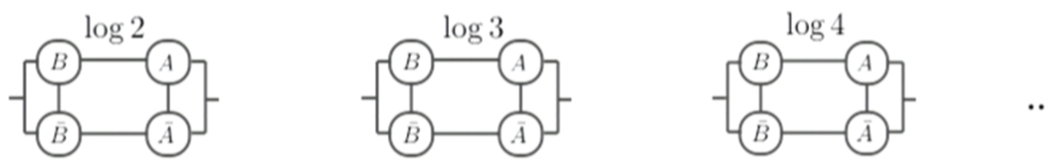


for classical states

Gouveia, Parrilo, Thomas, arXiv:1111.3164

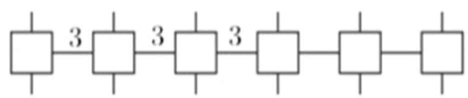
Hence, there does not exist an upper bound of the rank that depends only on the positive semidefinite rank

A multipartite counterexample

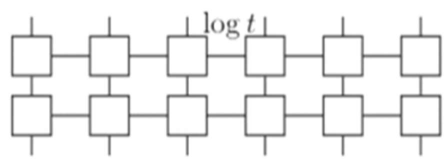
The slack matrix of regular t-gons in 2 dimensions such that $t = 2^m$

$$\rho_t = \sum_{x,y=1}^{t} S_t(x,y)|x,y\rangle\langle x,y|$$

Small Operator Schmidt rank across every cut



Unbounded purification rank across every cut



Upper bounds

The purification rank is upper bounded by

1. the OSR times the number of eigenvalues

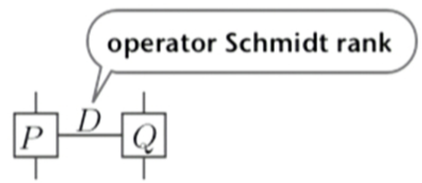
2. the OSR to the power of the number of different eigenvalues

Upper bound 1

Let ρ denote a density matrix with n eigenvalues. Then

purification rank (ρ) $\leq$ Operator Schmidt rank(ρ) $\times\, n$

Proof (informal, 1):

1. **Operator Schmidt decomposition:** $\rho =$ 

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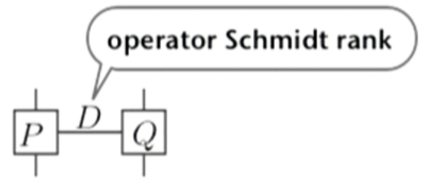
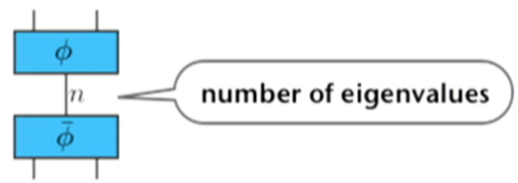


2. **Eigenvalue decomposition:** $\rho = \sum_{i=1}^{n} \lambda_i |\phi_i\rangle\langle\phi_i| \quad =$



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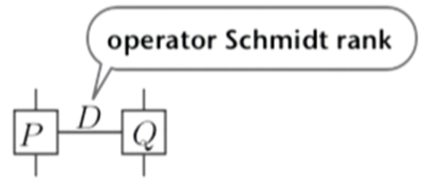
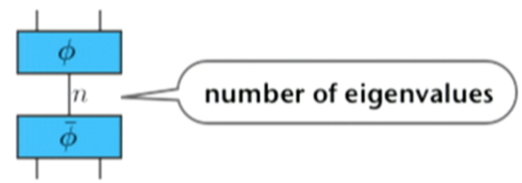
1. Operator Schmidt decomposition: $\rho =$ 

2. Eigenvalue decomposition: $\rho = \sum_{i=1}^{n} \lambda_i |\phi_i\rangle\langle\phi_i| \;=$ 

This already provides a purification:

purification rank(ρ) $\leq$ rank($|\phi_i\rangle$)

Upper bound 1

Let ρ denote a density matrix with n eigenvalues. Then

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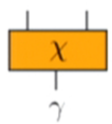
Proof (informal, 2):

- **Project ρ onto a product state:**

$\rho(|\mu_\gamma\rangle \otimes |\nu_\gamma\rangle) =$ 

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Let ρ denote a density matrix with n eigenvalues. Then

purification rank $(\rho) \leq$ Operator Schmidt rank$(\rho) \times n$

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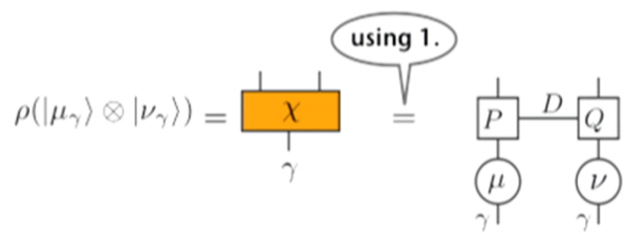

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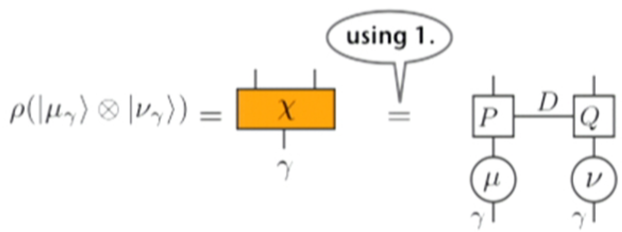

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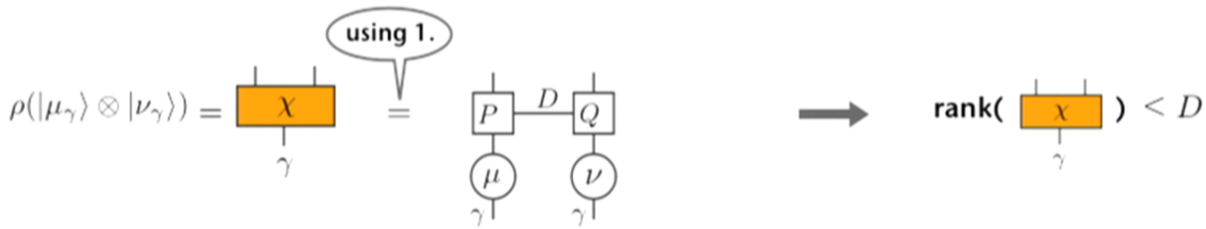

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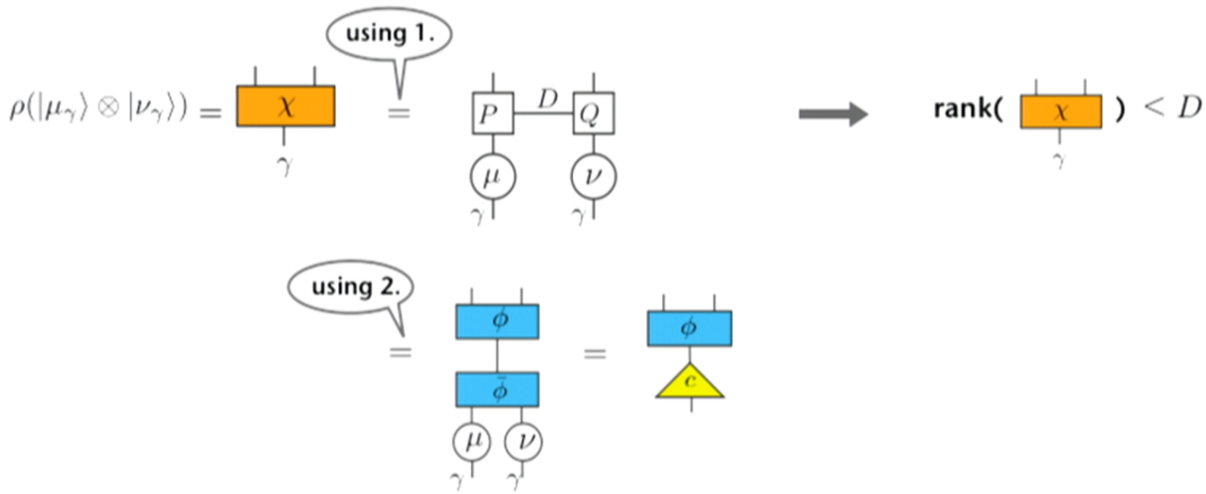

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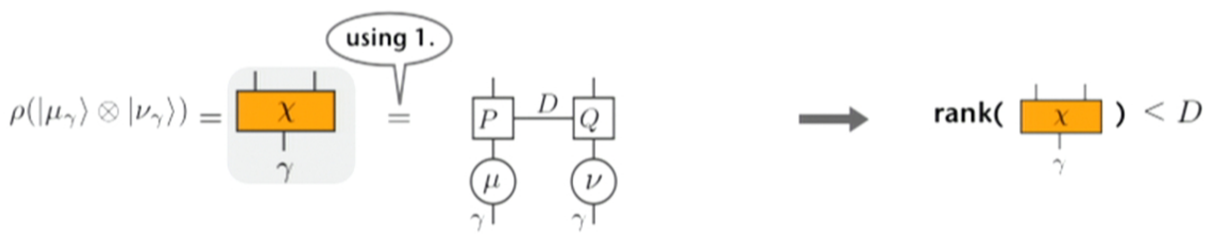
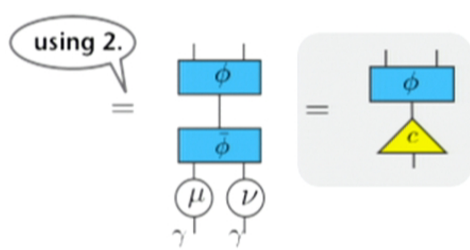




$|\chi_\gamma\rangle$ is expressed as a linear combination of eigenvectors $|\phi_i\rangle$: we only need to invert this relation...

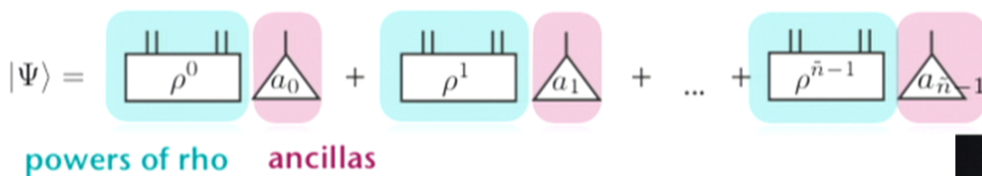
Upper bound 2

Let ρ denote a density matrix with n eigenvalues, $\tilde{n}$ of which are different.

purification rank (ρ) $\leq$ (Operator Schmidt rank(ρ))$^{\tilde{n}-1}$

Proof (informal, 1):

- Consider the purifying state



$$\rho' = \mathrm{tr}_{\mathrm{anc}} |\Psi\rangle\langle\Psi|$$

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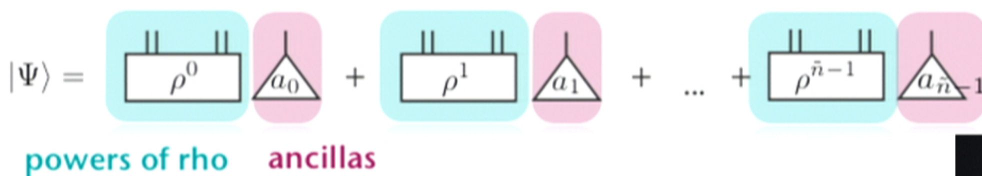
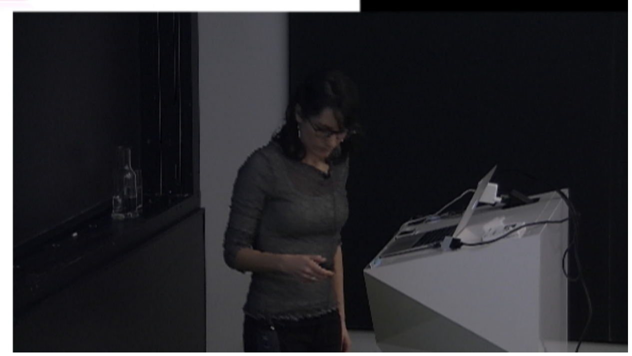


$$\rho' = \mathrm{tr}_{\mathrm{anc}} |\Psi\rangle\langle\Psi|$$

purif. rank (ρ') $\leq$ rank($|\Psi\rangle$) $\leq O(D^{\tilde{n}-1})$



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Proof (informal, 2):

- ρ' **has the same eigenvectors as** ρ **, and its eigenvalues are a polynomial of those of** ρ **.**

$$\rho' = \sum_{i=1}^{n} p(\lambda_i)|\phi_i\rangle\langle\phi_i|$$

$$p(\lambda_i) = \sum_{k=0}^{2(\tilde{n}-1)} c_k \lambda_i^k$$

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The coefficients are the sums of the antidiagonals of a pos. semidef. matrix.

$$R = \begin{pmatrix} R_{00} & R_{01} & R_{02} \\ R_{10} & R_{11} & R_{12} \\ R_{20} & R_{21} & R_{22} \end{pmatrix}$$

c_0 c_1

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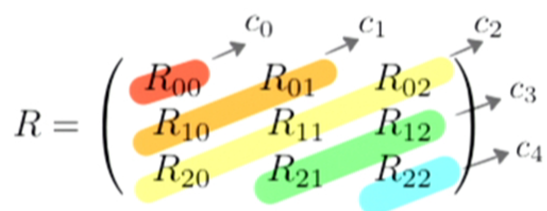
R is the Gram matrix of the ancillary states!

$$R_{ij} = \langle a_i | a_j \rangle$$



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Proof (informal, 3):

- **The polynomial can be written as** $p(\lambda_i) = [\lambda_i^0 \, \lambda_i^1 \ldots \lambda_i^{\tilde{n}-1}] R \begin{bmatrix} \lambda_i^0 \\ \lambda_i^1 \\ \vdots \\ \lambda_i^{\tilde{n}-1} \end{bmatrix} = \langle v_i | R | v_i \rangle$

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  Hence there exists a biorthogonal basis $\{|w_1\rangle, \ldots, |w_{\tilde{n}}\rangle\}$ such that $\langle v_i | w_j \rangle = \delta_{ij}$

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- **Choose** $R = \sum_{j=1}^{\tilde{n}} \lambda_j |w_j\rangle\langle w_j|$

  This satisfies $p(\lambda_i) = \lambda_i$

- **Hence,** $\rho' = \rho$ **. Thus, purif. rank (** ρ **)** $\leq O(D^{\tilde{n}-1})$ ■

Approximate solutions

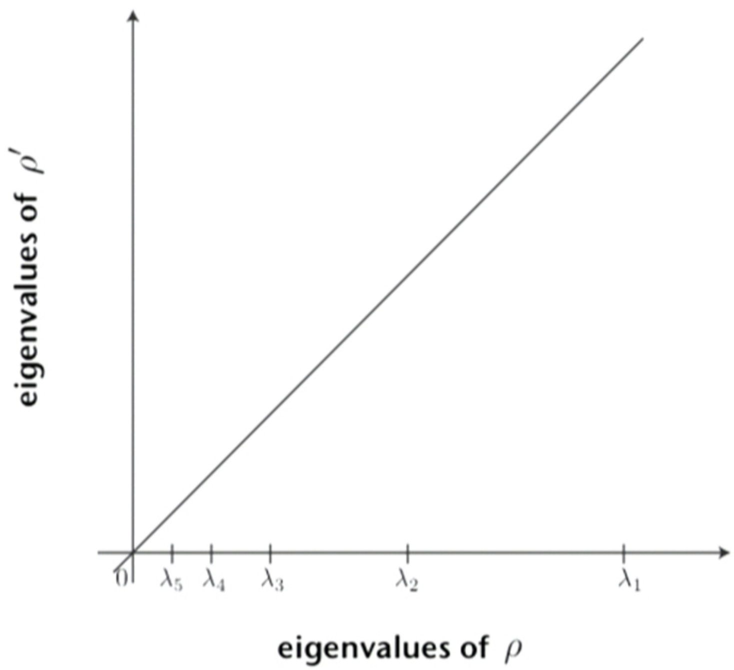
Finding the closest density matrix with a maximum purification rank

is formulated as a Semidefinite Program.

Exact solution

Constructrive proof
of upper bound 2

$p(\lambda_i) = \lambda_i$ **for all i.**



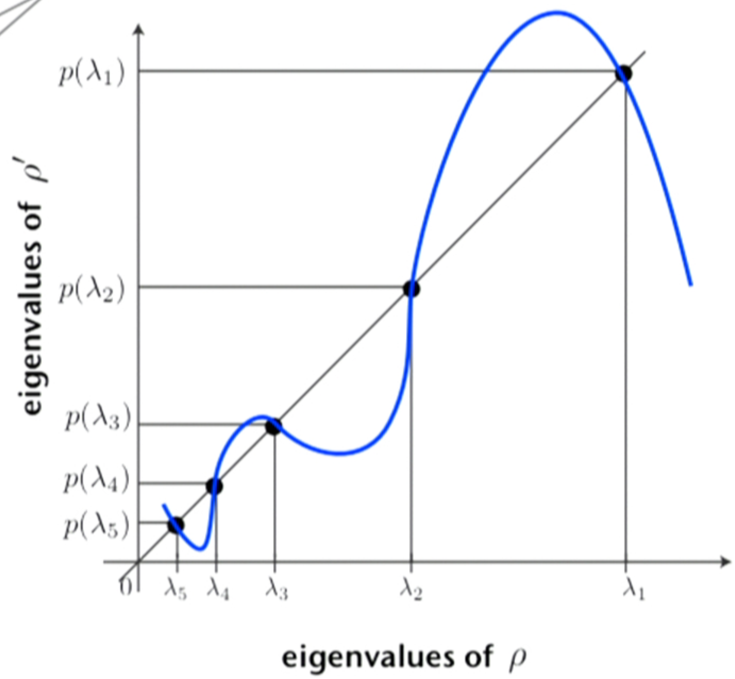
Exact solution

Constructrive proof of upper bound 2

$p(\lambda_i) = \lambda_i$ **for all i.**

There's always a polynomial of degree $2(\tilde{n}-1)$ that passes through $\tilde{n}$ points.

whose coefficients are the sums of the antidiagonals of a positive semidef. matrix



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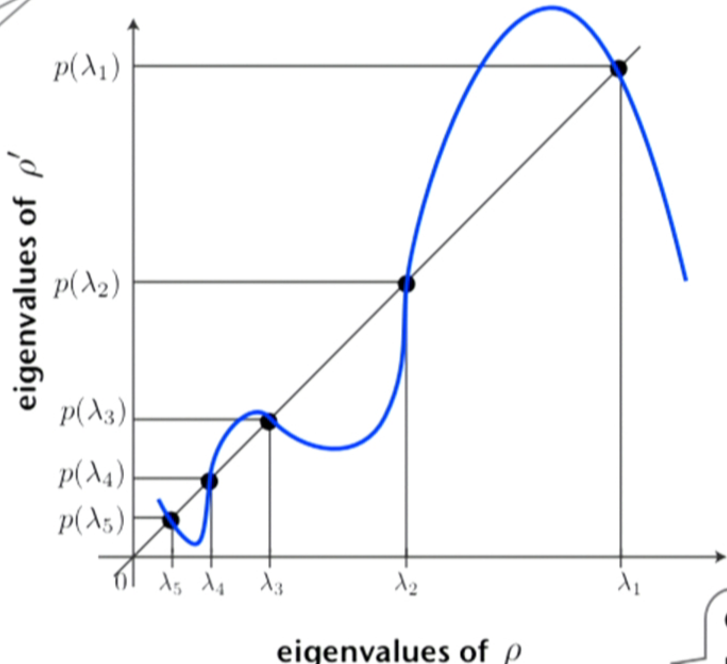


Only different eigenvalues matter ($\tilde{n}$)

Approximate solution

Given ρ with OSR D,

provide ρ' that is closest (in 1-norm) to ρ

and such that purif. rank(ρ') $\leq D^{k-1}$

Approximate solution

We have formulated it as a Semidefinite Program.

Given ρ with OSR D,

provide ρ' that is closest (in 1-norm) to ρ

and such that purif. rank(ρ') $\leq D^{k-1}$

Approximate solution

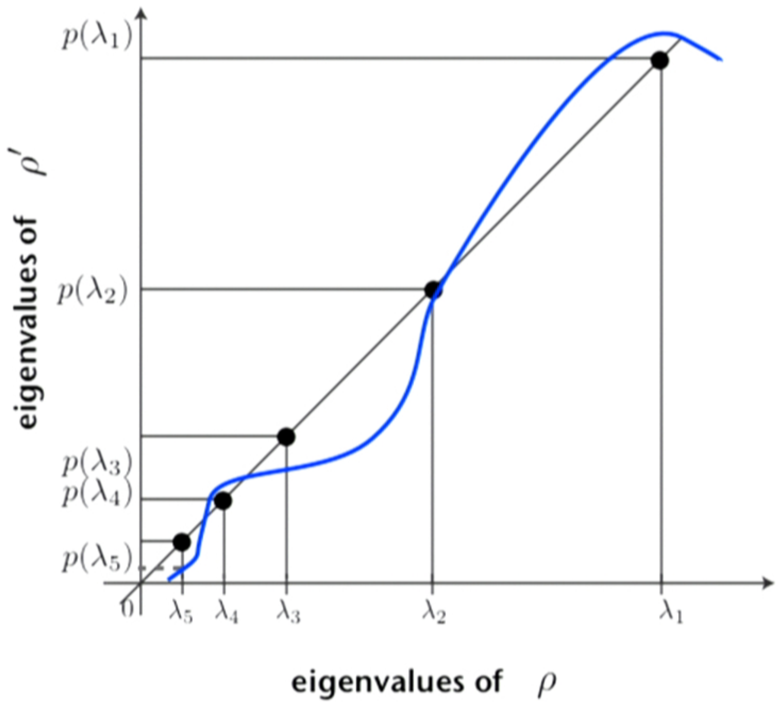
purification rank(ρ') $\leq D^{k-1}$ ➡ polynomial of degree $2(k-1)$

A polynomial of degree $2(k-1)$ can only cross the line $2(k-1)$ times.

Find the polynomial of degree $2(k-1)$ that minimizes the distance (in 1-norm) to the $\tilde{n}$ points.

whose coefficients are the sums of the antidiagonals of a positive semidef. matrix

Approximate solution



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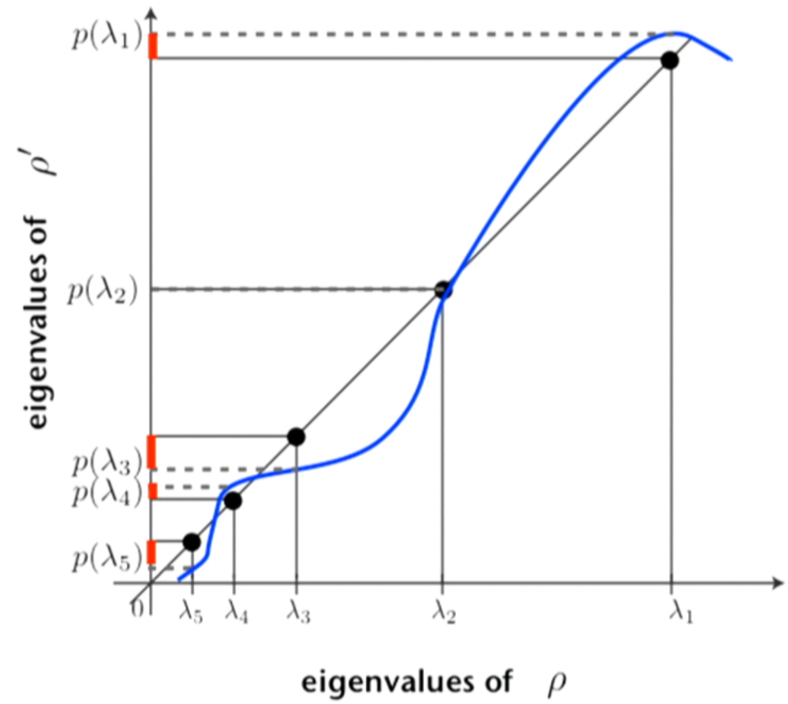
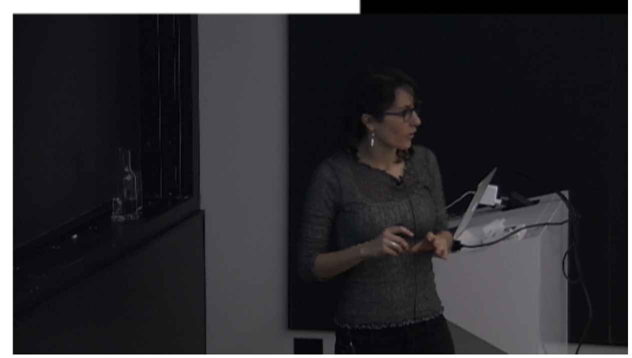


- **Easy distributions:**
  eig. cluster around some points.

- **Hardest distribution:**
  all eigenvalues equally separated.



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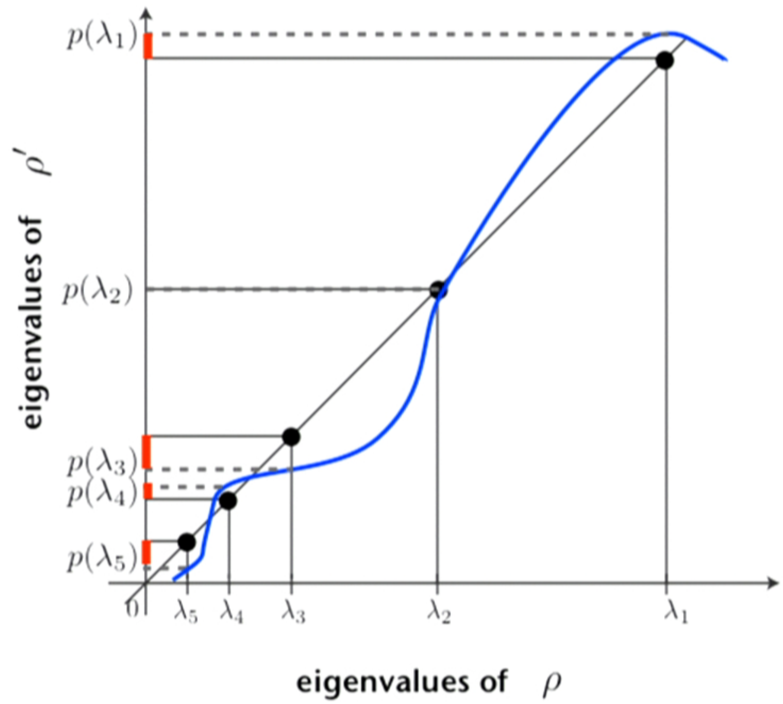

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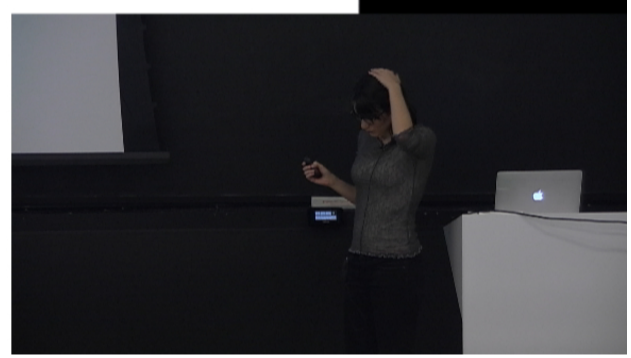

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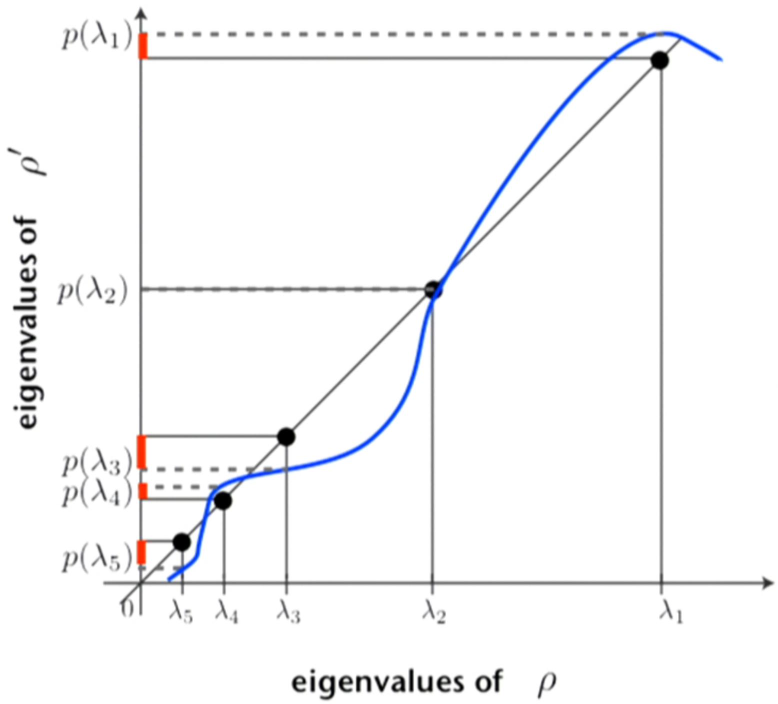

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Towards: **Given** ρ **, provide** ρ' **such that** $||\rho - \rho'||_1 \leq \epsilon$ **and purif. rank(** ρ'**)** $\leq f(\epsilon)$

Conclusions

Develop a good theoretical description of mixed states with tensor networks

↓

Find a canonical form for Matrix Product Density Operators

↓

Relate the two decompositions of Matrix Product Density Operators

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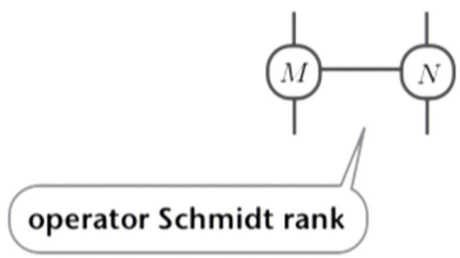
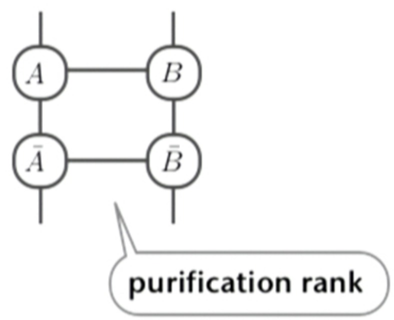
↓

Relate the two decompositions of Matrix Product Density Operators

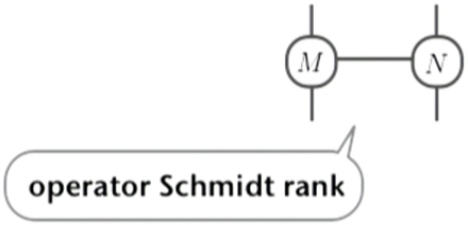
Operator Schmidt decomposition

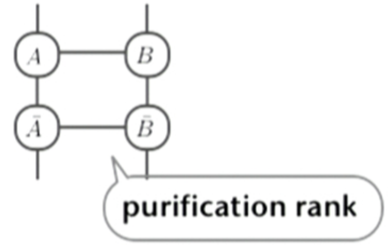


Local purification



Conclusions (2)





The purification rank cannot be upper bounded by a function of the OSR only.

The purification rank is upper bounded by:

1. **the OSR times the number of eigenvalues**
2. **the OSR to the power of the number of different eigenvalues**

Outlook

- Potential applications
  - canonical form for MPDOs ?
  - thermal Hamiltonians
  - symmetries
  - numerical algorithms
  - ...

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  - numerical algorithms
  - ...

- Collateral implications
  - Divisibility of CP maps
  - Communication complexity
  - ...

Thank you!