Diagonal Unitary and Orthogonal Symmetries in Quantum Theory

joint work with Satvik Singh (Cambridge UK —> Munich)

A graphical calculus for integration over random diagonal unitary matrices - LAA 613 (2021) [arXiv:2010.07898]
Diagonal unitary and orthogonal symmetries in quantum theory - Quantum 5, 519 (2021) [arXiv:2112.11123]
The PPT² conjecture holds for all Choi-type maps - Annales Henri Poincaré 23 (2022) [arxiv:2011.03809]
Random covariant quantum channels - joint work with Sang-Jun Park [arXiv:2403.03667]
Entanglement in cyclic sign invariant quantum states - joint work with Aabhas Gulati [arXiv:2501.04786]

Ion Nechita (CNRS, LPT Toulouse)
Quantum Meets IIIT - June 16th 2025

Plan of the talk

1. Unitary symmetry in quantum information
2. Diagonal unitary / orthogonal symmetry
3. Separability of symmetric states
4. The PPT^2 conjecture

Unitary symmetry in quantum information

Symmetry in quantum theory

- Quantum states are modeled mathematically by density matrices

$$\{\rho \in \mathcal{M}_d(\mathbb{C}) \ : \ \rho \geq 0 \text{ and } \operatorname{Tr} \rho = 1\}$$

- Unitary operators encode time evolution

$$\rho \mapsto U\rho U^*, \quad \text{for } U \in \mathcal{U}_d$$

- We would like to consider quantum states which are left invariant by a certain class of unitary operators

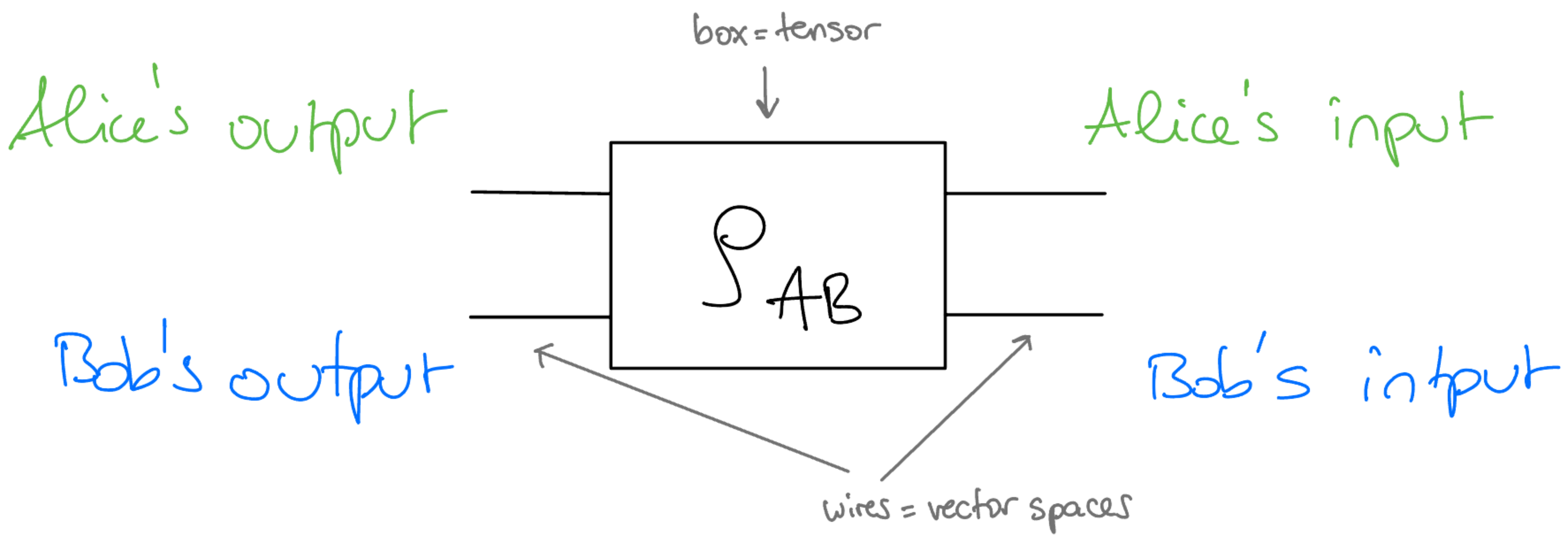
Example. If $UXU^* = X$ for all $U \in \mathcal{U}_d$, then X must be a scalar matrix, i.e. $X = cI_d$ for some constant $c \in \mathbb{C}$. For density matrices, $c = 1/d$.

Bipartite operators

- Quantum entanglement is of the key features of quantum theory. It appears when one considers two quantum systems.

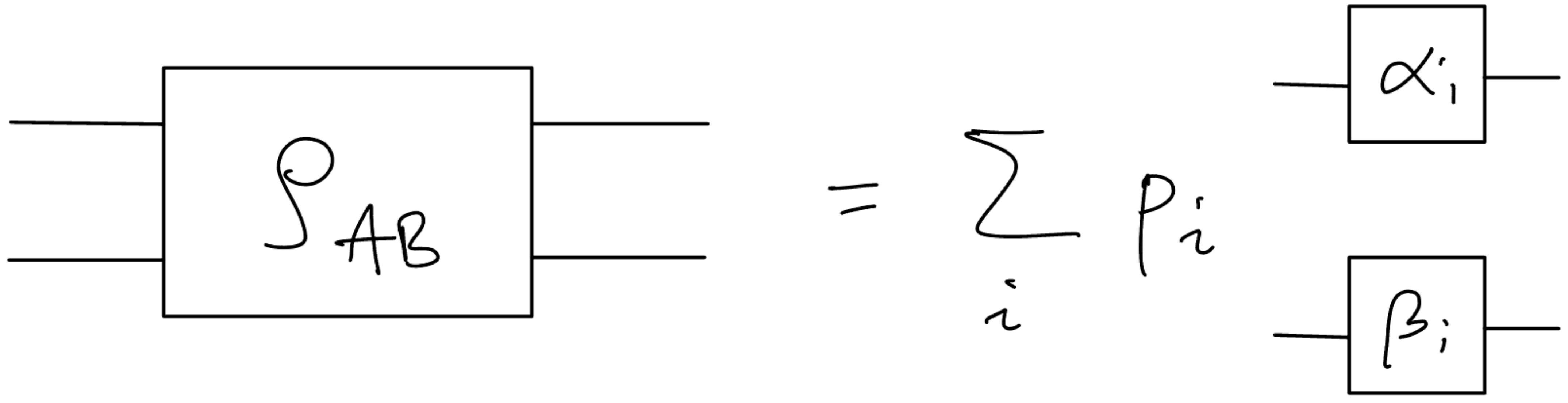
- In this case, the set of quantum states is given by bipartite matrices:

$$\{\rho_{AB} \in \mathcal{M}_d \otimes \mathcal{M}_d \cong \mathcal{M}_{d^2} \ : \ \rho \geq 0 \ \text{and} \ \operatorname{Tr} \rho = 1\}$$

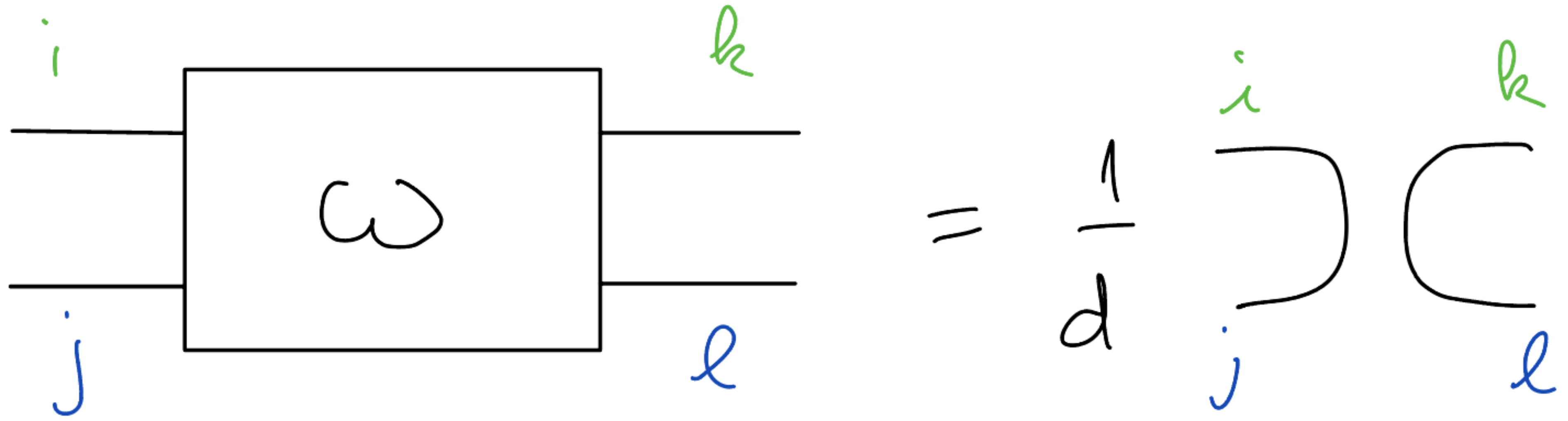


Quantum Entanglement

- Separable states are bipartite quantum states which can be written as convex combinations of product states $\rho_A \otimes \rho_B$



- Entangled states are the non-separable states. The most important example is the *maximally entangled state*



$$\omega = \frac{1}{d} \sum_{i,j=1}^{d} |ii\rangle\langle jj|$$

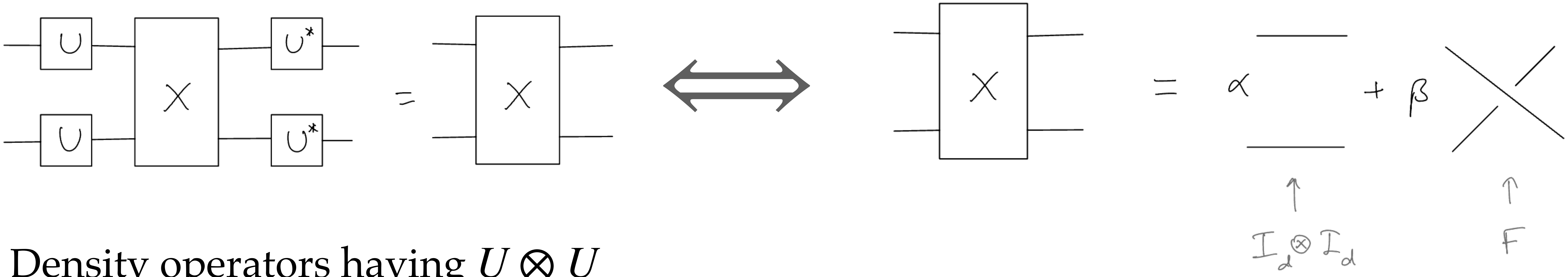
$$\omega_{ijkl} = \frac{1}{d} \delta_{ij} \delta_{kl}$$

(Full) Unitary symmetry in the bipartite case

Theorem. Let $X \in \mathcal{M}_d \otimes \mathcal{M}_d$ be a bipartite operator. Then

$$\forall U \in \mathcal{U}_d, (U \otimes U)X(U \otimes U)^* = X \iff X = \alpha I_{d^2} + \beta F \text{ for } \alpha, \beta \in \mathbb{C}$$

where the (unitary) flip operator is defined by $F\, x \otimes y = y \otimes x$. Note that the property above is equivalent to $[X, U \otimes U] = 0$ for all $U \in \mathcal{U}_d$.



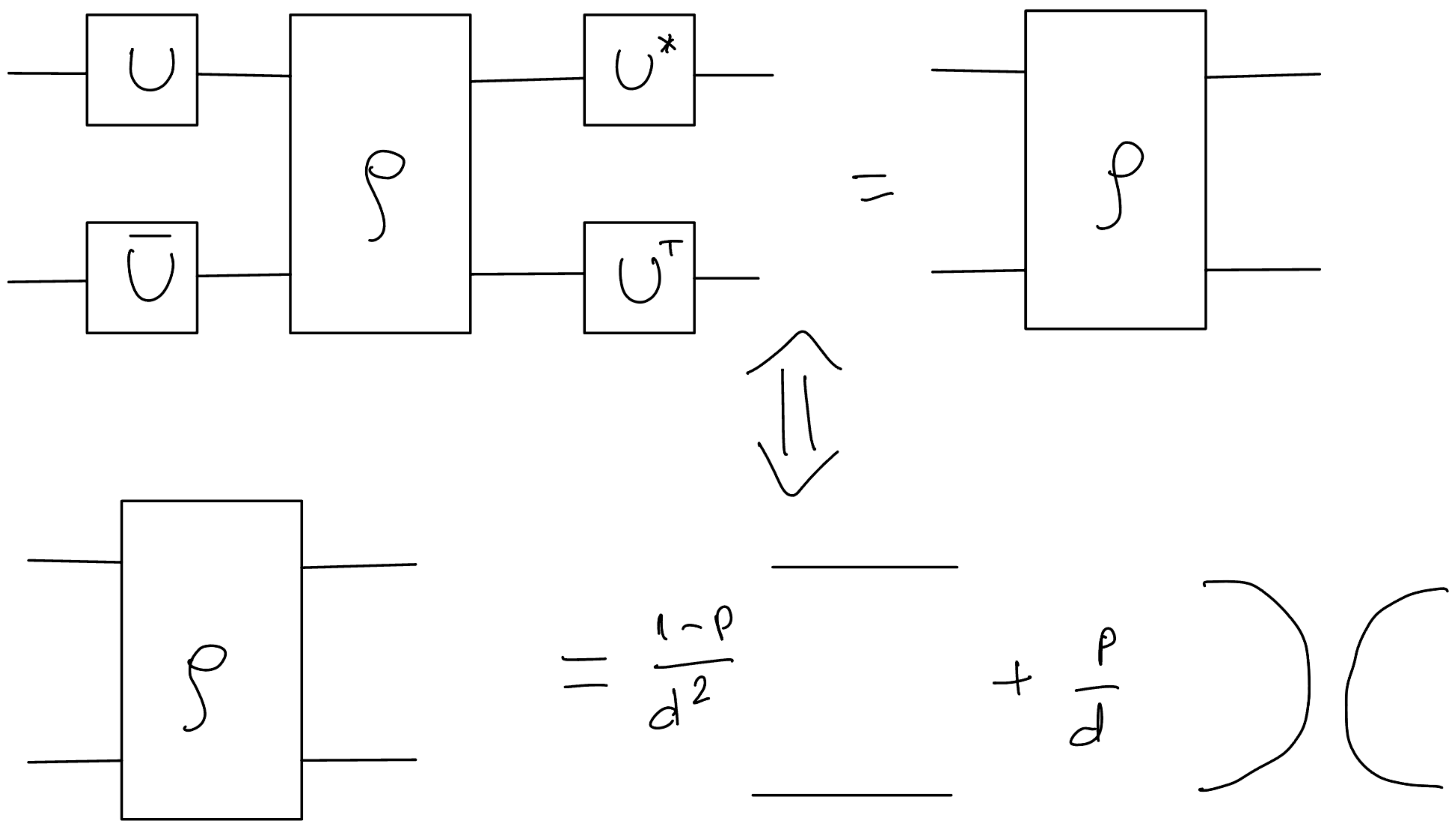
Density operators having $U \otimes U$ symmetry are called Werner states

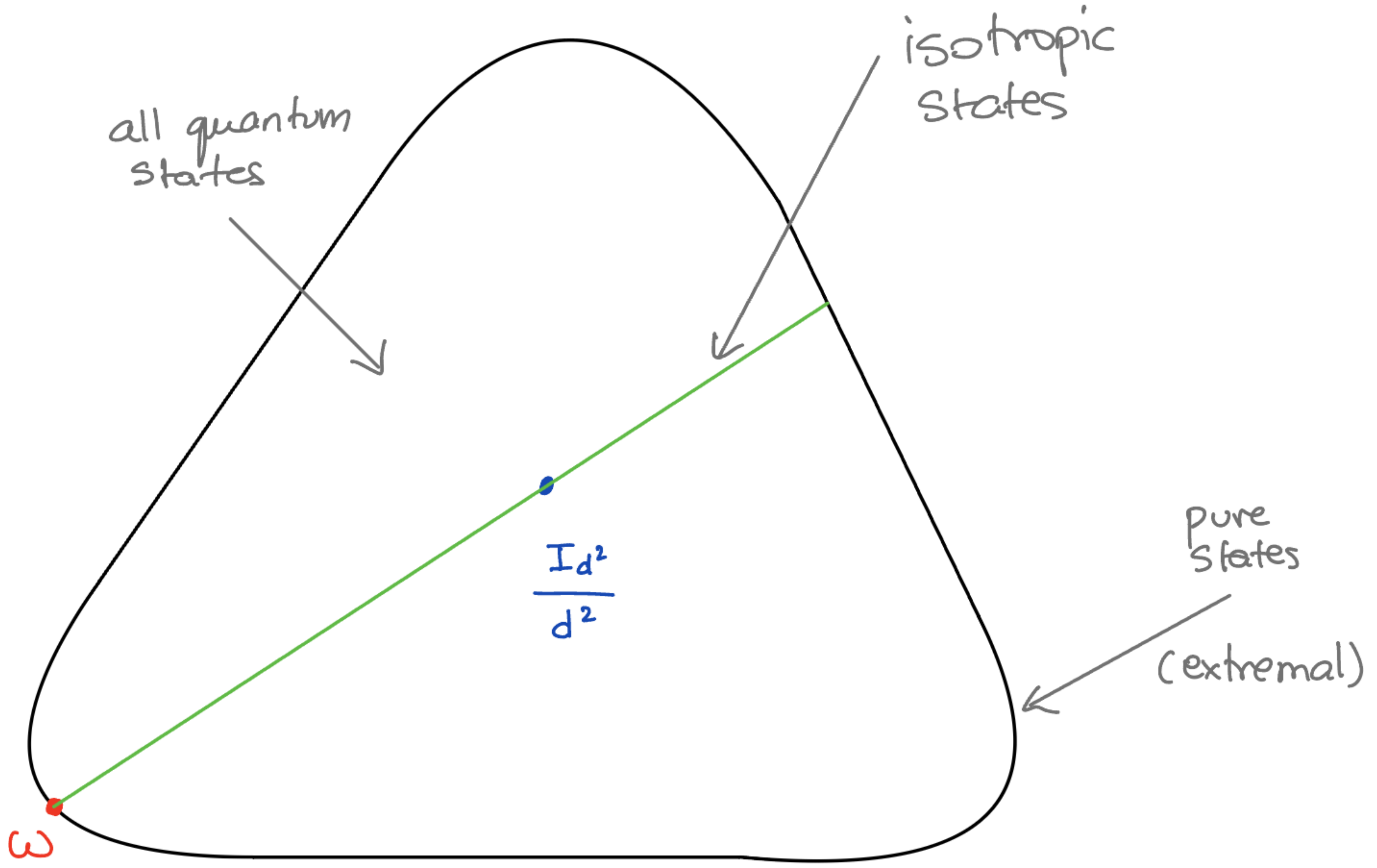
Isotropic quantum states

Theorem. Let $\rho \in \mathcal{M}_d \otimes \mathcal{M}_d$ be a bipartite density matrix. Then

$$\forall U \in \mathcal{U}_d, (U \otimes \bar{U})\rho(U^* \otimes U^\top) = \rho \iff \rho = (1-p)\frac{I}{d^2} + p\omega \text{ for } p \in [-1/(d^2-1), 1]$$

i.e. ρ must be a convex combination of the maximally mixed state and the maximally entangled state. Such quantum states are called isotropic.

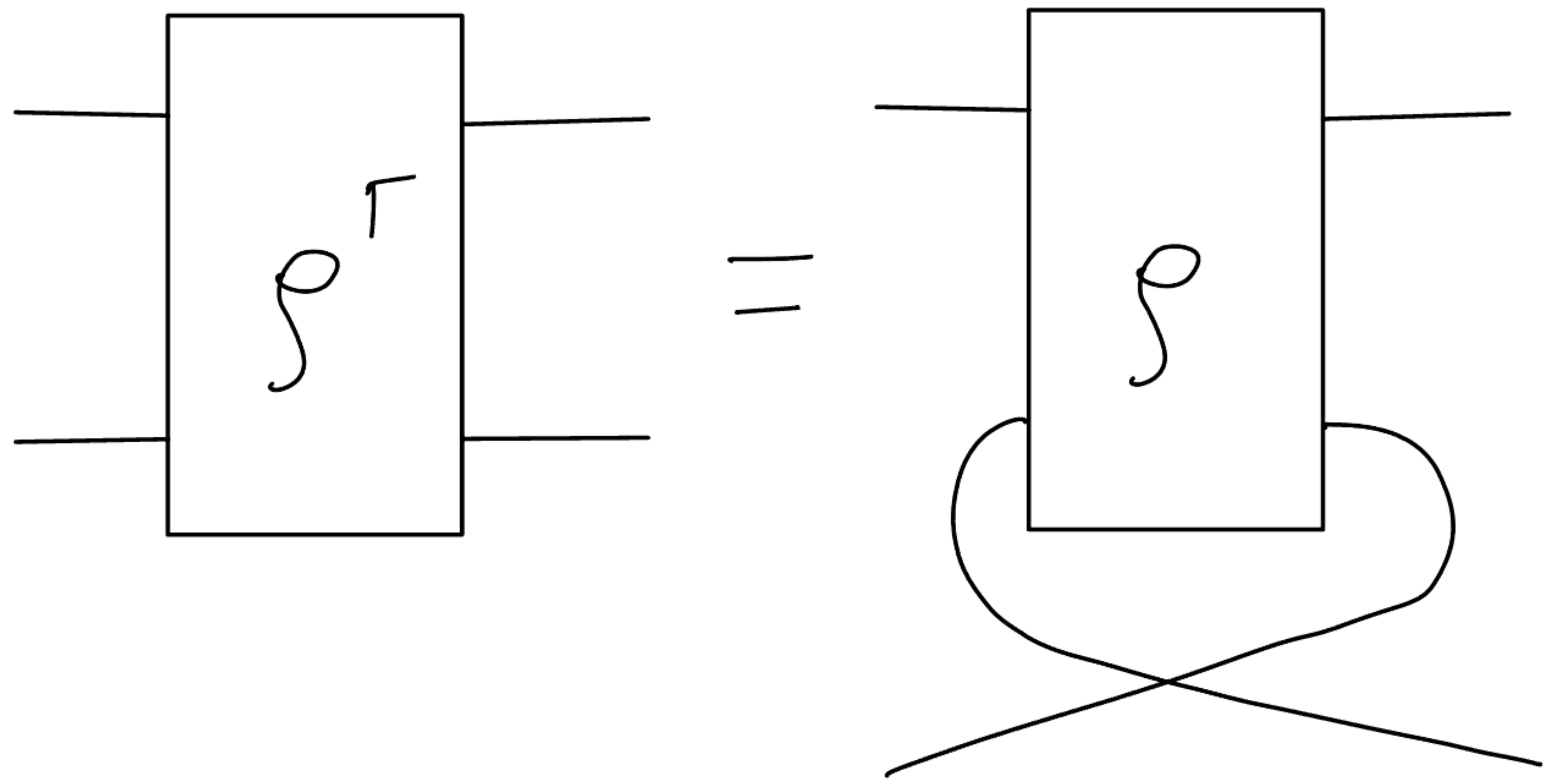




The partial transposition criterion

Given a separable state $\rho = \sum_i p_i \alpha_i \otimes \beta_i$, we have that

$$\rho^\Gamma := [\mathrm{id} \otimes \top\,](\rho) = \sum_i p_i \alpha_i \otimes \beta_i^\top \geq 0.$$



A state ρ such that $\rho^\Gamma \geq 0$ is said to have a positive partial transpose (PPT). A state that is not PPT is necessarily entangled. The PPT criterion is sufficient only for $d_A \cdot d_B \leq 6$.

An isotropic state ρ is separable iff it is PPT iff $p \leq 1/(d+1)$.
Similarly, a Werner state ρ_W is separable iff it is PPT.
In conclusion, there are no PPT entangled states that are $U \otimes U$ or $U \otimes \bar{U}$ symmetric. The same is true for $O \otimes O$ symmetric states (Brauer states) and even the more general hyperoctahedral states.

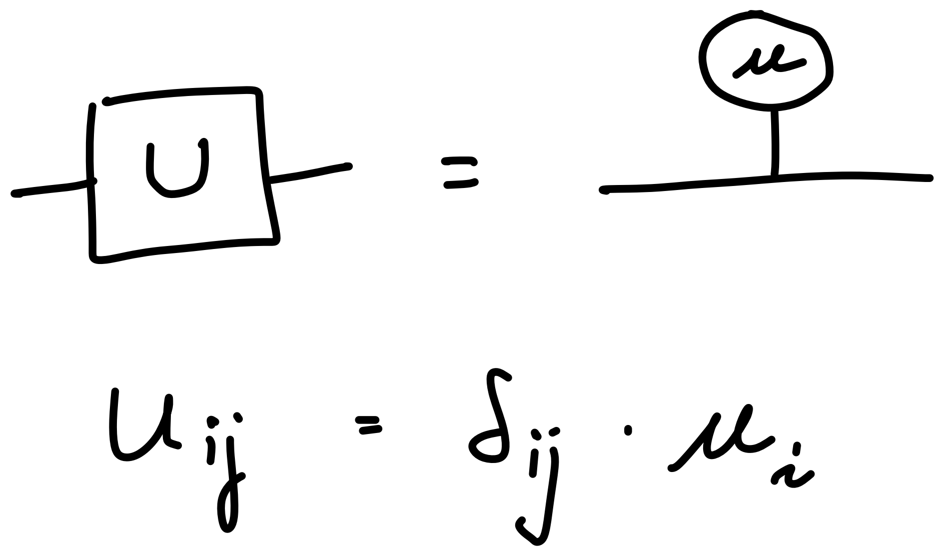
Diagonal unitary / orthogonal symmetry

The diagonal subgroup

- Since requiring the full unitary symmetry yields matrices (resp. quantum states) with only 2 parameters, we shall consider the much smaller subgroups

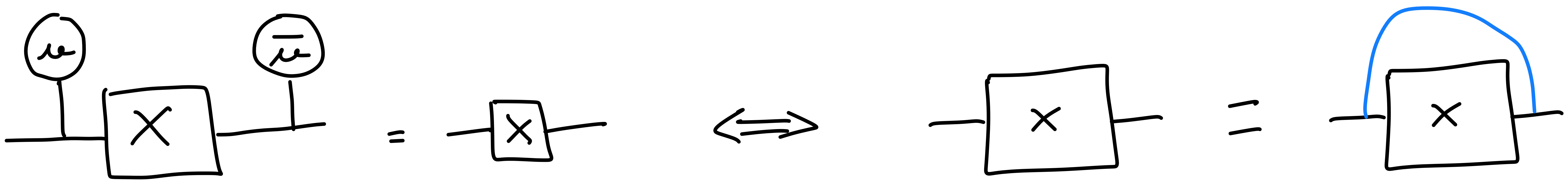
$$\mathscr{DU}_d := \{\mathrm{diag}(e^{i\theta_1}, \ldots, e^{i\theta_d}) \;:\; \theta \in \mathbb{R}^d\}$$

$$\mathscr{DO}_d := \{\mathrm{diag}(\epsilon_1, \ldots, \epsilon_d) \;:\; \epsilon \in \{\pm 1\}^d\}$$



- In the case of a single tensor factor, we have

$$\forall U \in \mathscr{DU}_d, \quad UXU^* = X \iff X = \mathrm{diag}(X)$$

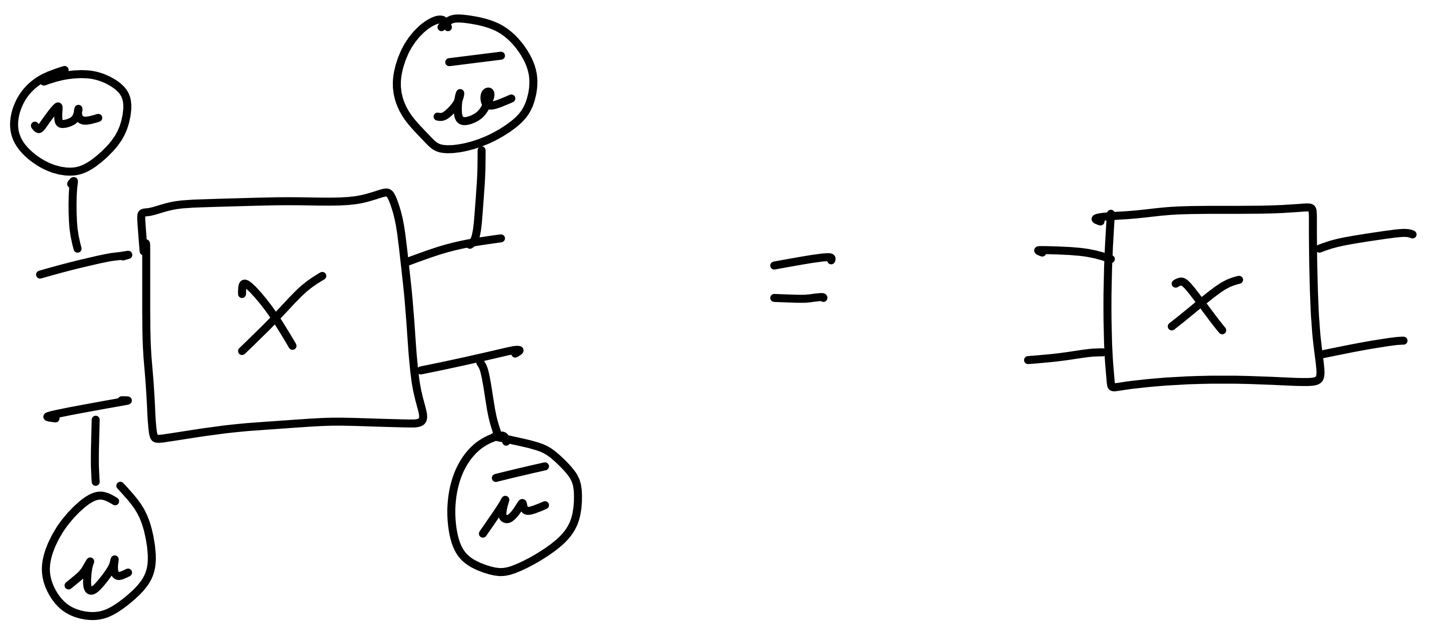


Diagonally symmetric bipartite matrices

Definition. A bipartite matrix $X \in \mathcal{M}_d \otimes \mathcal{M}_d$ is called:

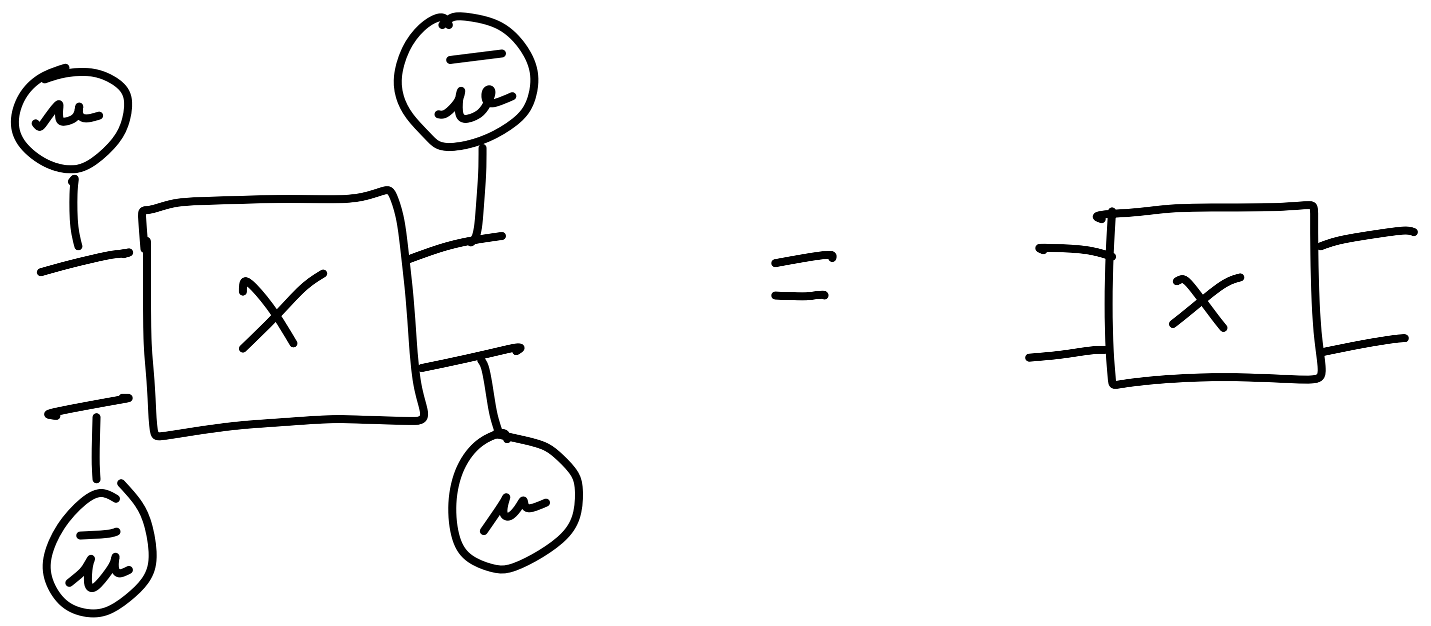
- LDUI (local diagonal unitary invariant) if

$$\forall U \in \mathcal{DU}_d, \quad (U \otimes U)X(U^* \otimes U^*) = X$$



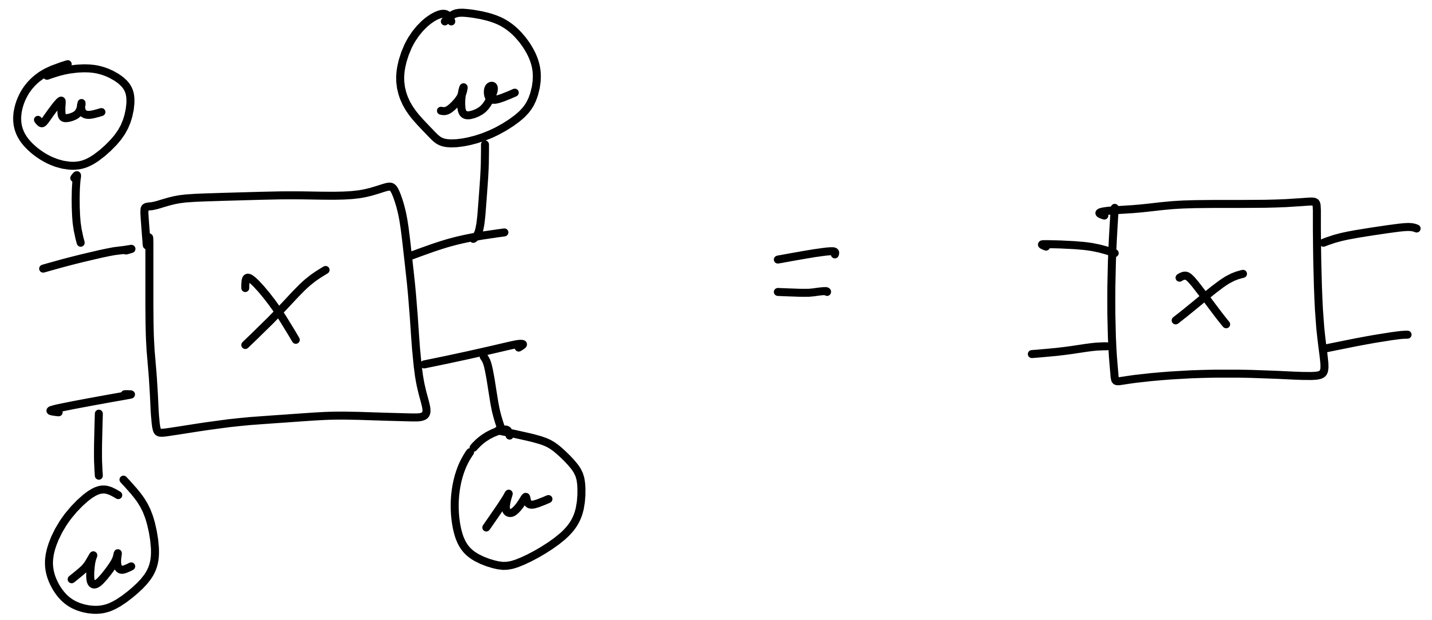
- CLDUI (conjugate LDUI) if

$$\forall U \in \mathcal{DU}_d, \quad (U \otimes \bar{U})X(U^* \otimes U^\top) = X$$



- LDOI (local diagonal orthogonal invariant) if

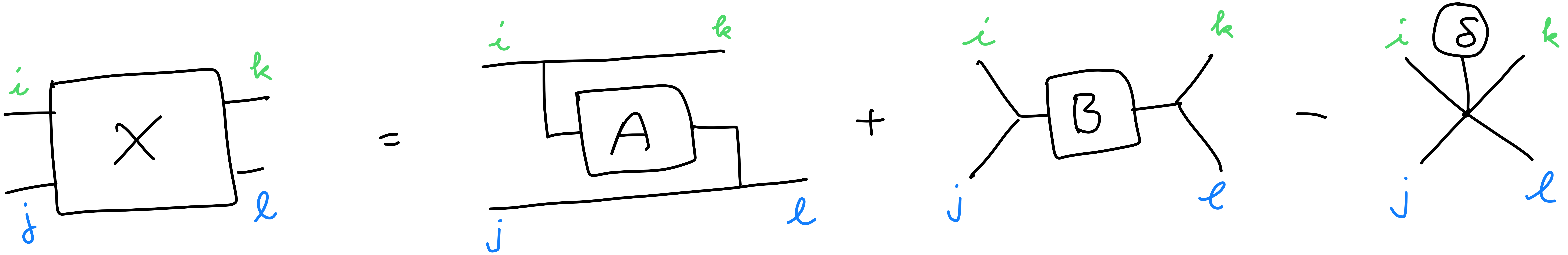
$$\forall U \in \mathcal{DO}_d, \quad (U \otimes U)X(U^\top \otimes U^\top) = X$$

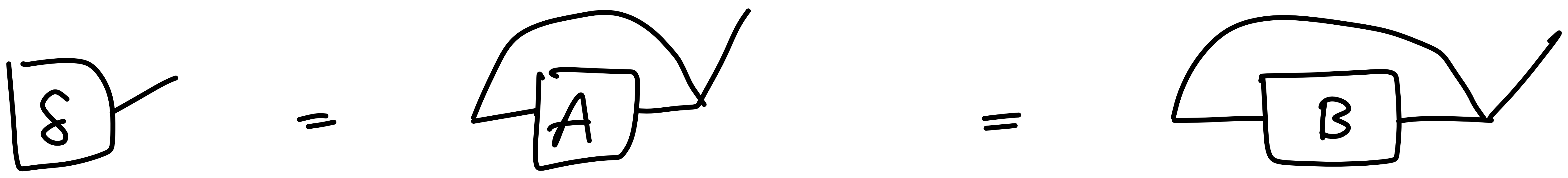


Characterization theorem — CDLUI case

Theorem. A matrix $X \in \mathcal{M}_d \otimes \mathcal{M}_d$ is CLDUI iff there exist matrices $A, B \in \mathcal{M}_d$ having the same diagonal $\operatorname{diag} A = \operatorname{diag} B =: \delta \in \mathbb{C}^d$ such that

$$X_{ij,kl} = \mathbf{1}_{i=k,j=l} A_{ij} + \mathbf{1}_{i=j,k=l} B_{ik} - \mathbf{1}_{i=j=k=l} \delta_i$$





Characterization theorem - LDUI and LDOI

Theorem. A matrix $X \in \mathscr{M}_d \otimes \mathscr{M}_d$ is LDUI iff there exist matrices $A, C \in \mathscr{M}_d$ having the same diagonal $\operatorname{diag} A = \operatorname{diag} C =: \delta \in \mathbb{C}^d$ such that

$$X_{ij,kl} = \mathbf{1}_{i=k,j=l} A_{ij} + \mathbf{1}_{i=l,j=k} C_{ij} - \mathbf{1}_{i=j=k=l} \delta_i$$

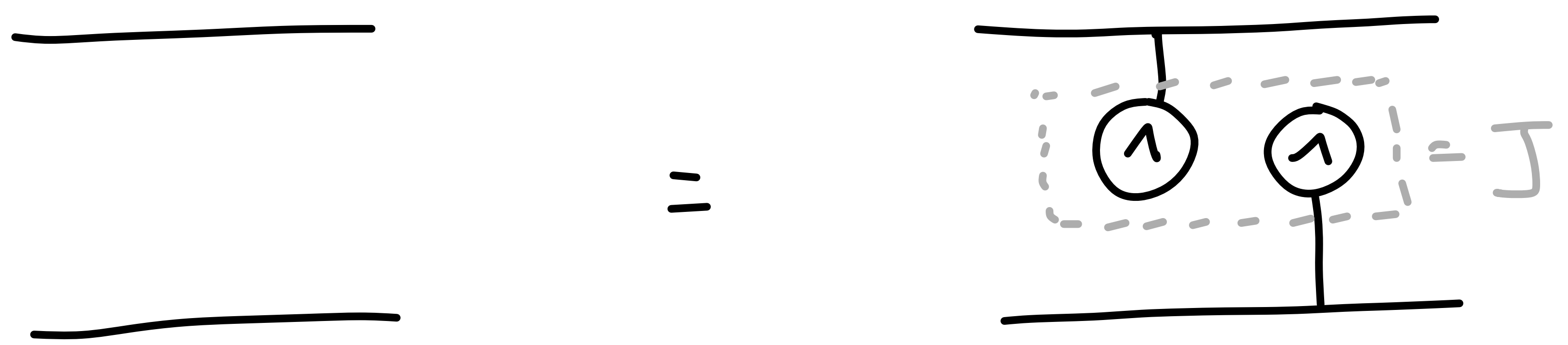
Theorem. A matrix $X \in \mathscr{M}_d \otimes \mathscr{M}_d$ is LDOI iff there exist matrices $A, B, C \in \mathscr{M}_d$ having the same diagonal $\operatorname{diag} A = \operatorname{diag} B = \operatorname{diag} C =: \delta \in \mathbb{C}^d$ such that

$$X_{ij,kl} = \mathbf{1}_{i=k,j=l} A_{ij} + \mathbf{1}_{i=j,k=l} B_{ik} + \mathbf{1}_{i=l,j=k} C_{ij} - 2\mathbf{1}_{i=j=k=l} \delta_i$$

Three examples

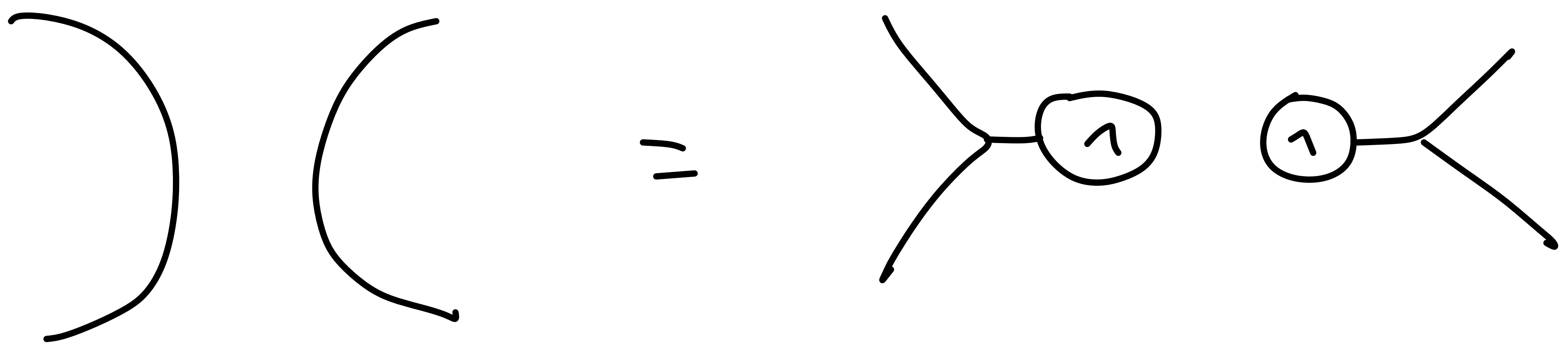
- The identity matrix is CLDUI with

  $A = J_d, B = I_d$



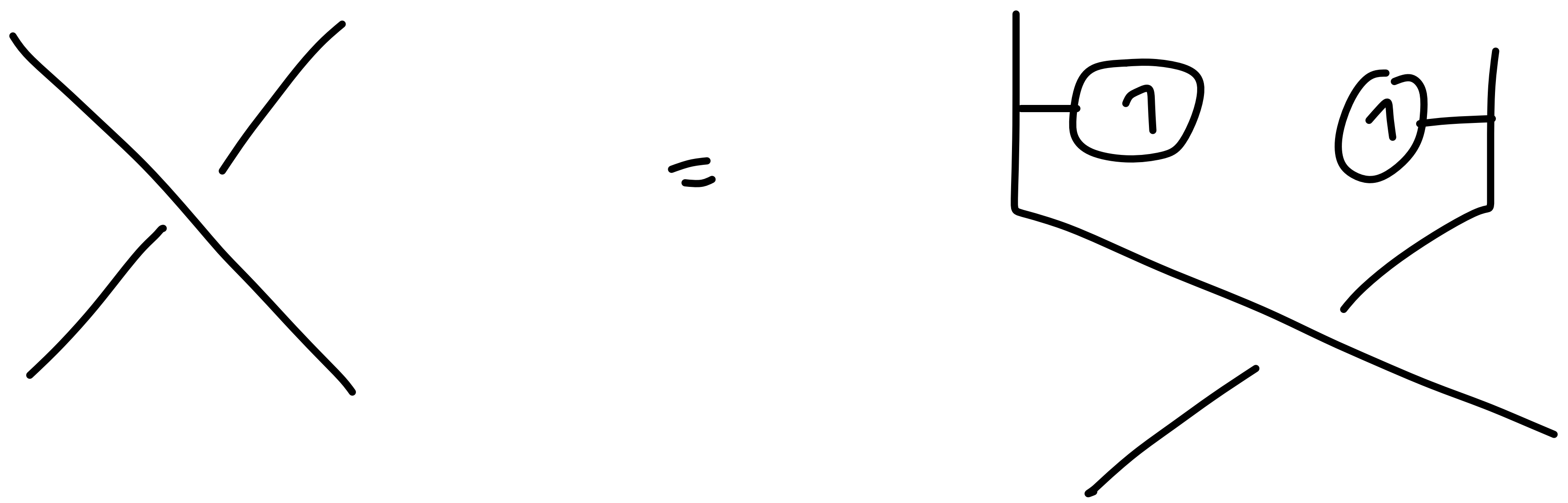
- The maximally entangled state is

  CLDUI with $A = I_d, B = J_d$



- The flip operator is LDUI with

  $A = I_d, B = J_d$



More examples

Werner and isotropic states

$X_{a,b}^{\text{wer}} = a(I_d \otimes I_d) + b \sum_{i,j=1}^{d} |ij\rangle\langle ji|$ and $X_{a,b}^{\text{iso}} = a(I_d \otimes I_d) + b \sum_{i,j=1}^{d} |ii\rangle\langle jj|$ are,

respectively, LDUI and CLDUI, with $A = bI_d + aJ_d$ and $B = aI_d + bJ_d$.

Mixtures of Dicke states or diagonal symmetric matrices

$X_Y^{\text{dicke}} = \sum_{1\le i\le j\le d} Y_{ij} |\psi_{ij}\rangle\langle\psi_{ij}|$ are LDUI, with $A = B = \text{diag}(Y) + (Y - \text{diag}(Y))/2$.

Here, $\psi_{ii} = |ii\rangle$ and $\psi_{ij} = (|ij\rangle + |ji\rangle)/\sqrt{2}$.

Symmetric bipartite PSD operators

Properties of symmetric operators

Theorem. A bipartite LDOI operator $X = X_{A,B,C}$ is

- self-adjoint iff A is real and B, C are self-adjoint
- positive semidefinite iff the following three conditions hold:
    1. A is entry-wise non-negative ($A_{ij} \geq 0$ for all i, j)
    2. B is positive semidefinite
    3. $A_{ij}A_{ji} \geq |C_{ij}|^2$ for all i, j

Note that LDUI operators correspond to B diagonal, and CLDUI operators correspond to C diagonal.

Further properties

Proposition. The set of LDOI matrices is stable under tensor leg operations:

$$F X_{A,B,C} F = X_{A^\top,B,C^\top} \qquad X^T_{A,B,C} = X_{A,B^\top,C^\top} \qquad X^\Gamma_{A,B,C} = X_{A,C,B}$$

In particular, a CLDUI matrix $X_{A,A}$ is PPT iff A is doubly non-negative

$$A \in \mathrm{DNN}_d := \{A \in \mathscr{M}_n(\mathbb{R}) \,:\, A_{ij} \geq 0 \, \forall i,j \text{ and } A \geq 0\}$$

Similarly, different normalizations of LDOI matrices can be read off A:

$$\operatorname{Tr} X_{A,B,C} = \langle 1 \,|\, A \,|\, 1 \rangle \qquad \operatorname{Tr}_2 X_{A,B,C} = \operatorname{diag}(A \cdot 1) \qquad \operatorname{Tr}_1 X_{A,B,C} = \operatorname{diag}(1^\top \cdot A)$$

Conclusion. The set of LDOI, CLDUI, and LDUI matrices form a $O(d^2)$-parameter family of bipartite matrices $X_{A,B,C} \in \mathscr{M}_{d^2}$ for which many of the properties relevant to quantum information theory can be easily read off the parameters $A, B, C \in \mathscr{M}_d$.

Separability for diagonal symmetric matrices

Theorem. A bipartite CLDUI operator of the form $X = X_{A,A} \in \mathscr{M}_d(\mathbb{C}) \otimes \mathscr{M}_d(\mathbb{C})$ is separable iff the matrix A is completely positive, i.e.

$$\exists R \in \mathscr{M}_{d\times k}(\mathbb{R}_+) \quad \text{s.t.} \quad A = RR^\top .$$

The columns of the non-negative square root R give the separable decomposition

$$X = \sum_{i=1}^{k} |r_i\rangle\langle r_i| \otimes |r_i\rangle\langle r_i| .$$

In this case, $A = \sum_{i=1}^{k} |r_i\rangle\langle r_i|$.

More on completely positive matrices

Completely positive matrices are doubly non-negative: they have non-negative entries and they are positive semidefinite:

$$\mathrm{CP}_d \subseteq \mathrm{DNN}_d = \{A \in \mathcal{M}_n(\mathbb{R}) \ : \ A_{ij} \geq 0 \, \forall i,j \text{ and } A \geq 0\} \, .$$

Recall that: $X_{A,A}$ is PPT iff $A \in \mathrm{DNN}_d$ and $X_{A,A}$ is SEP iff $A \in \mathrm{CP}_d$

For $d \leq 4$, $\mathrm{CP}_d = \mathrm{DNN}_d$, so, in particular, every PPT CLDUI $X_{A,A}$ state is separable.

For $d \geq 5$, there exist DNN matrices that are not completely positive, so there exist PPT entangled $X_{A,A}$ states.

$$A = \begin{bmatrix} 7 & 4 & 0 & 0 & 4 \\ 4 & 7 & 4 & 0 & 0 \\ 0 & 4 & 7 & 4 & 0 \\ 0 & 0 & 4 & 7 & 4 \\ 4 & 0 & 0 & 4 & 7 \end{bmatrix}$$

In general, it is NP-hard to detect membership in CP.

PCP and TCP matrices

Definition. A pair of matrices (A, B) is called pairwise completely positive (PCP) if there exist matrices $V, W \in \mathscr{M}_{d\times k}(\mathbb{C})$ such that

$$A = (V \odot \bar{V})(W \odot \bar{W})^* \quad \text{and} \quad B = (V \odot W)(V \odot W)^* .$$

A triple (A, B, C) is called triplewise completely positive (TCP) if, additionally, $C = (V \odot \bar{W})(V \odot \bar{W})^*$.

Theorem. A (C)LDUI matrix $X_{A,B}$ is separable iff the pair (A, B) is PCP. An LDOI matrix $X_{A,B,C}$ is separable iff the triple (A, B, C) is TCP.

Application: the PPT² conjecture

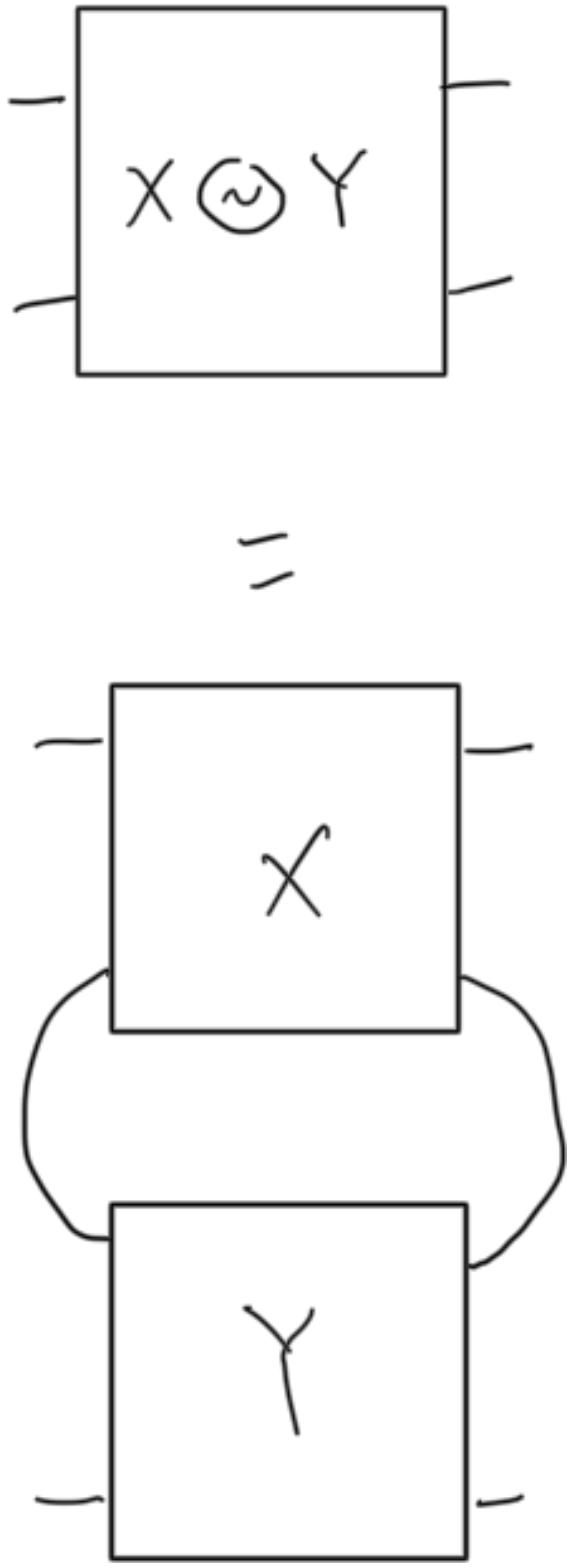
Conjecture. The link product of two PPT matrices is separable.

Recall that a (C)LDUI matrix $X_{A,B}$ is PPT (positive partial transpose) iff A is entrywise non-negative, B is PSD, and $\forall i, j, A_{ij}A_{j,i} \geq |B_{ij}|^2$.

Theorem. The PPT² conjecture holds for (C)LDUI matrices.

Proposition. Let $X_{A,B}$ be a PPT (C)LDUI matrix. If B is diagonally dominant (i.e. $\forall i, \quad A_{ii} = B_{ii} \geq \sum_{j \neq i} |B_{ij}|$), then (A, B) is PCP ($\iff \quad X_{A,B}$ is separable).

The proof of the proposition relies on the notion of factor width.



Factor width

Definition. A positive semidefinite matrix B is said to have factor width k if it admits a decomposition $B = \sum_i |v_i\rangle\langle v_i|$, where the complex vectors v_i have support at most k.

Matrices with factor width 1 are diagonal matrices. The comparison matrix M(B) of B is defined by $M(B)_{ii} = |B_{ii}|$ and $M(B)_{ij} = -|B_{ij}|$ for $i \neq j$.

Theorem. A positive semidefinite matrix B has factor width 2 if and only if M(B) is positive semidefinite. In particular, if B is diagonally dominant, then B has factor width 2.

Proposition. A pair (A, B) with A non-negative, B positive semidefinite such that $A_{ij}A_{ji} \geq |B_{ij}|^2$ and B has factor width 2 is PCP. (used in the proof of PPT^2)

Take home slide

- Multipartite quantum states that are symmetric with by conjugation with diagonal unitary (resp. orthogonal) matrices form a rich, interesting class.

- For states invariant w.r.t. the full unitary group, there are no PPT entangled states. One can consider slightly larger symmetry groups, e.g. by adding cyclic permutations of the phases.

- The CLDUI class is parametrized by two matrices A, B having a common diagonal. This class contains all classical (diagonal) states and the maximally entangled state.

- A CLDUI matrix $X_{A,B}$ is PSD iff A is entry-wise non-negative and B is PSD.

- A CLDUI matrix $X_{A,B}$ is separable iff the pair (A, B) is pairwise completely positive (PCP). This is a generalization of completely positive matrices.

- (C)LDUI matrices satisfy the PPT^2 conjecture; the proof uses the notion of factor width and its generalisation to the PCP setting.