

Title: From Pauli's Principle to Fermionic Entanglement

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Abstract: The Pauli exclusion principle is a constraint on the natural occupation numbers of fermionic states. It has been suspected for decades, and only proved very recently, that there is a multitude of further constraints on these numbers, generalizing the Pauli principle. Surprisingly, these constraints are linear: they cut out a geometric object known as a polytope. This is a beautiful mathematical result, but are there systems whose physics is governed by these constraints?

In order to address this question, we studied a system of a few fermions connected by springs. As we varied the spring constant, the occupation numbers moved within the polytope. The path they traced hugs very close to the boundary of the polytope, suggesting that the generalized constraints affect the system. I will mention the implications of these findings for the structure of few-fermion ground states and then discuss the relation between the geometry of the polytope and different types of fermionic entanglement.

From Pauli's Principle to Fermionic Entanglement

Matthias Christandl
ETH Zurich

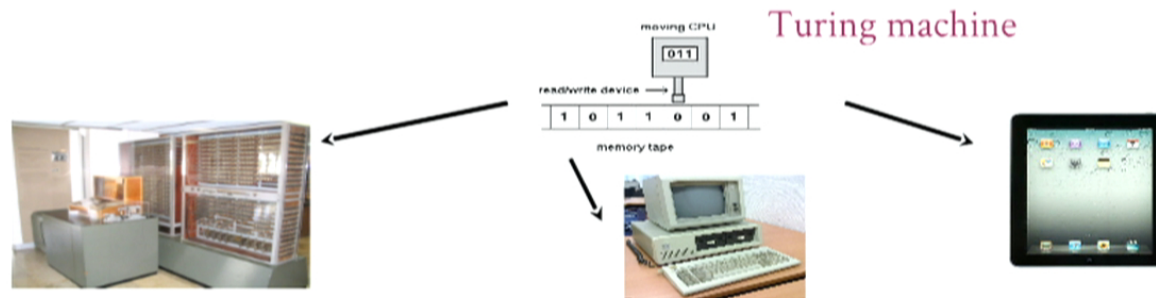
Information

Shannon, 1948

Computation

Turing, 1936

Concept „computation“ independent of physical implementation



All physical computation can be represented this way

→ Computer Science

Quantum Mechanics

Shannon & Turing's notions
based on classical physics
information has always definite value

01011010100

Quantum Mechanics (1900s)
atoms not governed by classical physics

Shannon/Turing do not
directly apply!

Quantum Information Theory

$$'0' \rightarrow |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad '1' \rightarrow |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

My Research in Quantum Information Theory

My Research in Quantum Information Theory

How are the whole and the parts
of a quantum state related?



density matrices

- quantum complexity theory
- condensed matter physics
- quantum chemistry

Schilling, Gross & Christandl
Physical Review Letters 2013

entanglement

- quantum cryptography
- foundations of physics
- algebraic complexity theory

entropy

- quantum coding theory
- mathematical physics
- optimization

Brandao, Christandl & Yard
Communications in Mathematical Physics 2011

Pauli's principle

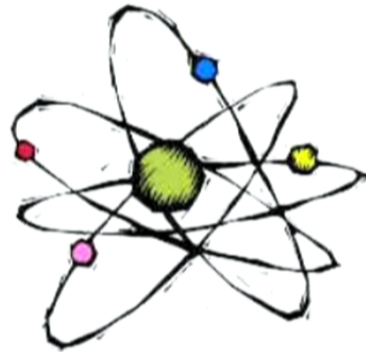
Pauli exclusion principle (1925)
 All fermions must occupy different quantum states

Occupation Numbers

\mathcal{H}_N (fixed particle number N)
 $\{|\varphi_i\rangle\} \in \Lambda^N(\mathcal{H})$

Natural Occupation Numbers

\mathcal{H}_N $|\Psi_N\rangle$
 occupation numbers
 $n_i = \langle \Psi_N | a_i^\dagger a_i | \Psi_N \rangle$



Physical relevance?

Pauli principle \rightarrow $\sigma = \pm 1/2$
 can prevent electrons from falling

Polytopes

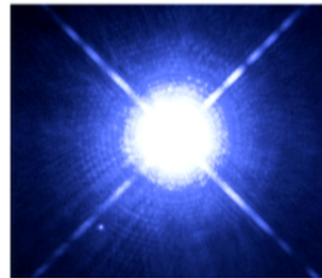
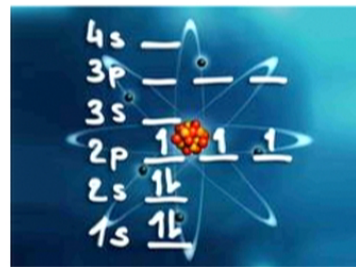
N fermions & k modes \rightarrow fermion simplex

Pauli's principle

Pauli's exclusion principle (1925):

`no two fermions in
the same quantum state'

$$0 \leq n_i \leq 1$$



strengthened by Dirac & Heisenberg in (1926):

`quantum states of fermions
are antisymmetric'

Occupation Numbers

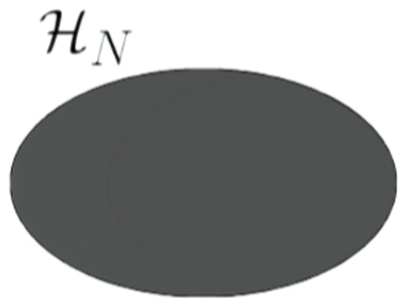
\mathcal{H}_N



fixed particle number N

$$|\Psi_N\rangle \in \Lambda^N(\mathcal{H})$$

Natural Occupation Numbers



$|\Psi_N\rangle$



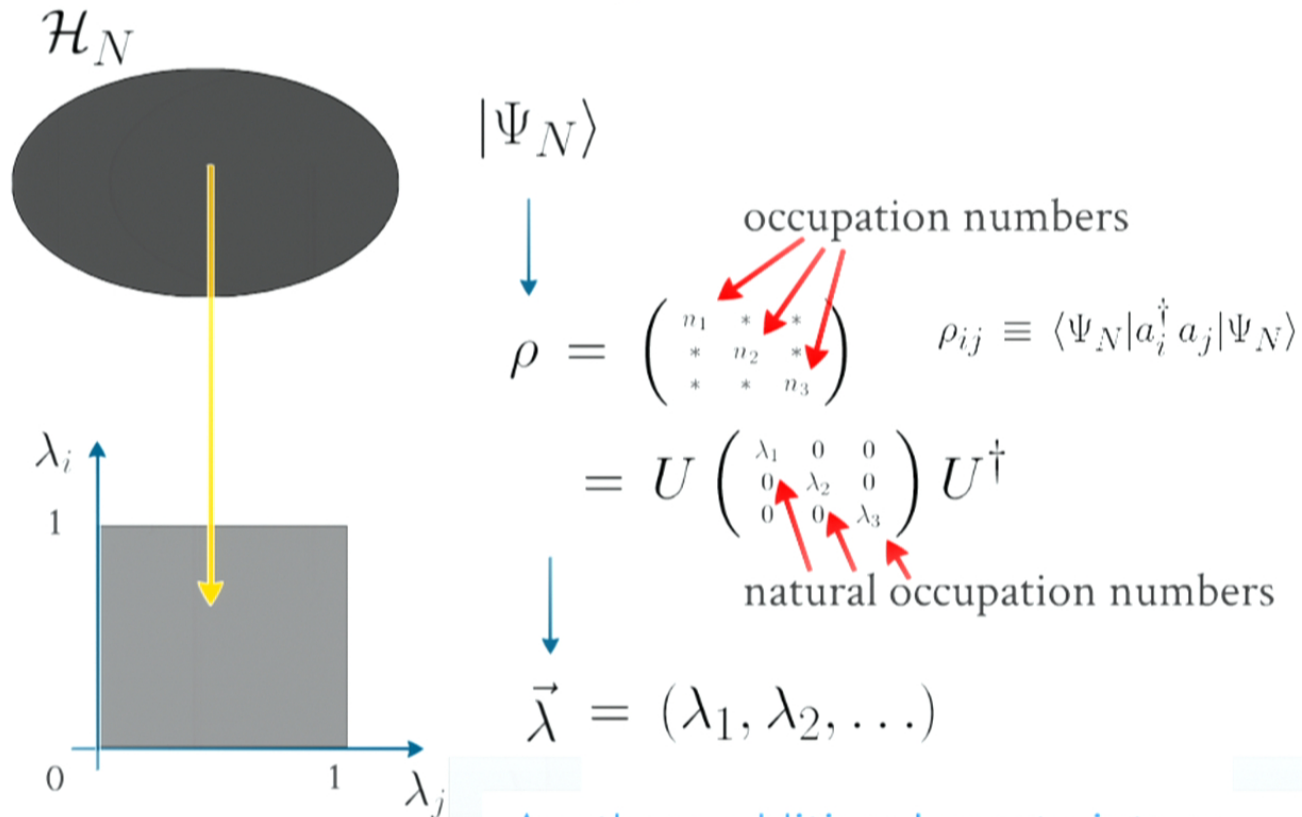
occupation numbers

$$\rho = \begin{pmatrix} n_1 & * & * \\ * & n_2 & * \\ * & * & n_3 \end{pmatrix} \quad \rho_{ij} \equiv \langle \Psi_N | a_i^\dagger a_j | \Psi_N \rangle$$

$$= U \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} U^\dagger$$

natural occupation numbers

Natural Occupation Numbers



Are there additional constraints on natural occupation numbers?

Polytopes

3 fermions & 6 modes

Dennis & Borland 1972

Polytopes

3 fermions & 6 modes

Dennis & Borland 1972

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6$$

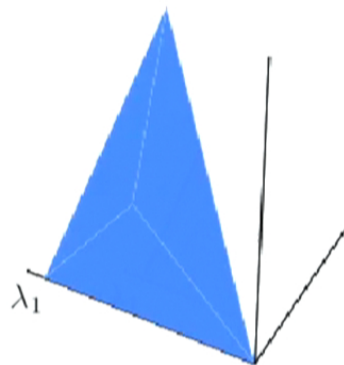
not implied by Pauli principle

$$\lambda_1 + \lambda_6 = 1$$

$$\lambda_2 + \lambda_5 = 1$$

$$\lambda_3 + \lambda_4 = 1$$

$$\lambda_1 + \lambda_2 + \lambda_4 \leq 2$$



Physical relevance?

Pauli principle $0 \leq n_i \leq 1$

can prevent electrons from falling

Kleber 2009

Beryllium?

Klyachko 2009

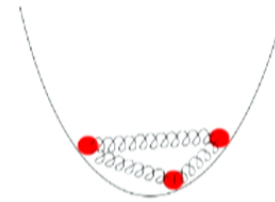
Beryllium? Harmonium!

Klyachko 2009

poisonous!



Group →	1	2	3	4
↓ Period				
1	1 H			
2	3 Li	4 Be		
3	11 Na	12 Mg		
4	19 K	20 Ca	21 Sc	22 Ti
5	37 Rb	38 Sr	39 Y	40 Zr



natural orbital



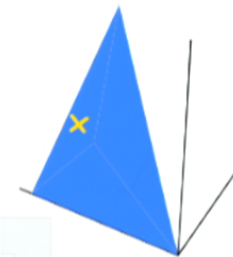
occupation

0.000004
0.000335
0.000339
0.999661
0.999665
0.999996



Is $\lambda_1 + \lambda_2 + \lambda_4 \leq 2$ saturated? Yes!

$$\lambda_4 \leq \lambda_5 + \lambda_6$$



Beryllium? Harmonium!

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approximation
error $O(\delta^8)$

Is $\lambda_1 + \lambda_2 + \lambda_4 \leq 2$ saturated? Yes!

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Schilling, Gross & Christandl
Phys. Rev. Lett. 110, 040404 (2013)

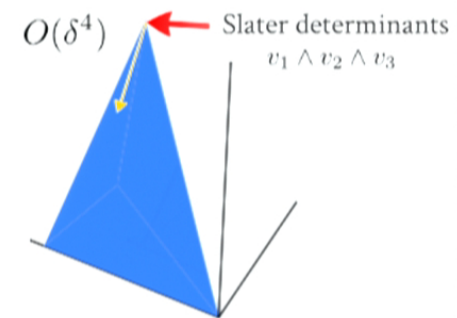


Wave function?

$$\dim \Lambda^3(\mathbb{C}^6) = \binom{6}{3} = 20$$

$$\text{general state } |\Psi\rangle = \sum_{ijk} c_{ijk} v_i \wedge v_j \wedge v_k$$

8 components!

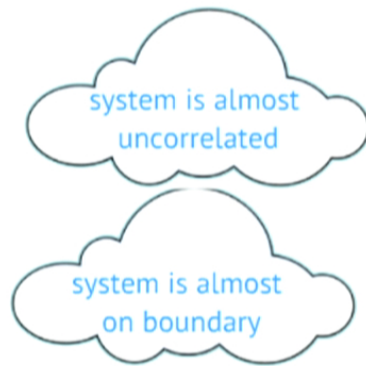
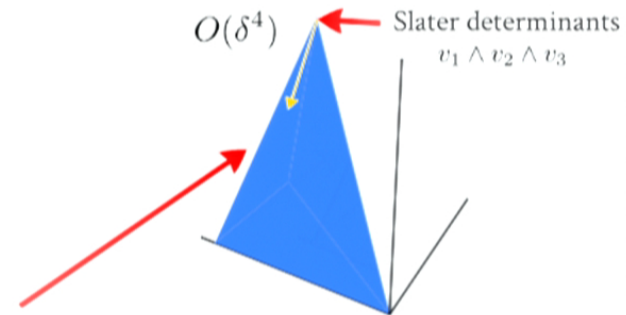


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8 components!

state on boundary $|\Psi\rangle = \alpha v_1 \wedge v_2 \wedge v_3 + \beta v_1 \wedge v_4 \wedge v_5 + \gamma v_2 \wedge v_4 \wedge v_6$
3 components!



Hartree-Fock method
optimize over Slater determinants

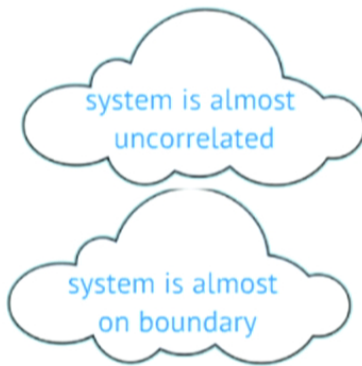
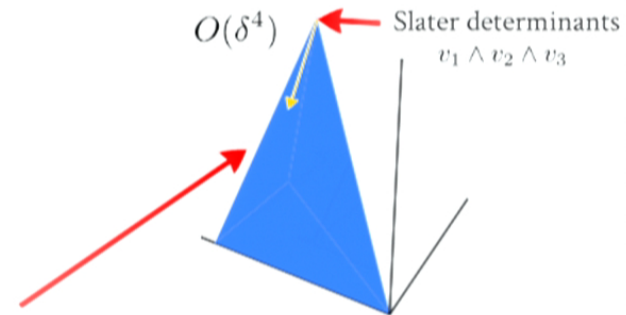
optimize over boundary states
result 4 orders of magnitude
better than Hartree-Fock!

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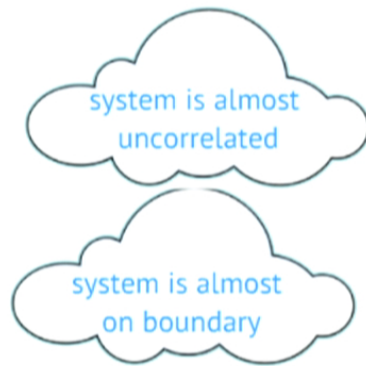
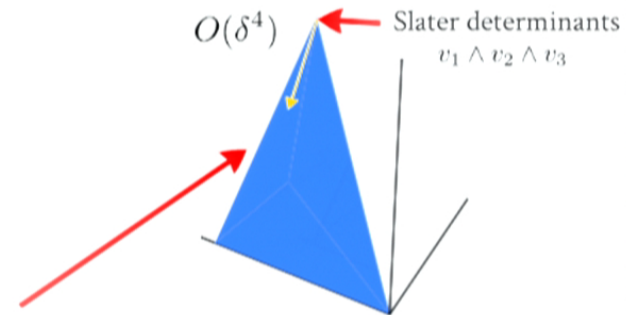
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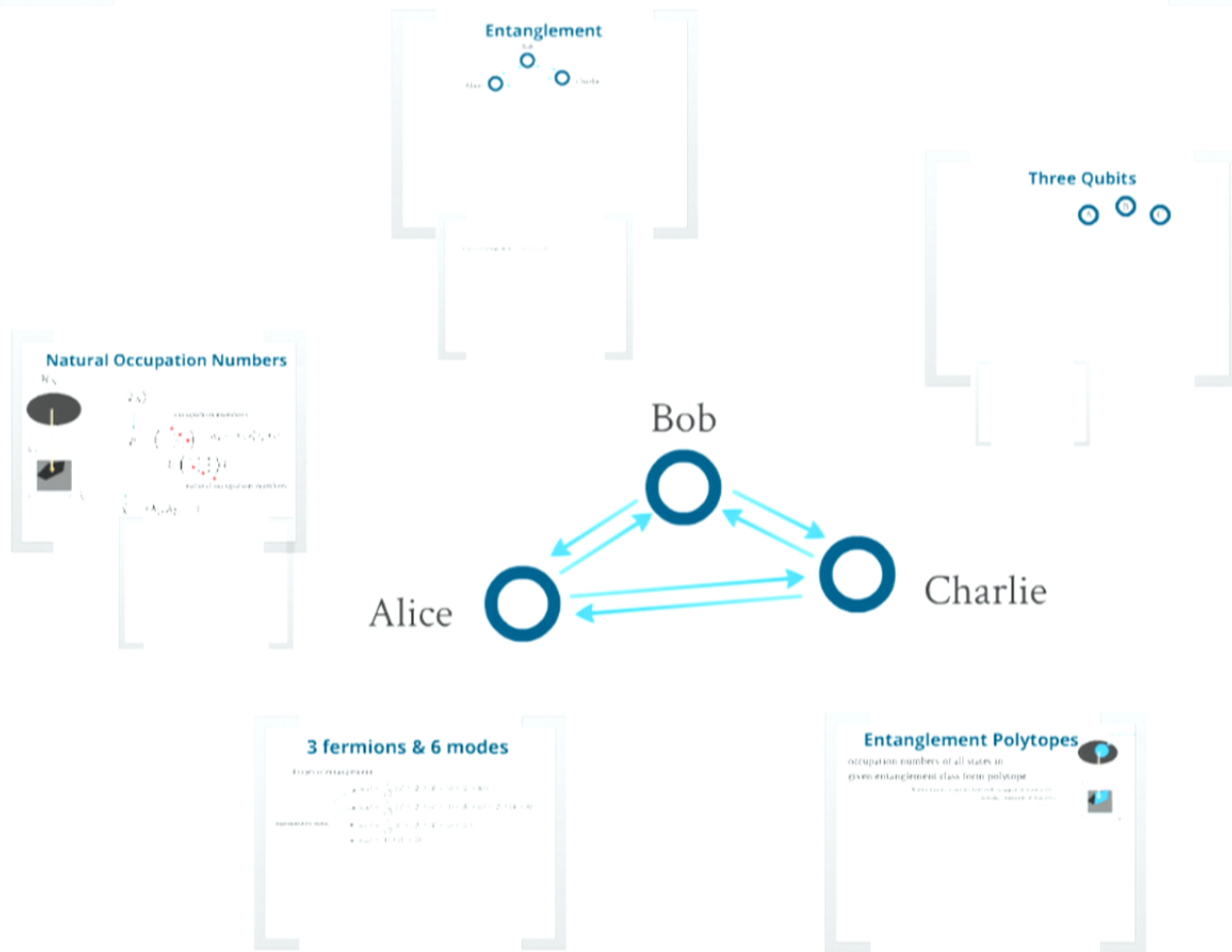
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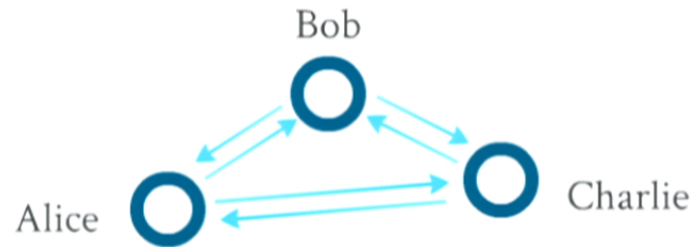
Hartree-Fock method
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Entanglement



Entanglement = unique quantum mechanical correlations

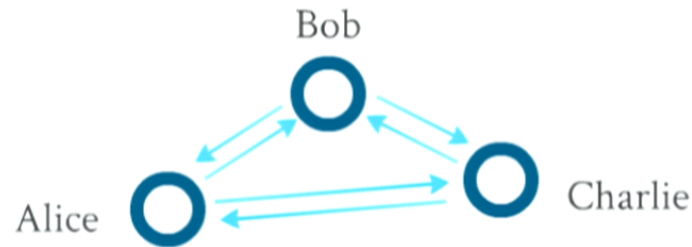
ψ and ϕ have same type of entanglement

\longleftrightarrow ψ and ϕ can be interconverted with
 stochastic local operations and classical
 communication

Dür, Vidal & Cirac 2000

fermions $\longleftrightarrow \psi = g.\phi$
 invertible linear transformation of modes

Entanglement



Entanglement = unique quantum mechanical correlations

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Dür, Vidal & Cirac 2000

fermions $\longleftrightarrow \psi = g.\phi$
invertible linear transformation of modes

3 fermions & 6 modes

4 types of entanglement Levay & Vrana 2008

representative states

$$\begin{aligned} |\psi_A\rangle &= \frac{1}{\sqrt{2}} (|1\rangle \wedge |2\rangle \wedge |3\rangle + |4\rangle \wedge |5\rangle \wedge |6\rangle), \\ |\psi_B\rangle &= \frac{1}{\sqrt{3}} (|1\rangle \wedge |2\rangle \wedge |4\rangle + |1\rangle \wedge |3\rangle \wedge |5\rangle + |2\rangle \wedge |3\rangle \wedge |6\rangle), \\ |\psi_C\rangle &= \frac{1}{\sqrt{2}} |1\rangle \wedge (|2\rangle \wedge |3\rangle + |4\rangle \wedge |5\rangle), \\ |\psi_D\rangle &= |1\rangle \wedge |2\rangle \wedge |3\rangle. \end{aligned}$$


infinite number of types

more fermions, more modes 

3 fermions & 6 modes

4 types of entanglement

representative states



The diagram shows the text "representative states" on the left. From this text, four curved arrows branch out to the right, each pointing to one of the four equations listed. The arrows originate from a single point and fan out towards the equations.

$$\begin{aligned} |\psi_A\rangle &= \frac{1}{\sqrt{2}} (|1\rangle \wedge |2\rangle \wedge |3\rangle + |4\rangle \wedge |5\rangle \wedge |6\rangle), \\ |\psi_B\rangle &= \frac{1}{\sqrt{3}} (|1\rangle \wedge |2\rangle \wedge |4\rangle + |1\rangle \wedge |3\rangle \wedge |5\rangle + |2\rangle \wedge |3\rangle \wedge |6\rangle) \\ |\psi_C\rangle &= \frac{1}{\sqrt{2}} |1\rangle \wedge (|2\rangle \wedge |3\rangle + |4\rangle \wedge |5\rangle), \\ |\psi_D\rangle &= |1\rangle \wedge |2\rangle \wedge |3\rangle. \end{aligned}$$

Entanglement Polytopes

occupation numbers of all states in
given entanglement class form polytope

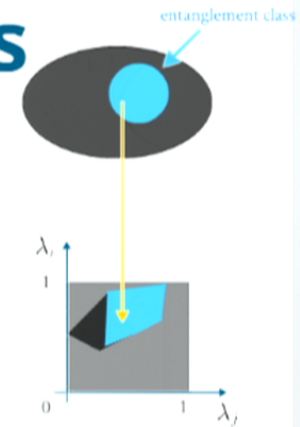
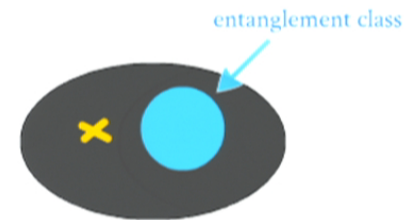
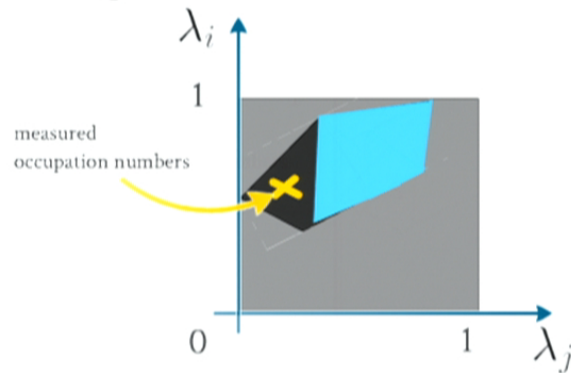
Walter, Doran, Gross & Christandl, to appear in Science 2013

Sawicki, Oszmaniec & Kus 2013

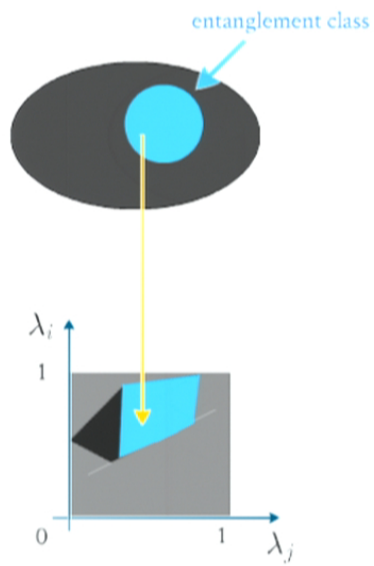
group representation theory

Brion's theorem

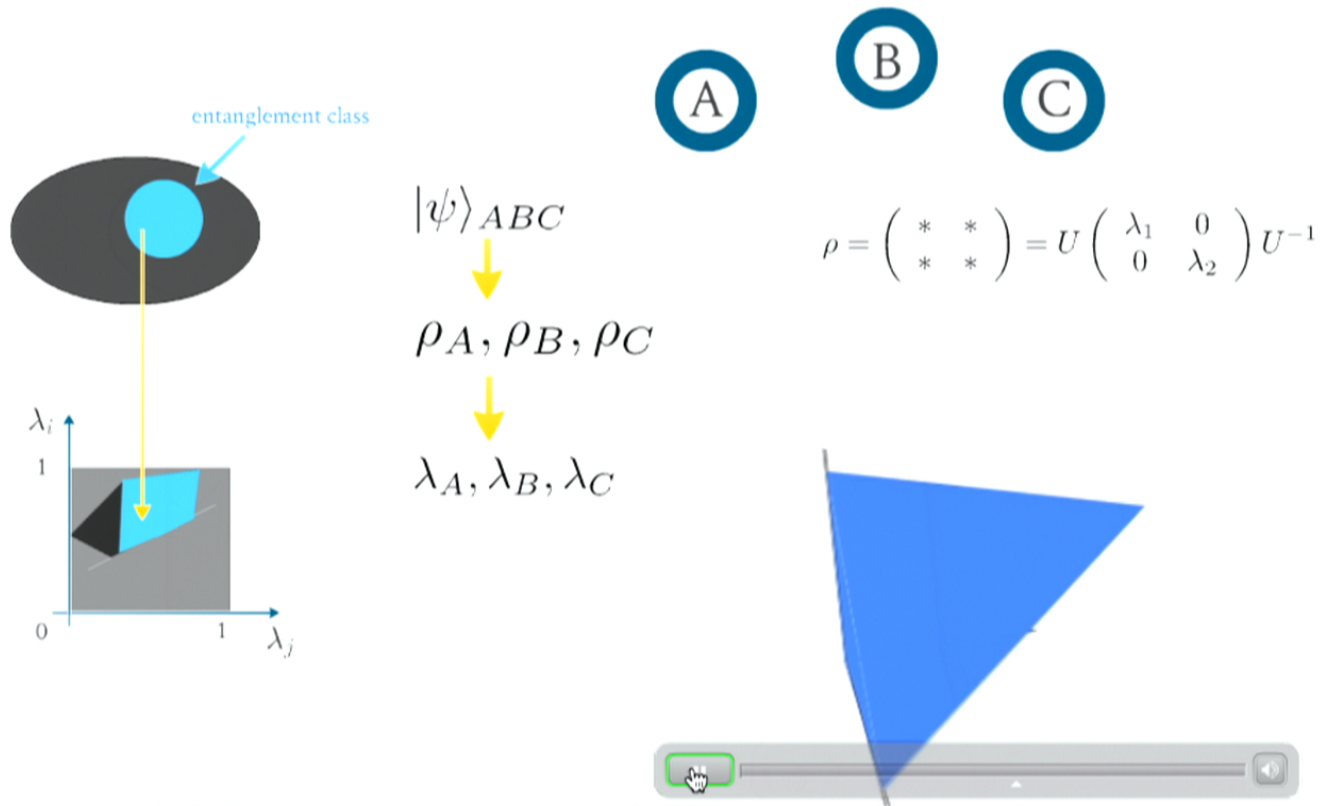
entanglement witness



Three Qubits



Three Qubits



Three Qubits

