

Title: From Pauli's Principle to Fermionic Entanglement

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URL: <http://pirsa.org/13050005>

Abstract: <span>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?

&nbsp;

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.</span>

# From Pauli's Principle to Fermionic Entanglement

Matthias Christandl  
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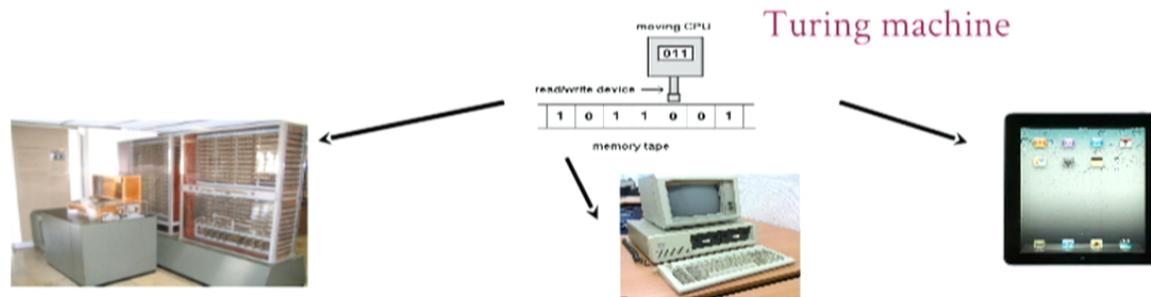
# Information

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

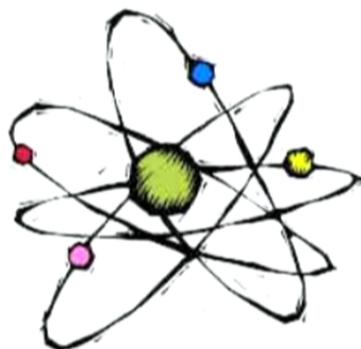
Pauli exclusion principle  
Two fermions cannot occupy the same quantum state

### Occupation Numbers

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

### Natural Occupation Numbers

$\mathcal{H}_N$   
 $|\Psi_N\rangle$   
occupation numbers  
 $\mu = (\mu_1, \mu_2, \dots)$   $\mu_i = \langle n_i | \Psi_N \rangle|^2$



### Physical relevance?

Pauli principle  $\rightarrow$  fermions  
can prevent electrons from falling

### Polytopes

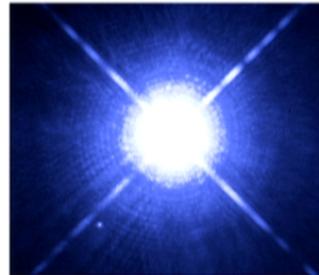
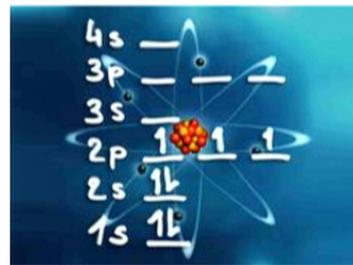
Alternating & k modes  $\rightarrow$  fermions

# 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

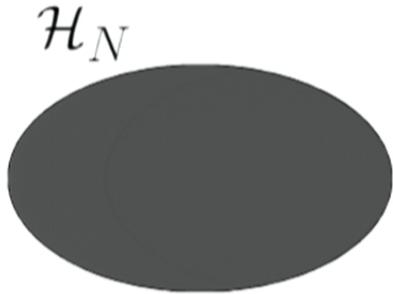
$\mathcal{H}_N$



fixed particle number  $N$

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

# Natural Occupation Numbers



$|\Psi_N\rangle$

↓

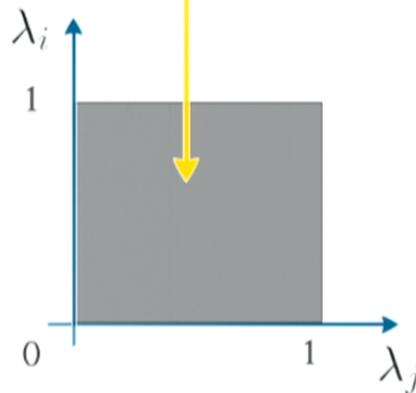
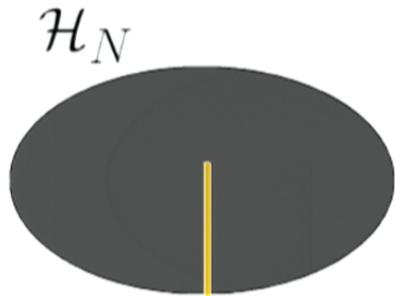
occupation numbers

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

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

natural occupation numbers

# Natural Occupation Numbers



$|\Psi_N\rangle$

↓

occupation numbers

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

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↓

natural occupation numbers

$$\vec{\lambda} = (\lambda_1, \lambda_2, \dots)$$

Are there additional constraints on natural occupation numbers?

# Polytopes

3 fermions & 6 modes Dennis & Borland 1972

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3 fermions & 6 modes Dennis & Borland 1972

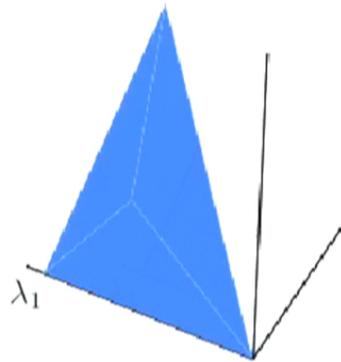
$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_6$  not implied by Pauli principle

$$\lambda_1 + \lambda_6 = 1$$

$$\lambda_2 + \lambda_5 = 1$$

$$\lambda_3 + \lambda_4 = 1$$

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



# Physical relevance?

Pauli principle  $0 \leq n_i \leq 1$   
can prevent electrons from falling

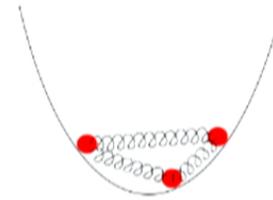
# Beryllium?

Klyachko 2009

# Beryllium? Harmonium!

Klyachko 2009

poisonous!

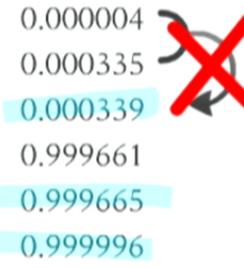


Group →	1	2	3	4
1	1 H			
2	3 Li	4 Be		
3	11 Na	12 Mg		
4	19 K	20 Ca	21 Sc	22 Ti
5	37 Rb	38 Sr	39 Y	40 Zr

natural orbital

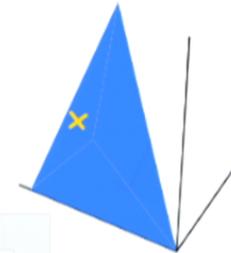


occupation



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

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



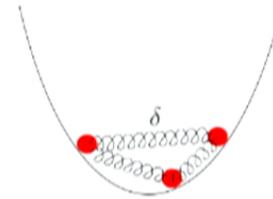
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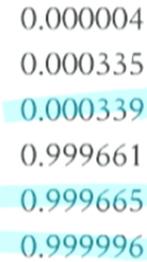
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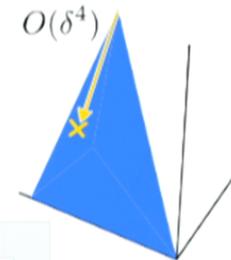
occupation



approximation  
error  $O(\delta^8)$

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

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



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

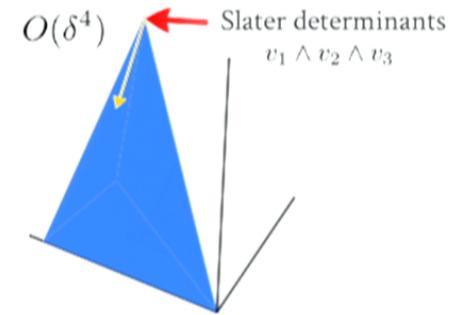


# Wave function?

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

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

8 components!



# Wave function?

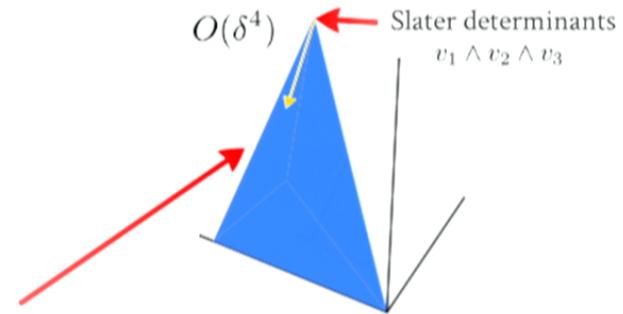
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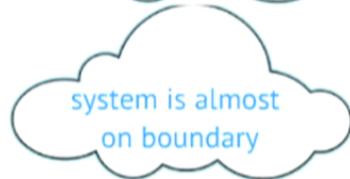
8 components!

$$\text{state on boundary } |\Psi\rangle = \alpha v_1 \wedge v_2 \wedge v_3 + \beta v_1 \wedge v_4 \wedge v_5 + \gamma v_2 \wedge v_4 \wedge v_6$$

3 components!



Hartree-Fock method  
optimize over Slater determinants



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

# Wave function?

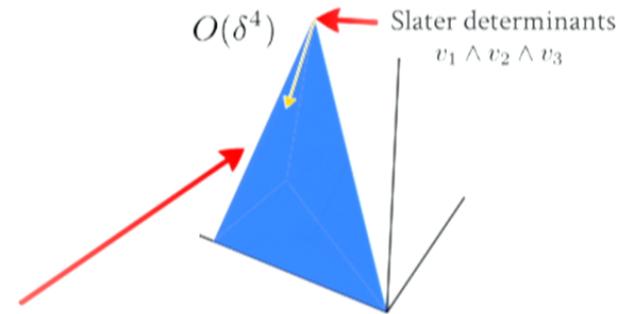
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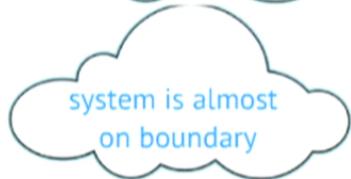
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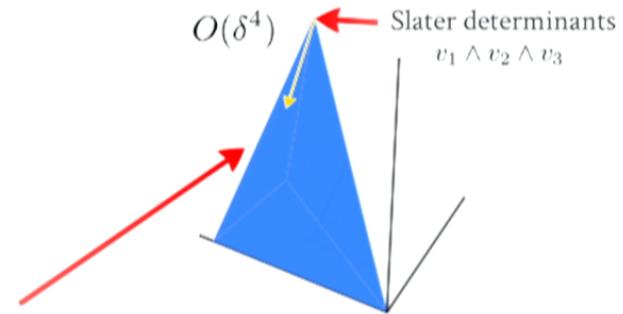
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# Wave function?

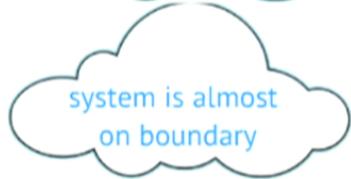
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general state  $|\Psi\rangle = \sum_{ijk} c_{ijk} v_i \wedge v_j \wedge v_k$   
8 components!

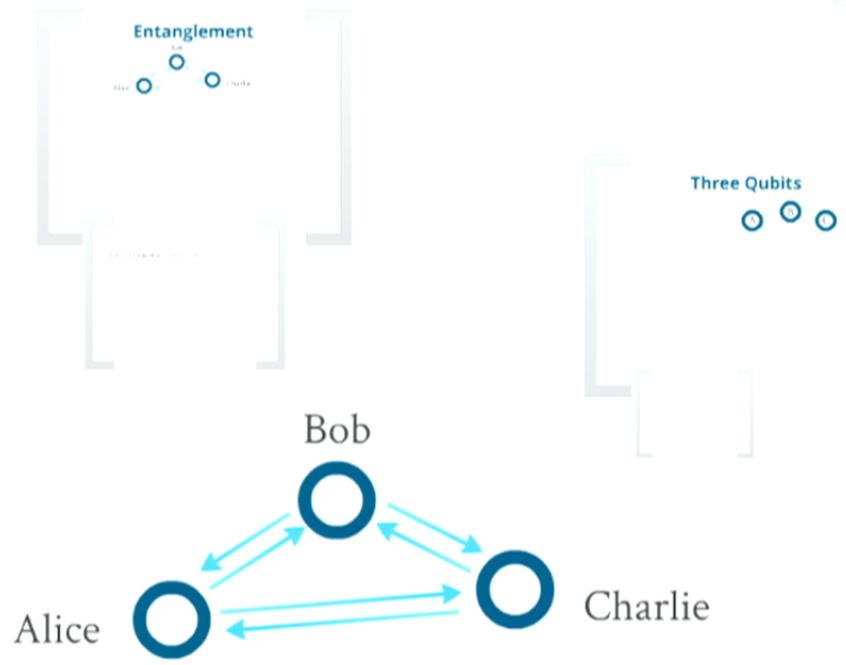
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Hartree-Fock method  
optimize over Slater determinants



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



### Natural Occupation Numbers

$n_{\alpha}$   
 $2 \times 2$   
 $\rho = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$   
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 $\sum_{\alpha} n_{\alpha} = 1$

### 3 fermions & 6 modes

Fermion occupation  
 •  $\sum_{\alpha} n_{\alpha} = 3$   
 •  $n_{\alpha} \in \{0, 1\}$   
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### Entanglement Polytopes

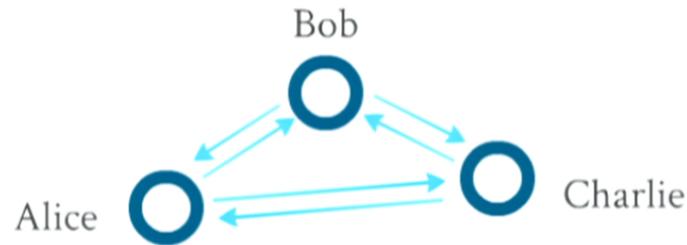
occupation numbers of all states in given entanglement class form polytope  
 •  $\rho = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$   
 •  $\rho = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

### Entanglement

Alice Bob Charlie

### Three Qubits

# Entanglement



Entanglement = unique quantum mechanical correlations

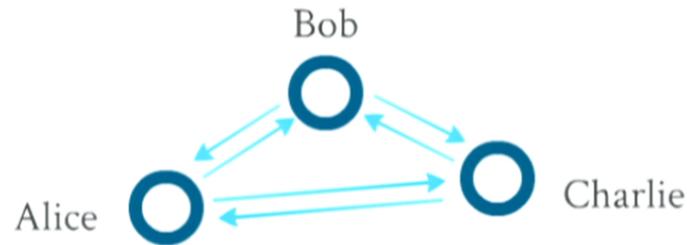
$\psi$  and  $\phi$  have same type of entanglement

$\longleftrightarrow$   $\psi$  and  $\phi$  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



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*fermions*  
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invertible linear transformation of modes

# 3 fermions & 6 modes

4 types of entanglement Levay & Vrana 2008

representative states

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

infinite number of types

more fermions, more modes →

# 3 fermions & 6 modes

4 types of entanglement

representative states

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

# Entanglement Polytopes

occupation numbers of all states in  
given entanglement class form polytope

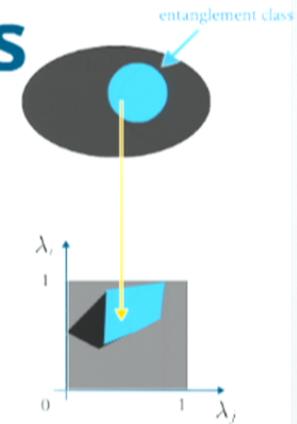
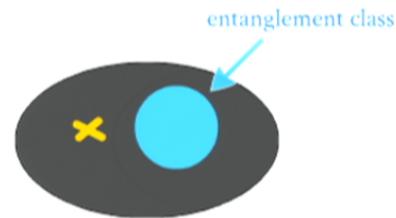
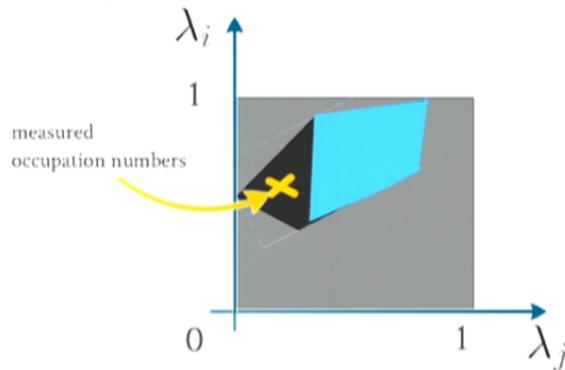
Walter, Doran, Gross & Christandl, to appear in Science 2013

Sawicki, Oszmaniec & Kus 2013

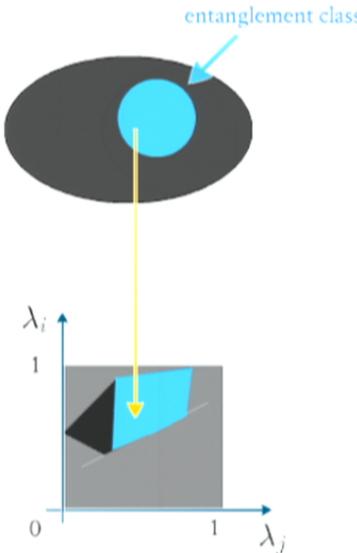
group representation theory

Brion's theorem

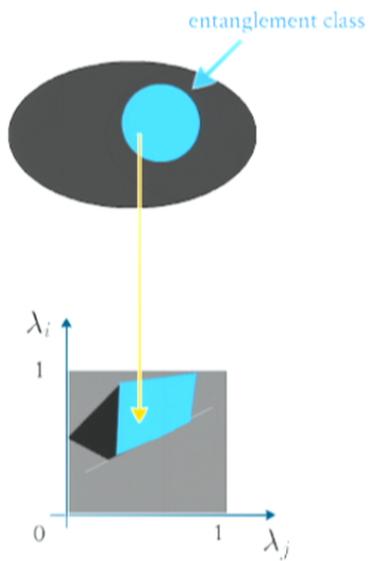
entanglement witness



# Three Qubits



# Three Qubits

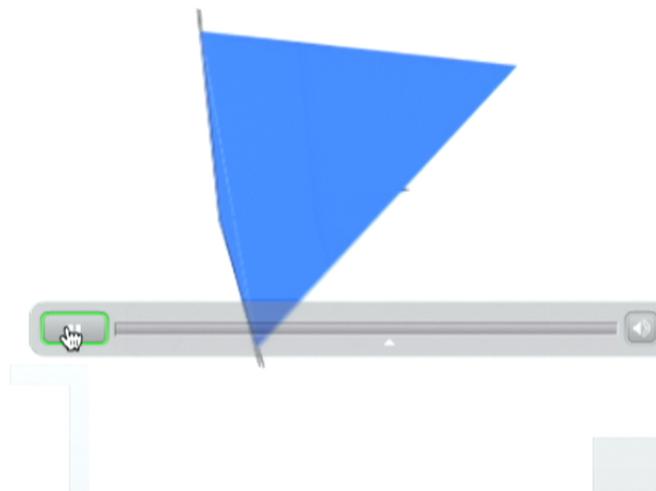


$|\psi\rangle_{ABC}$

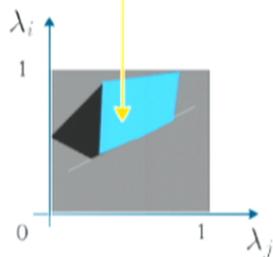
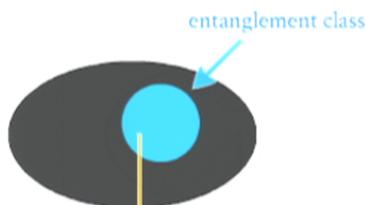
$\rho_A, \rho_B, \rho_C$

$\lambda_A, \lambda_B, \lambda_C$

$$\rho = \begin{pmatrix} * & * \\ * & * \end{pmatrix} = U \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} U^{-1}$$



# Three Qubits



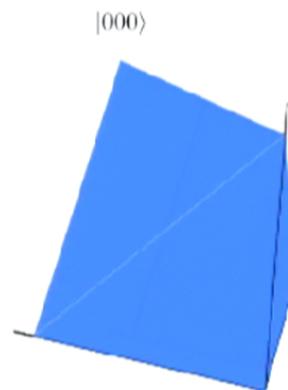
$$|\psi\rangle_{ABC}$$

$$\rho_A, \rho_B, \rho_C$$

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$$\rho = \begin{pmatrix} * & * \\ * & * \end{pmatrix} = U \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} U^{-1}$$

GHZ-type = whole polytope  
W-type = upper pyramid



$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)|0\rangle$$

$$\frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$$