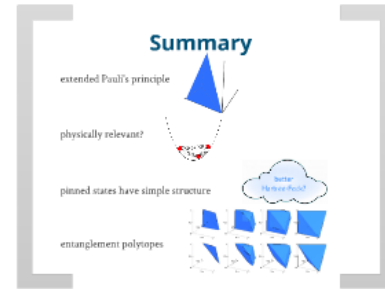
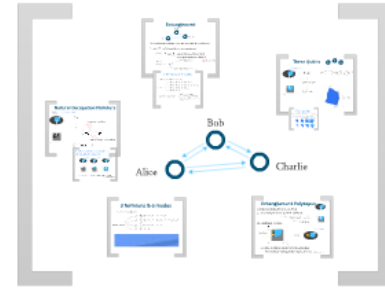
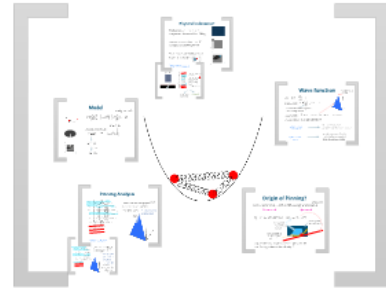
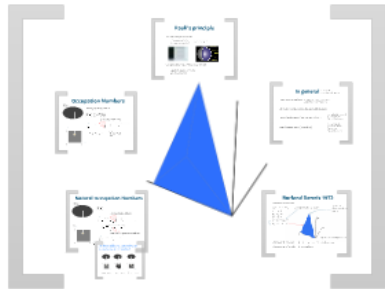


# From Pauli's Principle to Fermionic Entanglement

Matthias Christandl  
University of Copenhagen

based on work with Michael Walter, Christian Schilling & David Gross, Brent Doran



# From Pauli's Principle to Fermionic Entanglement

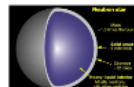
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## Pauli's principle

Pauli's exclusion principle (1925):

'no two fermions in the same quantum state'  $0 \leq n_i \leq 1$

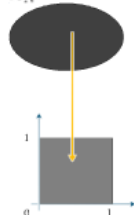


strengthened by Dirac & Heisenberg in (1926):

'quantum states of fermions are antisymmetric'

## Occupation Numbers

$\mathcal{H}_N$



fixed particle number  $N$

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

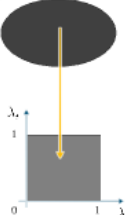
occupation numbers

$$\rho = \begin{pmatrix} n_1 \\ \vdots \\ n_i \\ \vdots \\ n_N \end{pmatrix} \quad \rho_i = \langle \Psi_N | a_i^\dagger a_i | \Psi_N \rangle$$

$$0 \leq n_i \leq 1 \quad \sum_i n_i = N$$

## Natural Occupation Numbers

$\mathcal{H}_N$



$|\Psi_N\rangle$

occupation numbers

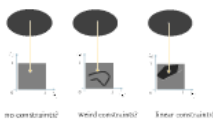
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$$= U \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_i \\ \vdots \\ \lambda_N \end{pmatrix} U^\dagger$$

natural occupation numbers

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

Are there additional constraints on natural occupation numbers?



## In general

distinguishable & indistinguishable particles

region is convex polytope partial trace operation is moment map  
apply Karwan's convexity theorem

depends on number of particles and local dimension

inner characterisation (representation theory)

Christandl & Mitchem, 2004  
Khavko 2004, 2006  
Datta & Hayden 2004

outer characterisation (inequalities)

Khavko 2004, 2006  
Datta & Hayden 2004  
Rosenz, 2008  
Vergne & Walter 2014

## Borland Dennis 1972

3 fermions & 6 modes

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_6$$

$$\lambda_1 + \lambda_6 = 1$$

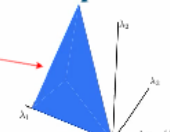
$$\lambda_2 + \lambda_5 = 1$$

$$\lambda_3 + \lambda_4 = 1$$

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

$$\lambda_1 + \lambda_2 \leq 1 + \lambda_3$$

not implied by Pauli principle  $e_1 \wedge e_2 \wedge e_3$   
Slater determinant  
(1,1,1)



<http://polytopes.lectspeak.org/>

3 fermions in 7 modes

$$\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2 \quad \text{and three others}$$

5 fermions in 10 modes

161 inequalities

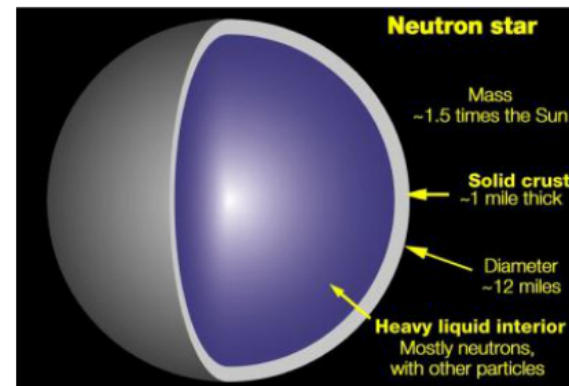
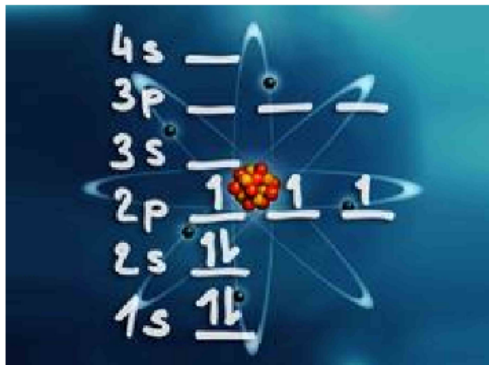
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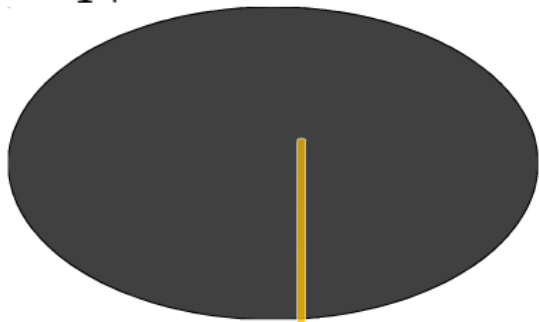


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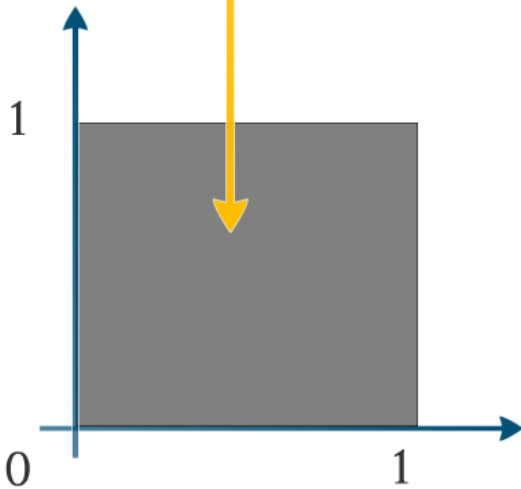
occupation numbers

$$\rho = \begin{pmatrix} n_1 & * & * \\ * & n_2 & * \\ * & * & n_3 \end{pmatrix}$$

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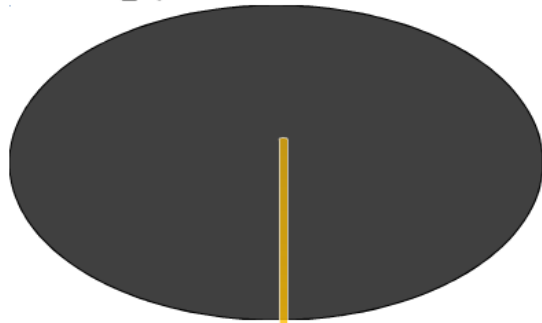
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# Natural Occupation Numbers

$\mathcal{H}_N$



$|\Psi_N\rangle$

↓

occupation numbers

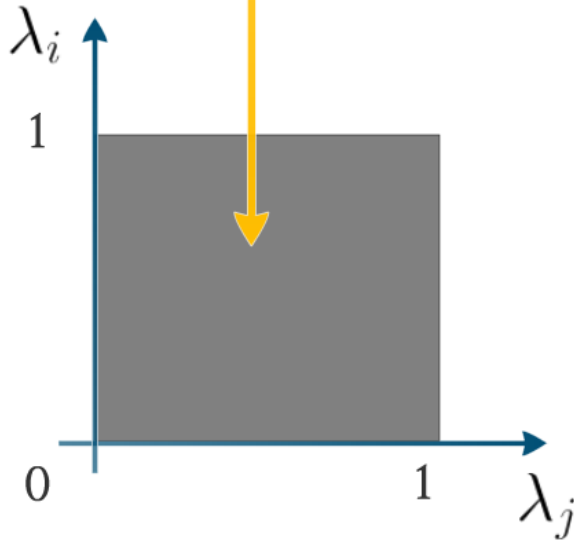
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natural occupation numbers

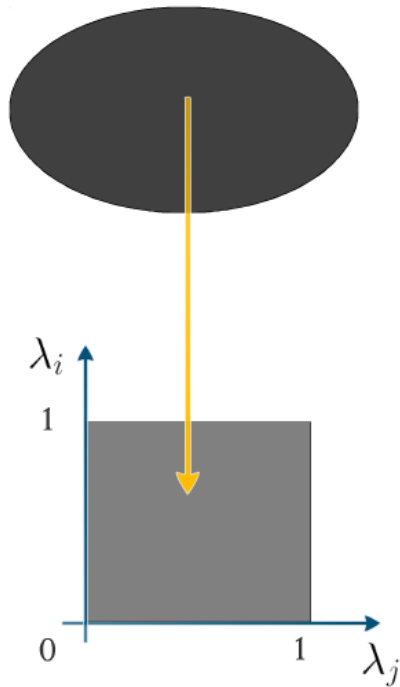
↓

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

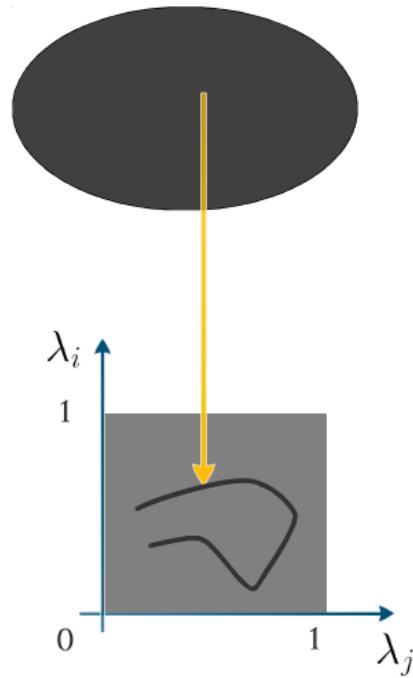


Are there additional constraints on natural occupation numbers?

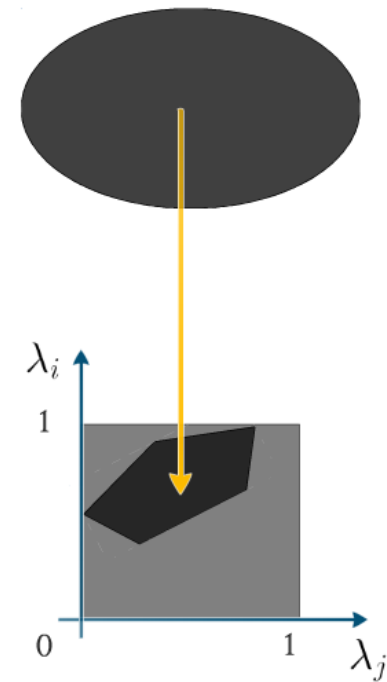
# Are there additional constraints on natural occupation numbers?



no constraints?



weird constraints?



linear constraints!

# Borland Dennis 1972

3 fermions & 6 modes

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_6$$

not implied by Pauli principle

$$\lambda_1 + \lambda_6 = 1$$

$$\lambda_2 + \lambda_5 = 1$$

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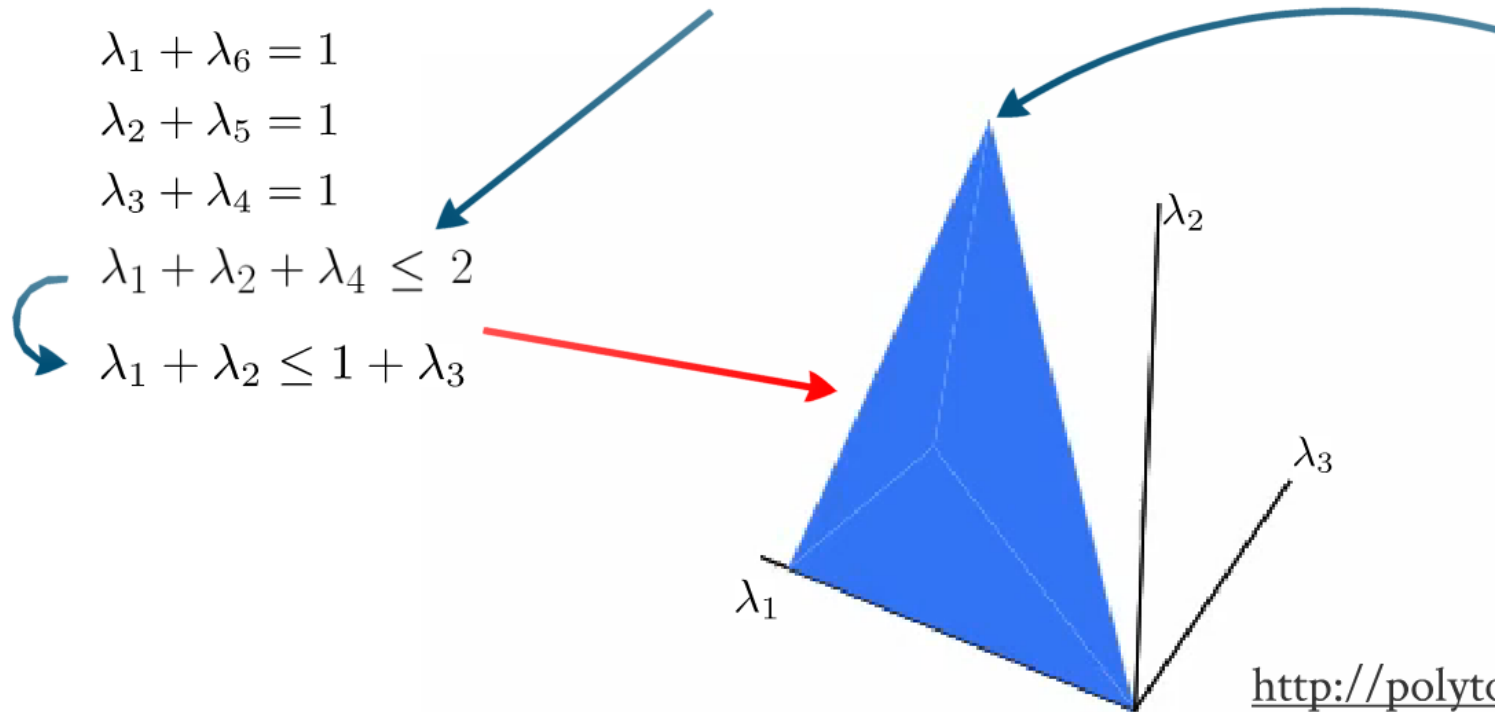
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$$\lambda_1 + \lambda_2 \leq 1 + \lambda_3$$

$$v_1 \wedge v_2 \wedge v_3$$

Slater determinant

$$(1,1,1)$$



3 fermions in 7 modes

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depends on number of particles and local dimension

inner characterisation (representation theory)

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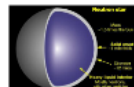
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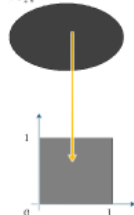


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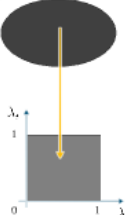
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## Natural Occupation Numbers

$\mathcal{H}_N$



$|\Psi_N\rangle$

occupation numbers

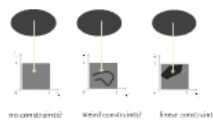
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$$= U \begin{pmatrix} n_1 \\ \vdots \\ n_i \\ \vdots \\ n_N \end{pmatrix} U^\dagger$$

natural occupation numbers

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

Are there additional constraints on natural occupation numbers?



no constraints, weak constraints, linear constraints

## Borland Dennis 1972

3 fermions & 6 modes

$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_6$

$\lambda_1 + \lambda_6 = 1$

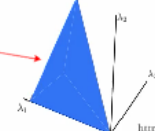
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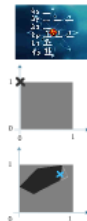
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### Physical relevance?

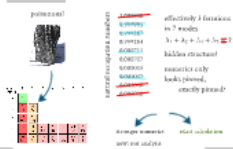
Pauli principle  $0 \leq n_i \leq 1$   
can prevent electrons from falling

constraints are active  $n_i = 0, 1$   
occupation numbers pinned

Are the new constraints active?  
E.g. Dennis-Borland:  $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$



### Beryllium $\epsilon_{\text{space}} = 2.0$



### Model

$$D = -\frac{\hbar^2}{2m} \nabla^2 + O(\delta^2)$$

$$H = \sum_{i=1}^N \left( \frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 x_i^2 \right) + \frac{1}{2} D \sum_{i=1}^N (x_i - x_j)^2$$

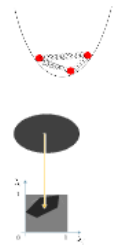
$$H = L^2(\mathbb{R})$$

fermionic ground state:

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

$$\rho_1(x, \vec{x}) \downarrow N-s$$

$$\vec{x} = \vec{x}(\delta)$$



### Wave function

Slater determinants  $\psi_1, \psi_2, \psi_3$

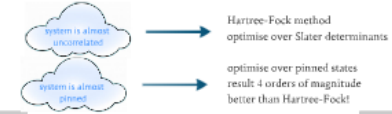
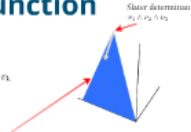
$$\dim \Lambda^3(\mathbb{C}^6) = \binom{6}{3} = 20$$

general state  $|\Psi\rangle = \sum_{i,j,k} c_{i,j,k} \psi_i \wedge \psi_j \wedge \psi_k$

can be written with 8 components when choosing the basis

pinned state  $|\Psi\rangle = \alpha \psi_1 \wedge \psi_2 \wedge \psi_3 + \beta \psi_1 \wedge \psi_4 \wedge \psi_5 + \gamma \psi_2 \wedge \psi_4 \wedge \psi_5$

3 components! true approximately!



### Pinning Analysis

$$\lambda_1 = \frac{40}{129} \delta^4 - \frac{1590}{59349} \delta^6 + O(\delta^8)$$

$$\lambda_2 = \frac{2}{9} \delta^4 - \frac{252}{1193} \delta^6 + \frac{2025}{11933} \delta^8 + O(\delta^{10})$$

$$1 - \lambda_3 = \frac{2}{9} \delta^4 - \frac{24}{253} \delta^6 + \frac{81902}{292315} \delta^8 + O(\delta^{10})$$

$$\lambda_4 = \frac{2}{9} \delta^4 - \frac{24}{253} \delta^6 + \frac{73902}{292315} \delta^8 + O(\delta^{10})$$

$$\lambda_5 = \frac{2}{9} \delta^4 - \frac{252}{1193} \delta^6 + \frac{2970}{11933} \delta^8 + O(\delta^{10})$$

$$\lambda_6 = \frac{40}{129} \delta^4 - \frac{1200}{59349} \delta^6 + O(\delta^8)$$

$$\lambda_7 = \frac{80}{1193} \delta^4 - O(\delta^6)$$

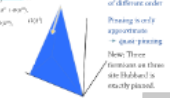
$$\lambda_8 = O(\delta^4)$$

Dennis-Borland setting up to  $O(\delta^4)$   
Is  $\lambda_1 = \lambda_2 = \lambda_3 \leq \lambda_4$  pinned?  
Yes, up to  $O(\delta^4)$ ! Pinning & setting of same order!



### Is Pinning Exact?

5 fermions in 7 modes up to  $O(\delta^7)$   
Is  $\lambda_1 = \lambda_2 = \lambda_3 \leq \lambda_4$  pinned?  
Yes, but set up to  $O(\delta^7)$ !  
Pinning & setting of different order  
Pinning itself approximate  
= exact pinning  
Now Three fermions in three states (3 modes) is exactly pinned.

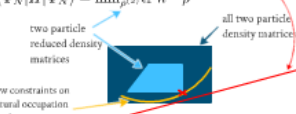


### Origin of Pinning?

new constraints in conflict with energy minimisation

kinematical dynamical

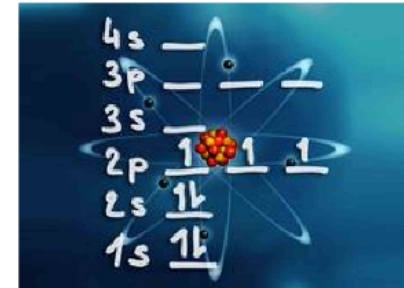
$$E_0 = \min_{\Psi_N} \langle \Psi_N | H | \Psi_N \rangle = \min_{\rho^{(2)}} \text{tr } h^{(2)} \rho^{(2)}$$



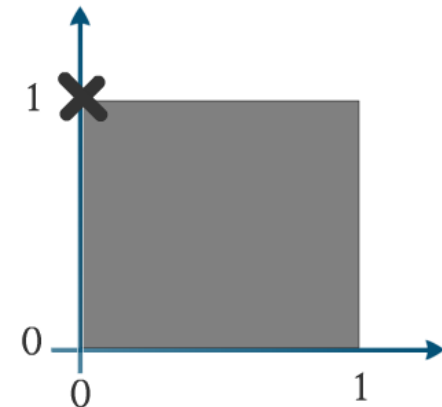
expectation: exactly pinned or not pinned at all!  
our findings: almost pinned! why...?

# Physical relevance?

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

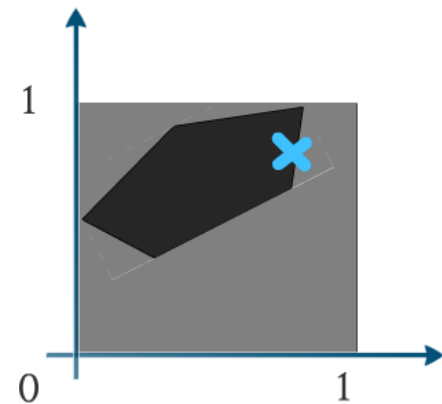
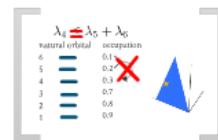


constraints are active  $n_i = 0, 1$   
 occupation numbers pinned



Are the new constraints active?

E.g. Dennis-Borland:



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

natural orbital

occupation

6



0.1

5



0.2

4



0.3

3



0.7

2

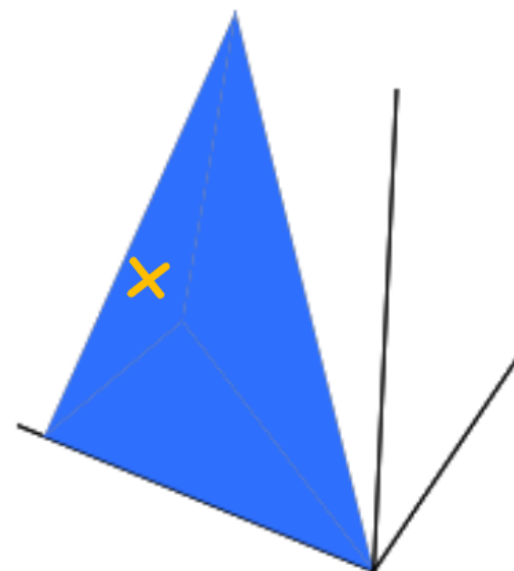


0.8

1

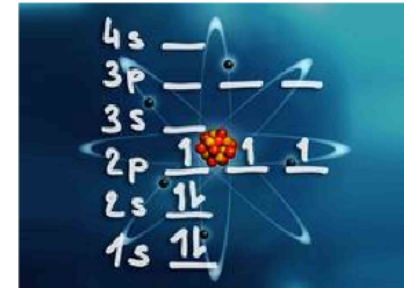


0.9

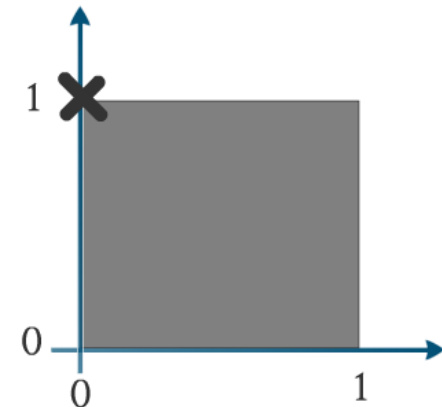


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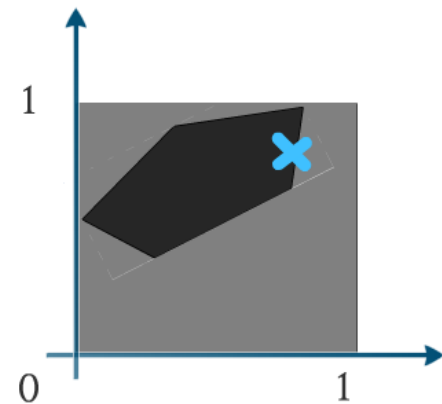
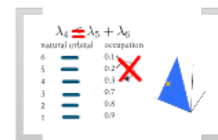


constraints are active  $n_i = 0, 1$   
 occupation numbers pinned



Are the new constraints active?

E.g. Dennis-Borland:



# Beryllium

Klyachko 2009

poisonous!



| Group → | 1        | 2        | 3        | 4        | 5        | 6        | 7        |
|---------|----------|----------|----------|----------|----------|----------|----------|
| 1       | 1<br>H   |          |          |          |          |          |          |
| 2       | 3<br>Li  | 4<br>Be  |          |          |          |          |          |
| 3       | 11<br>Na | 12<br>Mg |          |          |          |          |          |
| 4       | 19<br>K  | 20<br>Ca | 21<br>Sc | 22<br>Ti | 23<br>V  | 24<br>Cr | 25<br>Mn |
| 5       | 37<br>Rb | 38<br>Sr | 39<br>Y  | 40<br>Zr | 41<br>Nb | 42<br>Mo | 43<br>Tc |

natural occupation numbers

- ~~1.000000~~
- 0.999995
- 0.999287
- 0.999284
- 0.000711
- 0.000707
- 0.000009
- 0.000007
- ~~0.000000~~
- ~~0.000000~~

effectively 3 fermions  
in 7 modes

$$\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2$$

hidden structure!

numerics only

looks pinned,  
exactly pinned?

stronger numerics

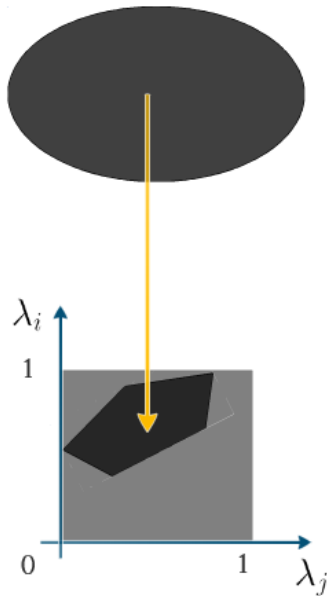
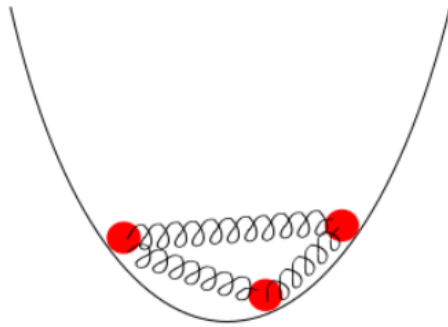
exact calculation

new: our analysis  
suggests no pinning

# Model

$$D = \frac{4m\omega^2}{N} \delta + O(\delta^2)$$

$$H = \sum_{i=1}^N \left( \frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 x_i^2 \right) + \frac{1}{2} D \sum_{i,j=1}^N (x_i - x_j)^2$$



fermionic ground state:

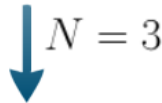
$$\mathcal{H} = L^2(\mathbb{R})$$



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



$$\rho_1(x, \tilde{x})$$



$$\vec{\lambda} \equiv \vec{\lambda}(\delta)$$



# Pinning Analysis

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$$\lambda_4 = \frac{2}{9} \delta^4 - \frac{64}{243} \delta^6 + \frac{73802}{295245} \delta^8 + O(\delta^{10}),$$

$$\lambda_5 = \frac{2}{9} \delta^4 - \frac{232}{729} \delta^6 + \frac{3976}{10935} \delta^8 + O(\delta^{10}),$$

$$\lambda_6 = \frac{40}{729} \delta^6 - \frac{2200}{59049} \delta^8 + O(\delta^{10}),$$

~~$$\lambda_7 = \frac{80}{2187} \delta^8 + O(\delta^{10}),$$~~

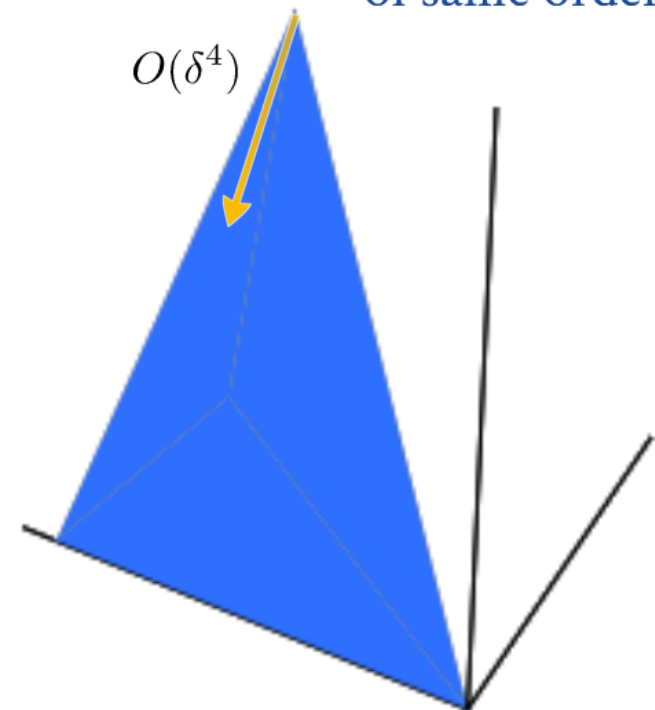
~~$$\lambda_8 = O(\delta^{10}),$$~~

~~$$\vdots$$~~

Dennis-Borland setting up to  $O(\delta^8)$

Is  $\lambda_1 + \lambda_2 + \lambda_4 \leq 2$  pinned?

Yes, up to  $O(\delta^8)$  ! Pinning & setting of same order!



Is Pinning Exact?

# Is Pinning Exact?

$$1 - \lambda_1 = \frac{40}{729} \delta^6 - \frac{1390}{59049} \delta^8 + O(\delta^{10}),$$

$$1 - \lambda_2 = \frac{2}{9} \delta^4 - \frac{232}{729} \delta^6 + \frac{3926}{10935} \delta^8 + O(\delta^{10}),$$

$$1 - \lambda_3 = \frac{2}{9} \delta^4 - \frac{64}{243} \delta^6 + \frac{81902}{295245} \delta^8 + O(\delta^{10}),$$

$$\lambda_4 = \frac{2}{9} \delta^4 - \frac{64}{243} \delta^6 + \frac{73802}{295245} \delta^8 + O(\delta^{10}),$$

$$\lambda_5 = \frac{2}{9} \delta^4 - \frac{232}{729} \delta^6 + \frac{3976}{10935} \delta^8 + O(\delta^{10}),$$

$$\lambda_6 = \frac{40}{729} \delta^6 - \frac{2200}{59049} \delta^8 + O(\delta^{10}),$$

$$\lambda_7 = \frac{80}{2187} \delta^8 + O(\delta^{10}),$$

$$\lambda_8 = O(\delta^{10}),$$

$\vdots$

3 fermions in 7 modes up to  $O(\delta^{10})$

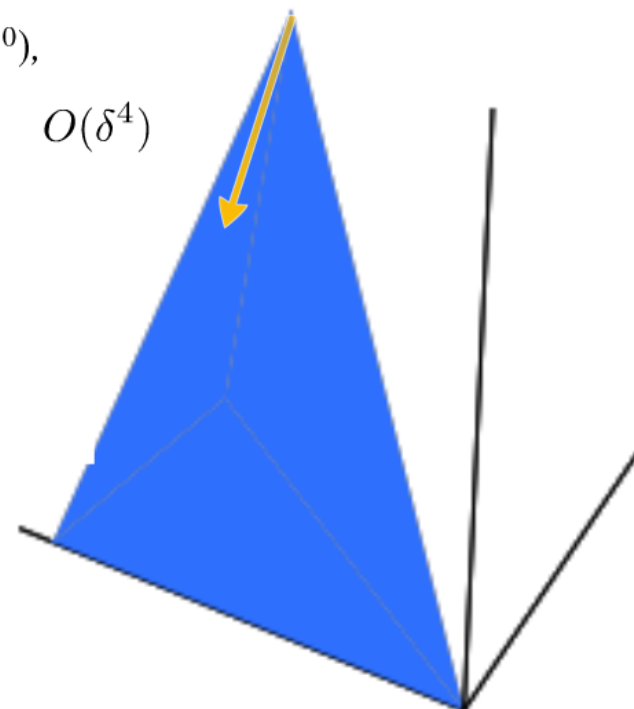
Is  $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2$  pinned?

Yes, but only up to  $O(\delta^8)$  !

Pinning & setting  
of different order

Pinning is only  
approximate  
→ quasi-pinning

New: Three  
fermions on three  
site Hubbard is  
exactly pinned.



# Origin of Pinning?

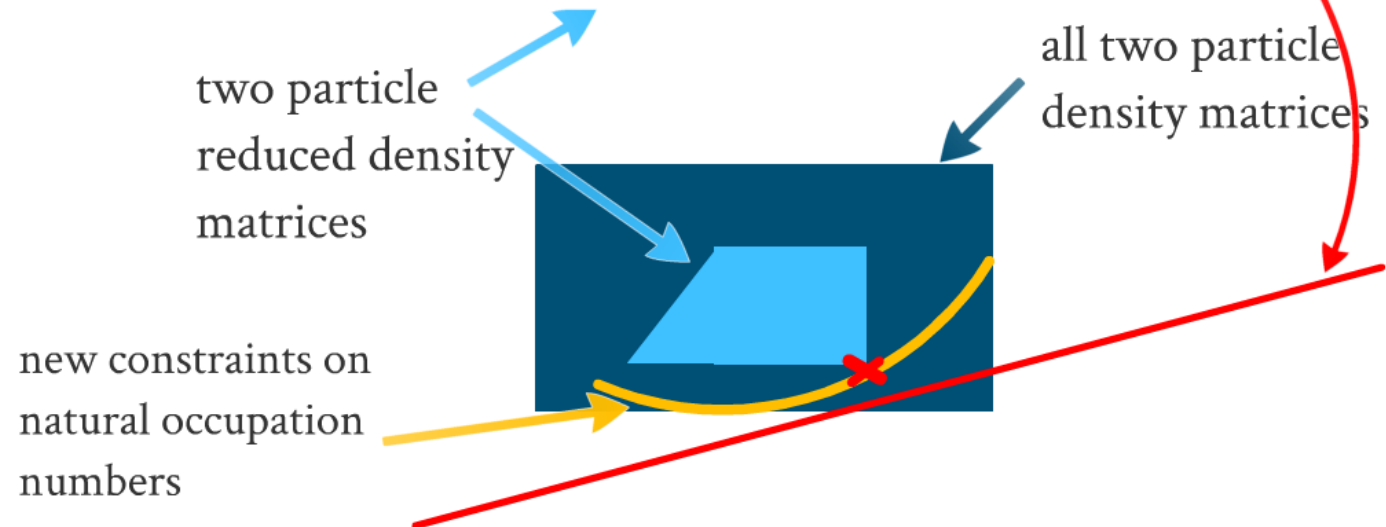
Klyachko 2009

new constraints in conflict with energy minimisation

kinematical

dynamical

$$E_g = \min_{\Psi_N} \langle \Psi_N | H | \Psi_N \rangle = \min_{\rho^{(2)}} \text{tr } h^{(2)} \rho^{(2)}$$



expectation: exactly pinned or not pinned at all!

our findings: almost pinned! why...?

# Wave function

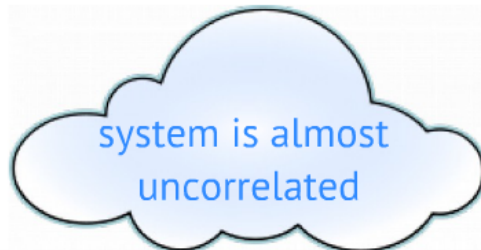
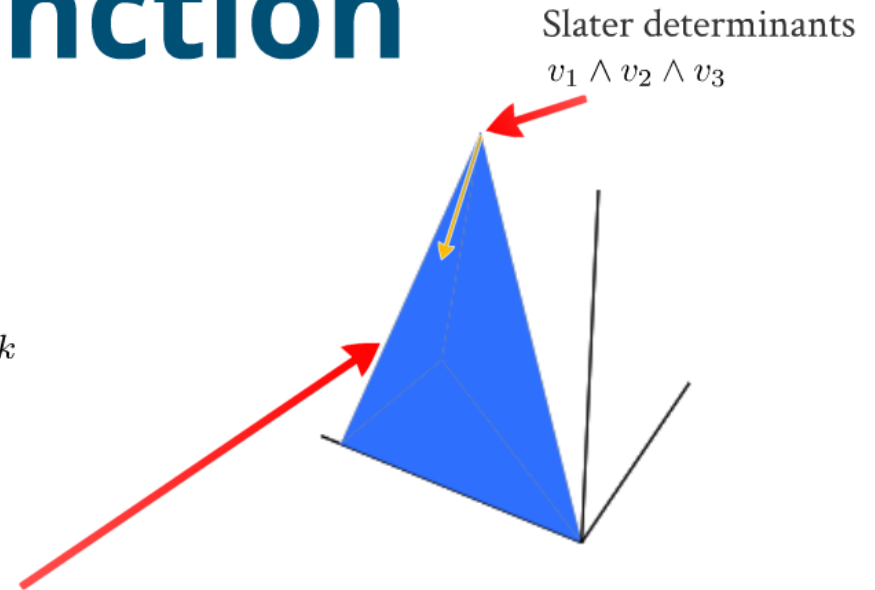
$$\dim \Lambda^3(\mathbb{C}^6) = \binom{6}{3} = 20$$

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

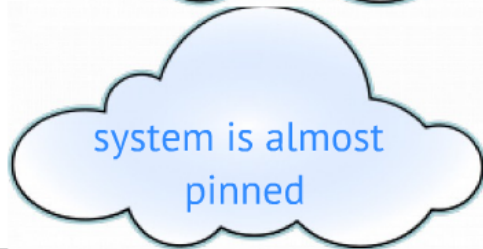
can be written with 8 components  
when choosing the basis

pinned state  $|\Psi\rangle = \alpha v_1 \wedge v_2 \wedge v_3 + \beta v_1 \wedge v_4 \wedge v_5 + \gamma v_2 \wedge v_4 \wedge v_6$

3 components! true approximately!



Hartree-Fock method  
optimise over Slater determinants



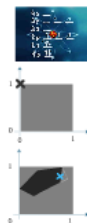
optimise over pinned states  
result 4 orders of magnitude  
better than Hartree-Fock!

### Physical relevance?

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

constraints are active  $n_i = 0, 1$   
occupation numbers pinned

Are the new constraints active?  
E.g. Dennis-Borland:  $\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$



### Beryllium $\epsilon_{\text{space}} = 28$



### Model

$$D = -\frac{\hbar^2}{2m} \nabla^2 \delta + O(\delta^2)$$

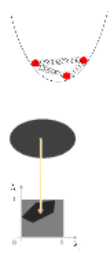
$$H = \sum_{i=1}^N \left( \frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 x_i^2 \right) + \frac{1}{2} D \sum_{i=1}^N (x_i - x_j)^2$$

fermionic ground state:

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

$$\rho_1(x, \vec{x}) \downarrow N-s$$

$$\vec{x} = \vec{x}(\delta)$$



### Wave function

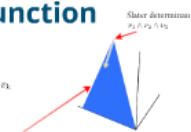
$\dim \Lambda^3(\mathbb{C}^6) = \binom{6}{3} = 20$

general state  $|\Psi\rangle = \sum_{i,j,k} c_{i,j,k} \phi_i \wedge \phi_j \wedge \phi_k$

can be written with 8 components when choosing the basis

pinned state  $|\Psi\rangle = \alpha \phi_1 \wedge \phi_2 \wedge \phi_3 + \beta \phi_1 \wedge \phi_4 \wedge \phi_5 + \gamma \phi_2 \wedge \phi_4 \wedge \phi_5$

3 components! true approximately!



Hartree-Fock method optimise over Slater determinants

system is almost uncorrelated

system is almost pinned

optimise over pinned states result 4 orders of magnitude better than Hartree-Fock!

### Pinning Analysis

$$\lambda_1 = \frac{40}{129} \delta^4 - \frac{1590}{59349} \delta^5 + O(\delta^6)$$

$$\lambda_2 = \frac{2}{9} \delta^4 - \frac{252}{1193} \delta^5 + \frac{2025}{11933} \delta^6 + O(\delta^7)$$

$$\lambda_3 = \frac{2}{9} \delta^4 - \frac{24}{253} \delta^5 + \frac{81902}{292315} \delta^6 + O(\delta^7)$$

$$\lambda_4 = \frac{2}{9} \delta^4 - \frac{24}{253} \delta^5 + \frac{73902}{292315} \delta^6 + O(\delta^7)$$

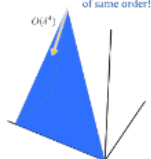
$$\lambda_5 = \frac{2}{9} \delta^4 - \frac{252}{1193} \delta^5 + \frac{2970}{11933} \delta^6 + O(\delta^7)$$

$$\lambda_6 = \frac{40}{129} \delta^4 - \frac{1280}{59349} \delta^5 + O(\delta^6)$$

$$\lambda_7 = \frac{80}{1193} \delta^4 - O(\delta^5)$$

$$\lambda_8 = O(\delta^4)$$

Dennis-Borland setting up to  $O(\delta^4)$   
Is  $\lambda_1 = \lambda_2 = \lambda_3 \leq \lambda_4$  pinned?  
Yes, up to  $O(\delta^4)$ ! Pinning & setting of same order!



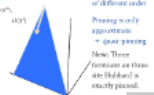
### Is Pinning Exact?

5 fermions in 7 modes up to  $O(\delta^7)$   
Is  $\lambda_1 = \lambda_2 = \lambda_3 \leq \lambda_4$  pinned?  
Yes, but set up to  $O(\delta^7)$ !

Pinning & setting of different order

Pinning itself approximate = exact pinning

Now Three fermions in three states (3 modes) is exactly pinned.

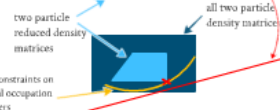


### Origin of Pinning?

new constraints in conflict with energy minimisation

kinematical dynamical

$$E_0 = \min_{\Psi_N} \langle \Psi_N | H | \Psi_N \rangle = \min_{\rho^{(2)}} \text{tr } h^{(2)} \rho^{(2)}$$



expectation: exactly pinned or not pinned at all!  
our findings: almost pinned! why...?

### Entanglement

Alice      Bob      Charlie

Entanglement = unique quantum mechanical correlations

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

$\longleftrightarrow$   $\psi$  and  $\phi$  can be interconverted with local operations and classical communication

$\longleftrightarrow$   $\psi = g \cdot \phi$  (invertible linear transformation of modes)

Dir. Vidal & Guse 2003

#### 3 fermions & 6 modes

4 types of entanglement

- $\rightarrow |\psi_1\rangle = \frac{1}{\sqrt{2}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle)$
- $\rightarrow |\psi_2\rangle = \frac{1}{\sqrt{3}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle + |1\rangle|4\rangle|5\rangle)$
- $\rightarrow |\psi_3\rangle = \frac{1}{\sqrt{2}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle)$
- $\rightarrow |\psi_4\rangle = |1\rangle|2\rangle|3\rangle$

same number of modes  $\rightarrow$  arbitrary number of types  
 necessarily many parameters  
 not locally accessible

### Three Qubits

$|\psi\rangle_{ABC}$

$\rho_{A^i}, \rho_{B^i}, \rho_{C^i}$

$\lambda_A, \lambda_B, \lambda_C$

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

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

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

#### Four Qubits

entanglement class

entanglement polytope

### Natural Occupation Numbers

$H_N$  entanglement class

$|\psi_N\rangle$

occupation numbers

$\rho = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix}$   $n_i = \langle \psi_N | a_i^\dagger a_i | \psi_N \rangle$

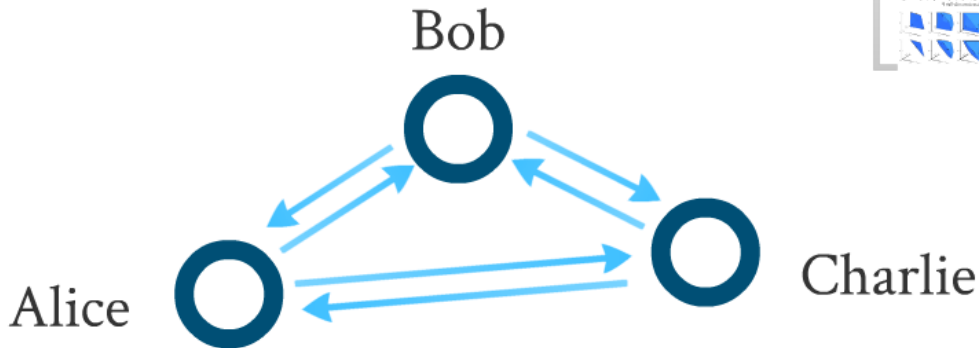
$= U \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} U^{-1}$

natural occupation numbers

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

Are there additional constraints on occupation numbers?

- no constraint
- weak constraint
- four constraint
- entanglement polytope



### 3 fermions & 6 modes

4 types of entanglement

- $\rightarrow |\psi_1\rangle = \frac{1}{\sqrt{2}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle)$
- $\rightarrow |\psi_2\rangle = \frac{1}{\sqrt{3}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle + |1\rangle|4\rangle|5\rangle)$
- $\rightarrow |\psi_3\rangle = \frac{1}{\sqrt{2}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle)$
- $\rightarrow |\psi_4\rangle = |1\rangle|2\rangle|3\rangle$

### Entanglement Polytopes

occupation numbers of all states in given entanglement class form polytope

Walter, Dorner, Gess & Christandl, Science 2012  
 Kosciuszko, Chaturvedi & Eis, 2012  
 group representation theory  
 Bric's theorem

entanglement witness

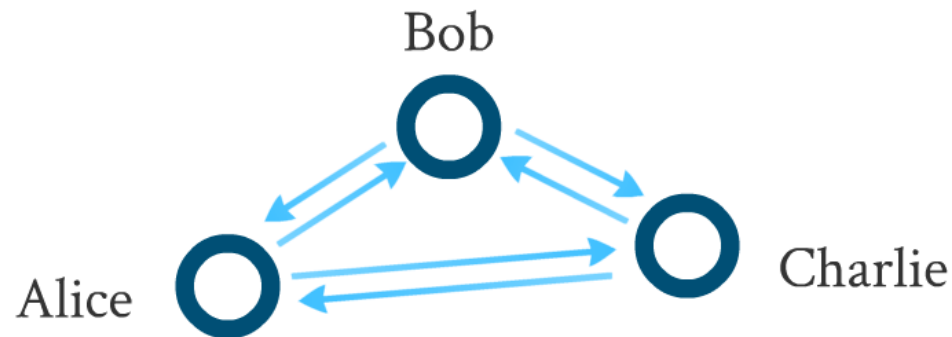
maximal multiparticle witnesses

entanglement class

systematic, finite, single-particle accessible  
 hierarchy of multiparticle entanglement

Calderbank, Gellman, Gisin, ...

# 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*  
 $\longleftrightarrow$   $\psi = g \cdot \phi$   
invertible linear transformation of modes

3 fermions & 6 modes

# 3 fermions & 6 modes

4 types of entanglement *Levay & Vrana 2008*

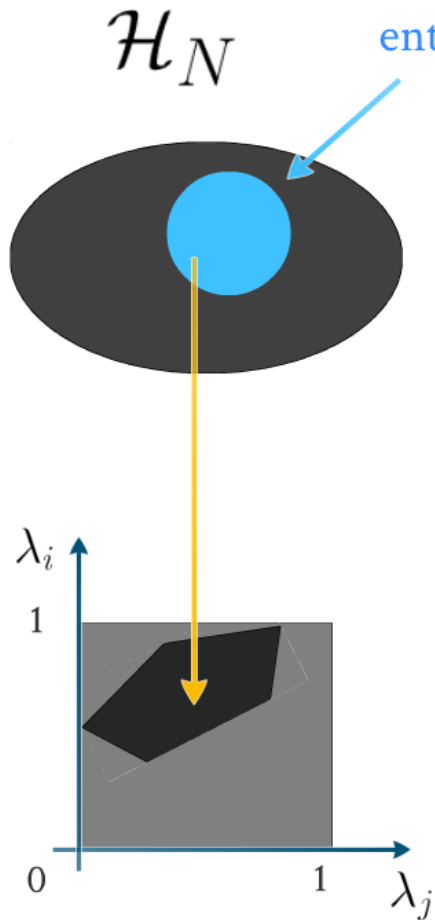
representative states

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

more fermions, more modes  $\longrightarrow$  infinite number of types  
exponentially many parameters  
not locally accessible *intractable!*



# Natural Occupation Numbers



$$|\Psi_N\rangle$$

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

occupation numbers

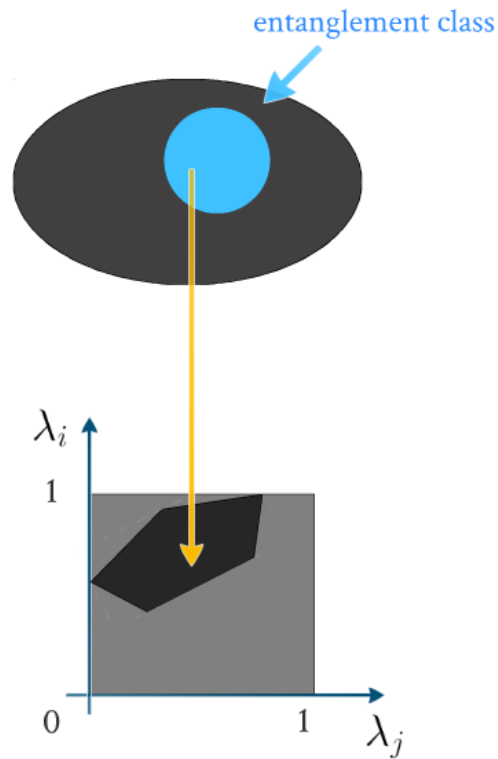
$$= U \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} U^\dagger$$

natural occupation numbers

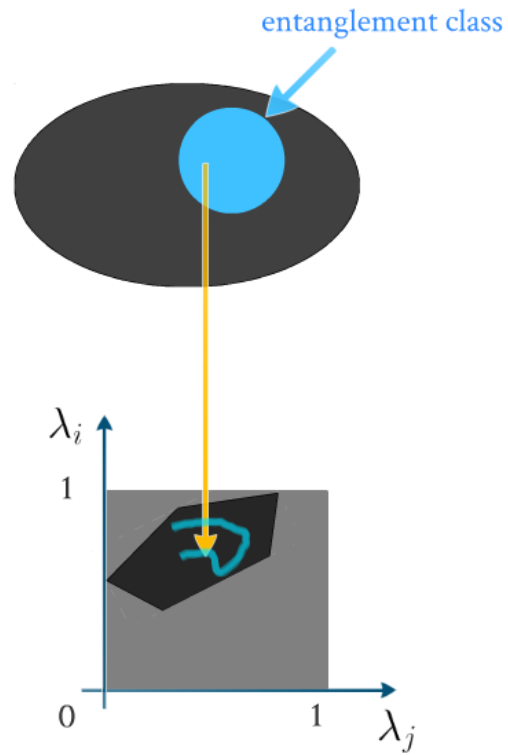
$$\vec{\lambda} = (\lambda_1, \lambda_2, \dots)$$

Are there additional constraints on occupation numbers?

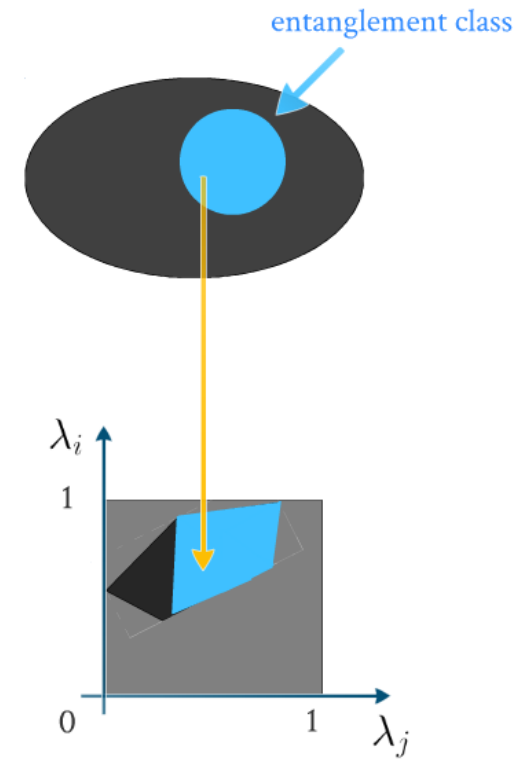
# Are there additional constraints on occupation numbers?



no constraints?



weird constraints?



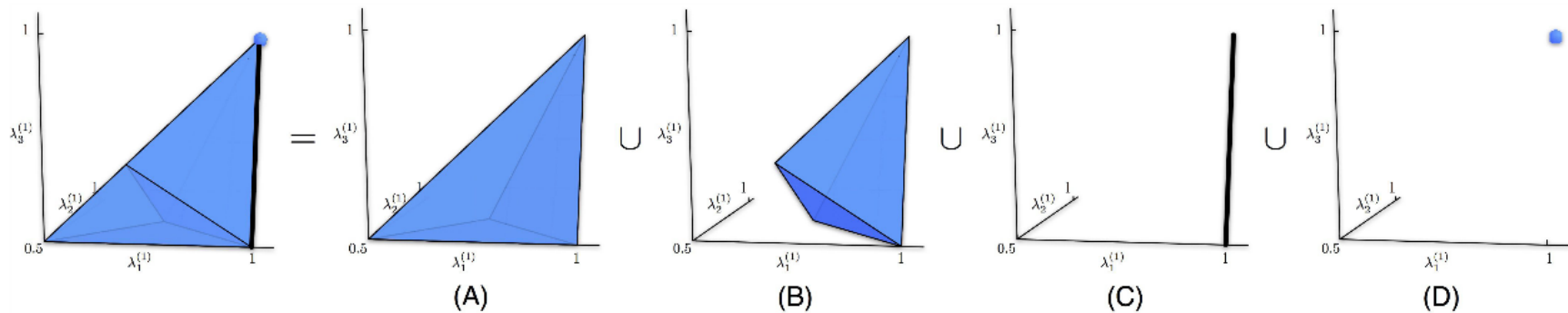
linear constraints!  
entanglement polytopes

# 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

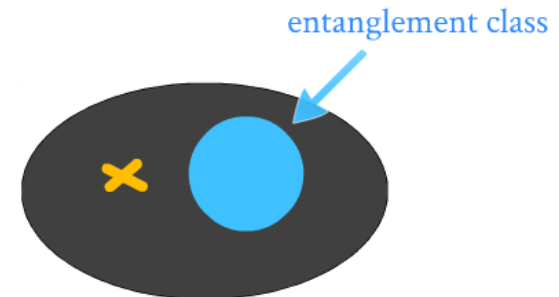
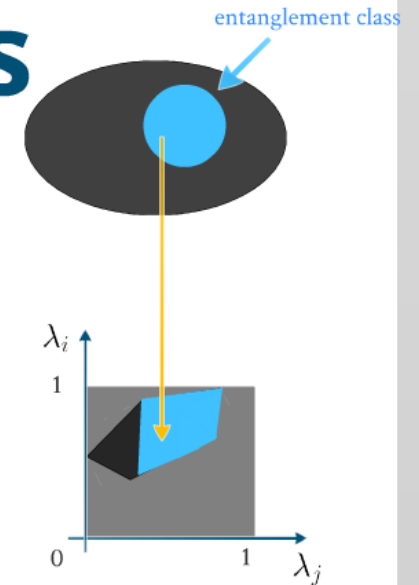
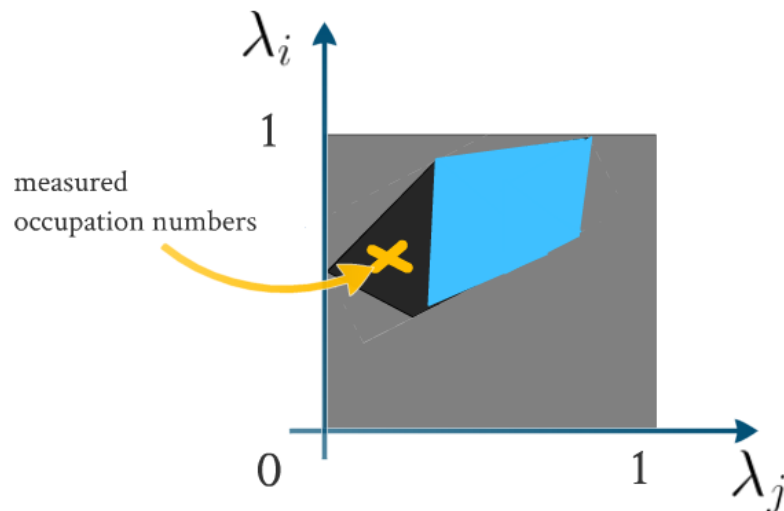
Walter, Doran, Gross & Christandl, Science 2013

Sawicki, Oszmaniec & Kus 2012

group representation theory

Brion's theorem

entanglement witness

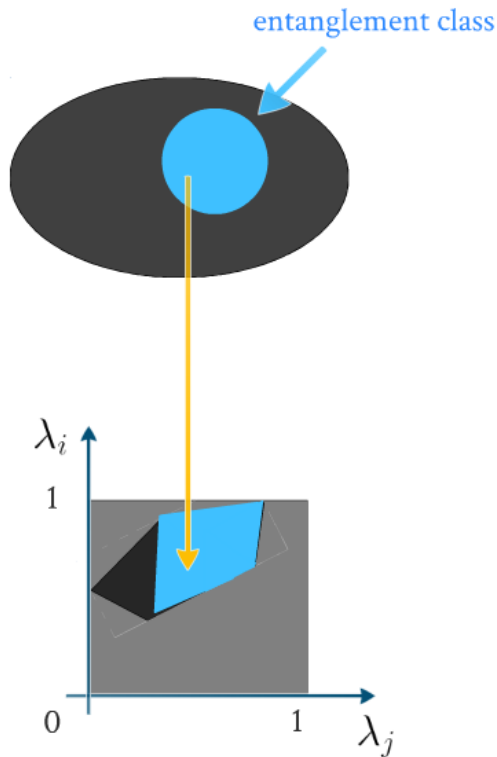


systematic, finite, single-particle accessible

hierarchy of multiparticle entanglement also for bosons, qubits, ...

# Three Qubits

Ⓐ   Ⓑ   Ⓒ



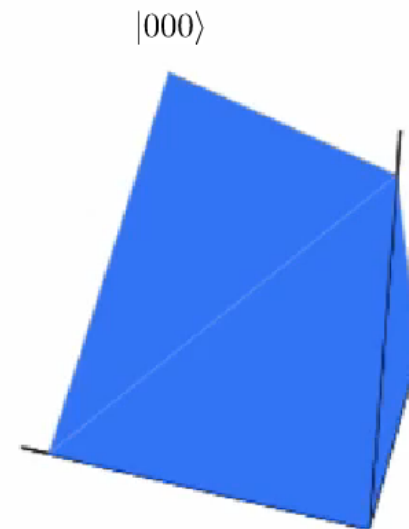
$$|\psi\rangle_{ABC}$$

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

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

$$\lambda_A, \lambda_B, \lambda_C$$

$$\frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle)$$



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

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

## Four Qubits

Entanglement classes: 9 infinite families of entanglement classes

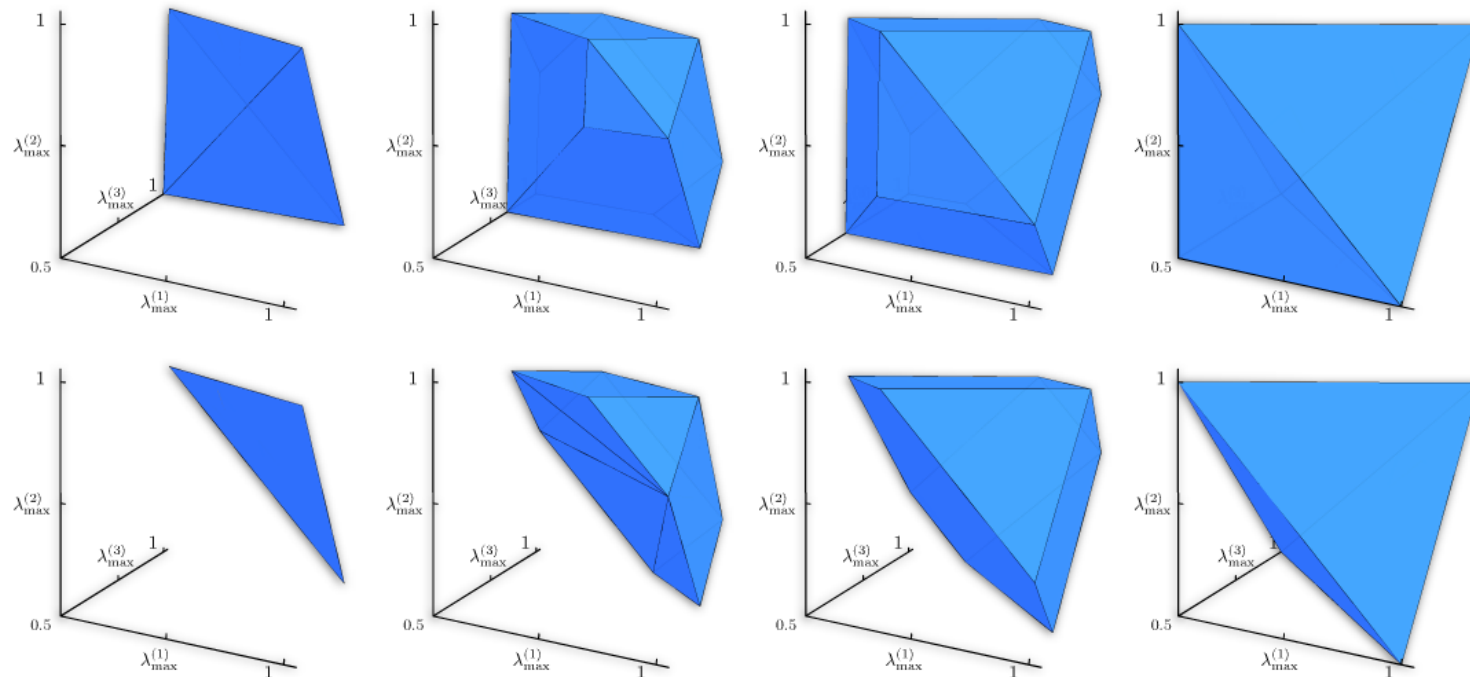
# Four Qubits

Entanglement classes: 9 infinite families of entanglement classes

Verstraete et al, 2002

Entanglement polytopes: 16 polytopes (up to permutation)

9 full-dimensional (genuine entangled)



### Entanglement

Entanglement = unique quantum mechanical correlations

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

$\longleftrightarrow$   $\psi$  and  $\phi$  can be interconverted with  
(local) local operations and classical communication

$\longleftrightarrow$   $\psi = g \cdot \phi$   
(global) invertible linear transformation of modes

Dir. Vidal & Guse 2003

#### 3 fermions & 6 modes

4 types of entanglement

- $\rightarrow |\psi_1\rangle = \frac{1}{\sqrt{2}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle)$
- $\rightarrow |\psi_2\rangle = \frac{1}{\sqrt{3}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle + |1\rangle|4\rangle|5\rangle)$
- $\rightarrow |\psi_3\rangle = \frac{1}{\sqrt{2}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle)$
- $\rightarrow |\psi_4\rangle = |1\rangle|2\rangle|3\rangle$

(arbitrary) number of types  
(arbitrary) necessarily many parameters  
(arbitrary) not locally accessible

### Three Qubits

$|\psi\rangle_{ABC}$       $\rho = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} = U \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} U^{-1}$

$\rho_A, \rho_B, \rho_C$   
 $\lambda_A, \lambda_B, \lambda_C$

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

#### Four Qubits

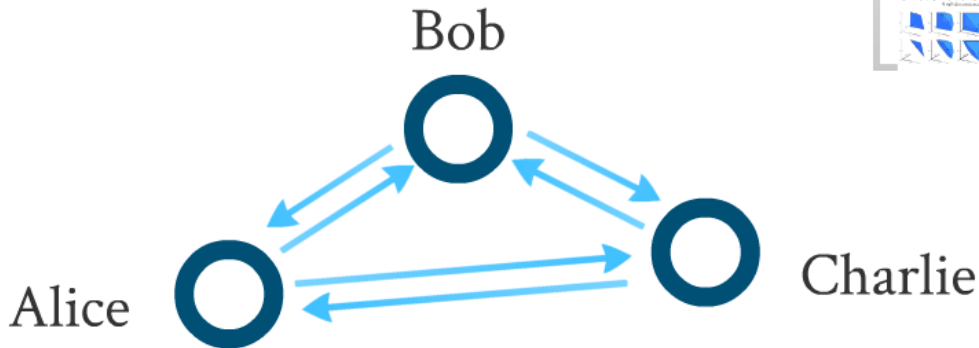
(arbitrary) number of types  
(arbitrary) necessarily many parameters  
(arbitrary) not locally accessible

### Natural Occupation Numbers

$|\psi_N\rangle$   
 occupation numbers  
 $\rho = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix}$       $n_i = \langle \psi_N | a_i^\dagger a_i | \psi_N \rangle$   
 $= U \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} U^{-1}$   
 natural occupation numbers  
 $\vec{\lambda} = (\lambda_1, \lambda_2, \dots)$

Are there additional constraints on occupation numbers?

- (no) no constraint
- (yes) well-ordered
- (yes) four constraints: arrangement polytope



### 3 fermions & 6 modes

4 types of entanglement

- $\rightarrow |\psi_1\rangle = \frac{1}{\sqrt{2}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle)$
- $\rightarrow |\psi_2\rangle = \frac{1}{\sqrt{3}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle + |1\rangle|4\rangle|5\rangle)$
- $\rightarrow |\psi_3\rangle = \frac{1}{\sqrt{2}}(|1\rangle|2\rangle|3\rangle + |4\rangle|5\rangle|6\rangle)$
- $\rightarrow |\psi_4\rangle = |1\rangle|2\rangle|3\rangle$

### Entanglement Polytopes

occupation numbers of all states in given entanglement class form polytope

Walter, Dorner, Gess & Christandl, Science 2012  
Kowalski, Chruściński & Eis, 2012  
group representation theory  
Brieno's theorem

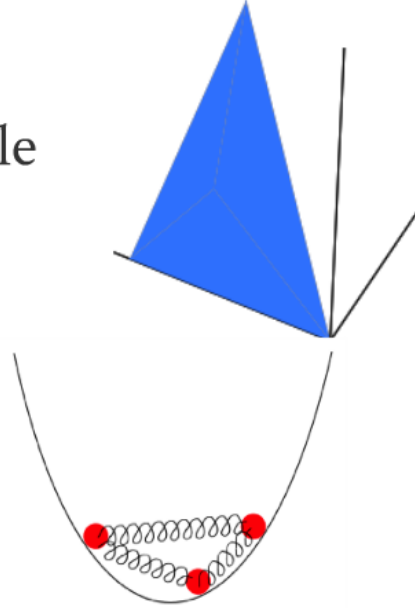
entanglement witness

systematic, finite, single-particle accessible  
hierarchy of multiparticle entanglement

Calderbank, Gellman, et al.

# Summary

extended Pauli's principle



physically relevant?

pinned states have simple structure



entanglement polytopes

