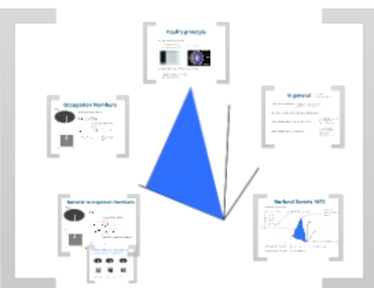
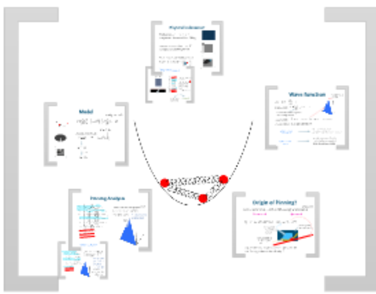
From Pauli's Principle to Fermionic Entanglement

Matthias Christandl
University of Copenhagen

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





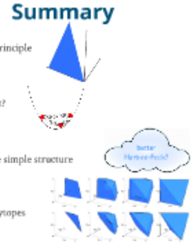
Summary

extended Pauli's principle

physically relevant?

pinned states have simple structure

entanglement polytopes



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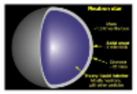
Pauli's exclusion principle (1925):

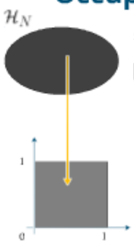
'no two fermions in the same quantum state' $0 \leq n_i \leq 1$



strengthened by Dirac & Heisenberg in (1926):

'quantum states of fermions are antisymmetric'

Occupation Numbers



fixed particle number N

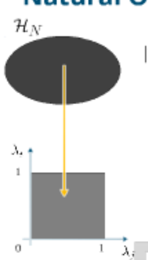
$|\Psi_N\rangle \in \Lambda^N(\mathcal{H})$

occupation numbers

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

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

Natural Occupation Numbers



$|\Psi_N\rangle$

occupation numbers

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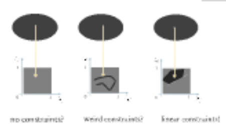
$= U \begin{pmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3 \end{pmatrix} U^\dagger$

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 Kirwan's convexity theorem

depends on number of particles and local dimension

inner characterisation (representation theory)   Christandl & Mitchison, 2004; Klyachko 2004, 2006; Daftuar & Hayden 2004

outer characterisation (inequalities)   Klyachko 2004, 2006; Daftuar & Hayden 2004; Ressayre, 2008; Vergne &Walter 2014

Borland Dennis 1972

3 fermions & 6 modes

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

$\lambda_1 + \lambda_6 = 1$

$\lambda_2 + \lambda_5 = 1$

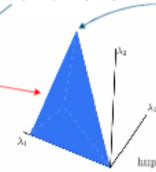
$\lambda_3 + \lambda_4 = 1$

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

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

not implied by Pauli principle

$e_1 \wedge e_2 \wedge e_3$ Slater determinant (1,1,1)

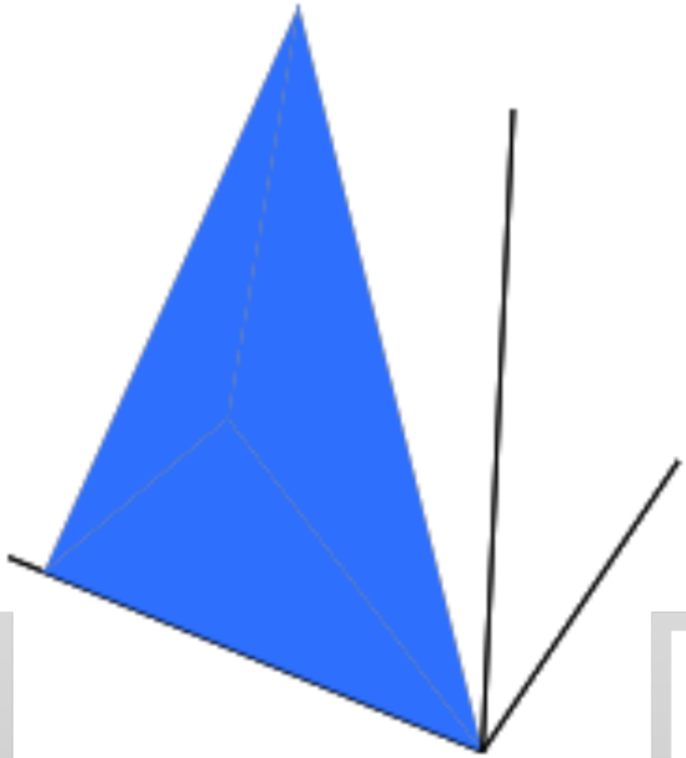


http://polytopes.leetspeak.org/

3 fermions in 7 modes $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2$ and three others

5 fermions in 10 modes   161 inequalities

...



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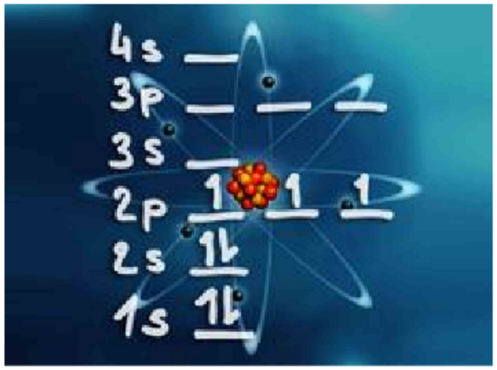

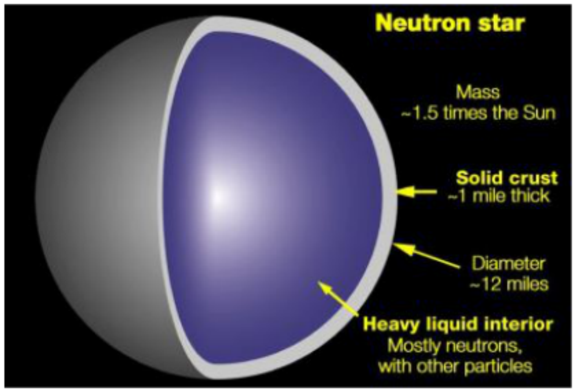

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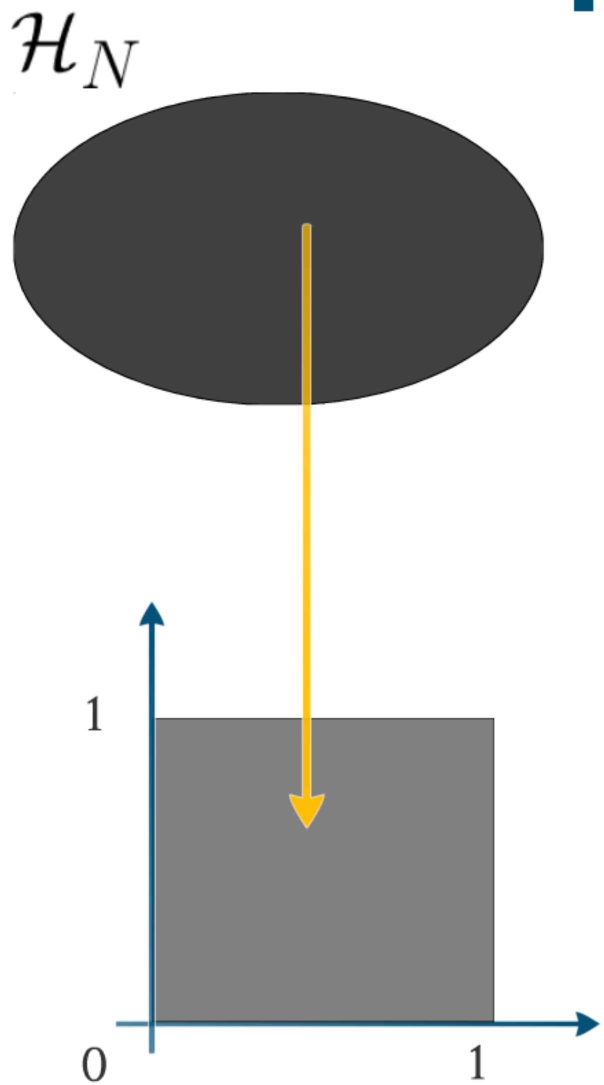

fixed particle number N

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

occupation numbers

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

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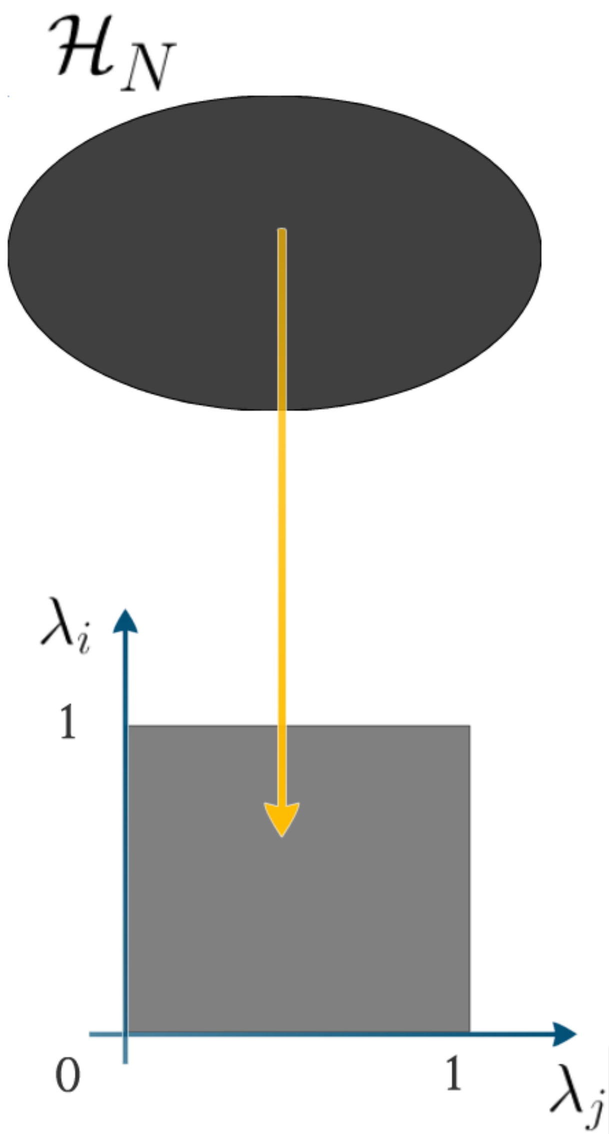

$$|\Psi_N\rangle$$

$$\downarrow$$

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Are there additional constraints on natural occupation numbers?

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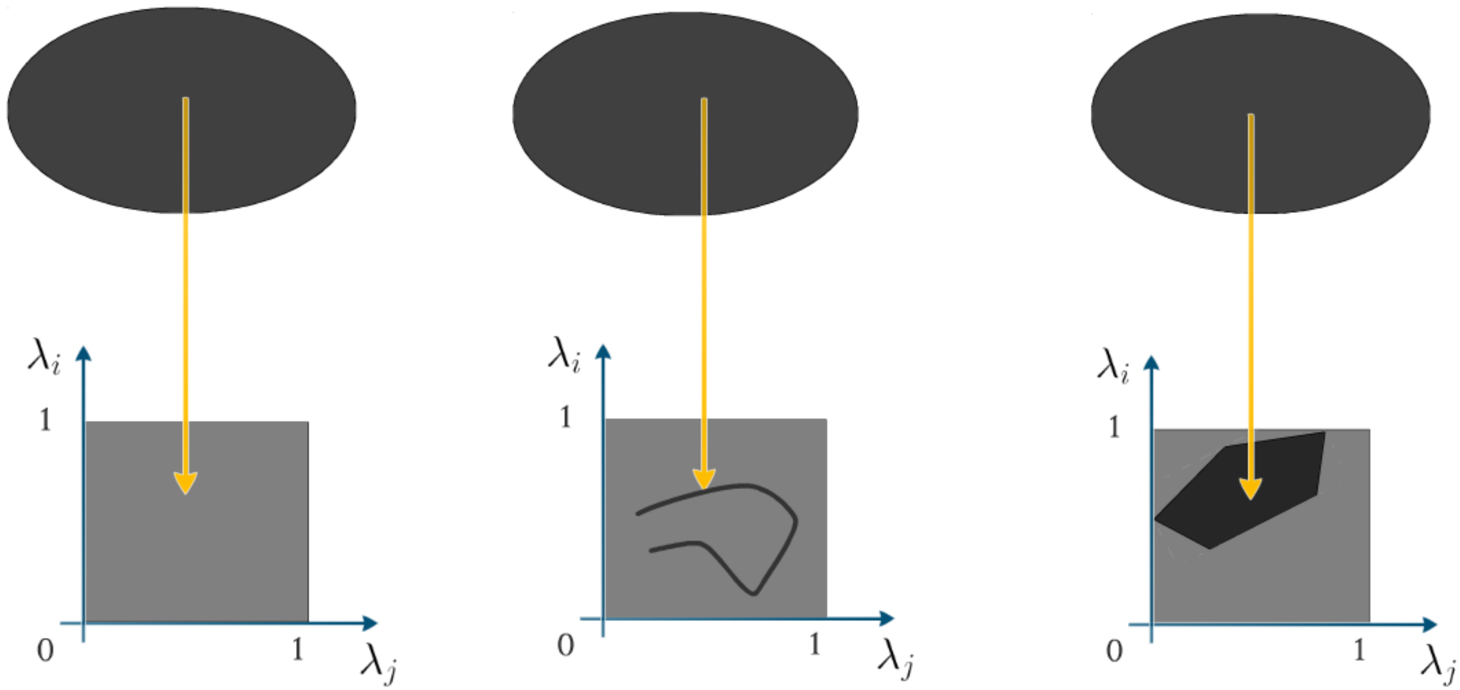

no constraints? weird constraints? linear constraints!

Borland Dennis 1972

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Slater determinant
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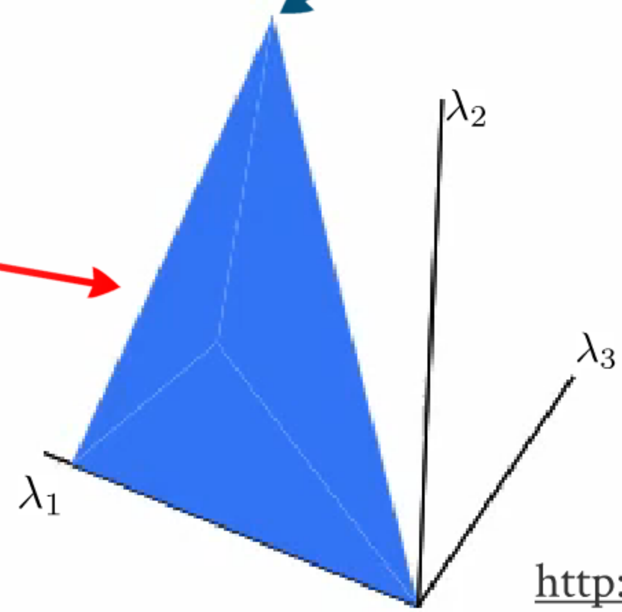

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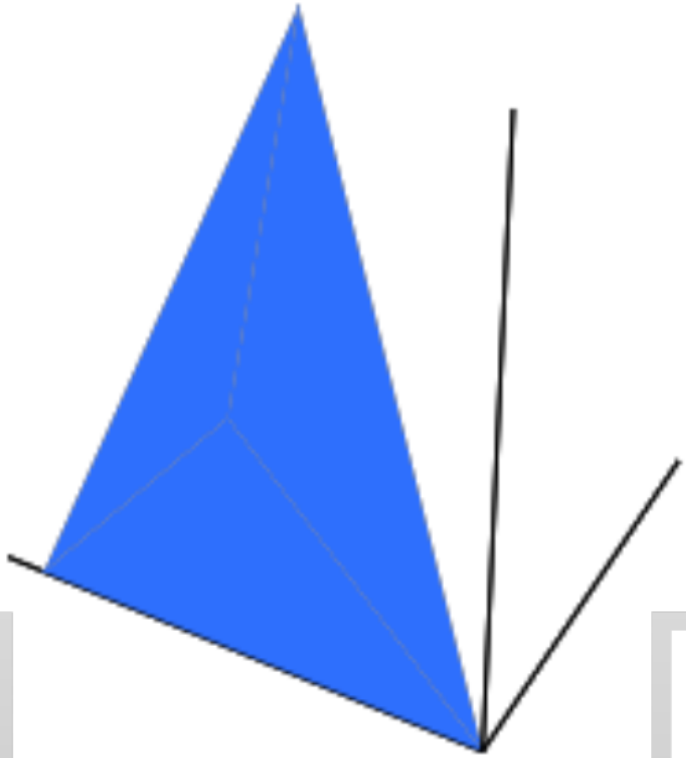

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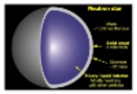

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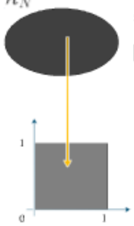

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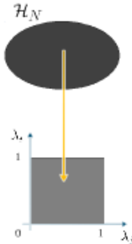

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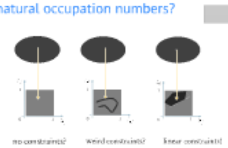

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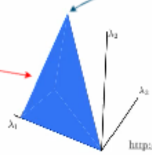

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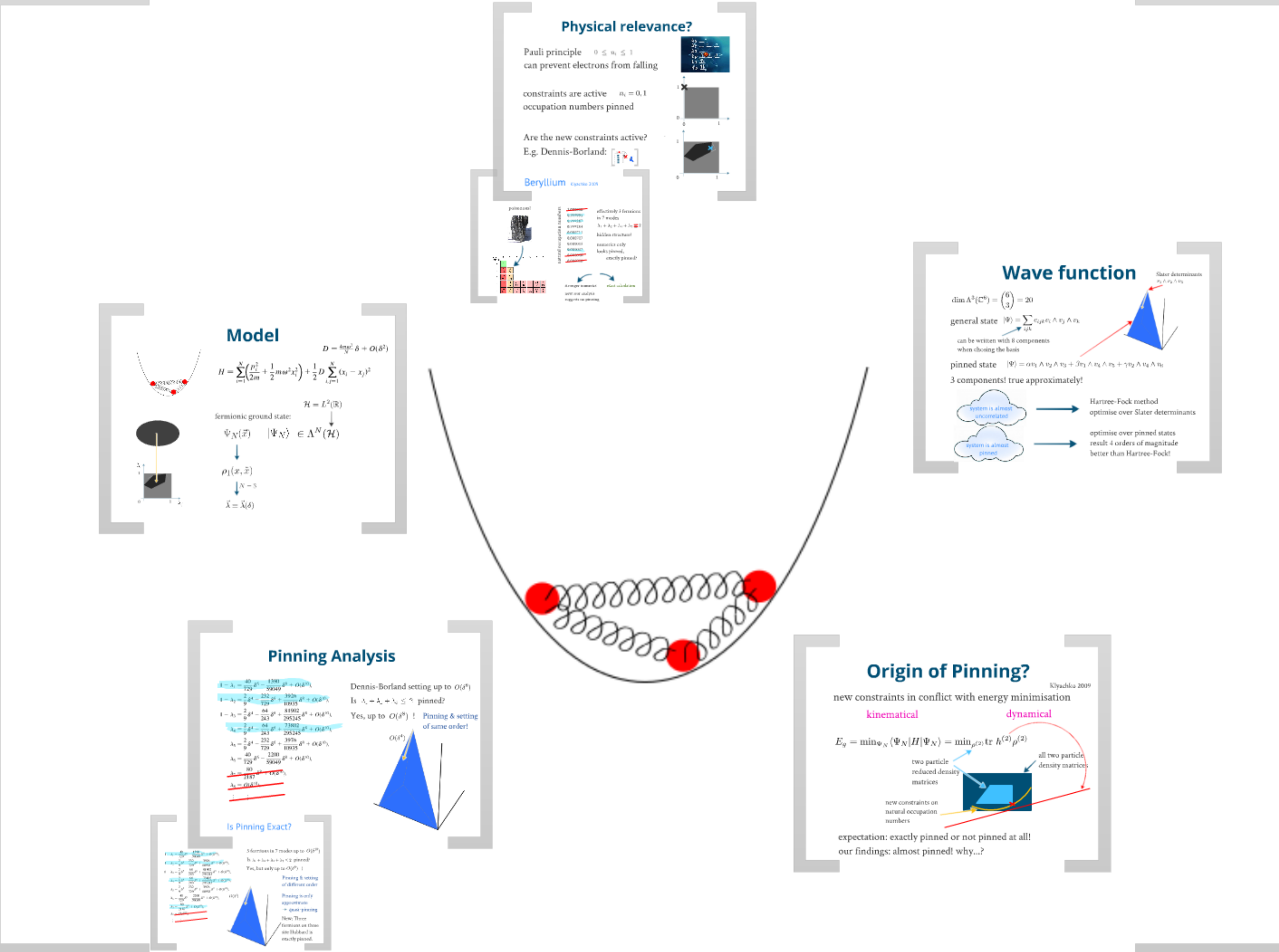

Physical relevance?
Pauli principle
can prevent electrons from falling
constraints are active
occupation numbers pinned
Are the new constraints active?
E.g. Dennis-Borland:
Beryllium
Wave function
general state
can be written with 8 components
when chosing the basis
pinned state
3 components! true approximately!
Hartree-Fock method
optimise over Slater determinants
optimise over pinned states
result 4 orders of magnitude
better than Hartree-Fock!
Model
fermionic ground state:
Pinning Analysis
Dennis-Borland setting up to
Yes, up to
Pinning & setting
of same order!
Is Pinning Exact?
Origin of Pinning?
new constraints in conflict with energy minimisation
kinematical
dynamical
two particle
reduced density
matrices
all two particle
density matrices
new constraints on
natural occupation
numbers
expectation: exactly pinned or not pinned at all!
our findings: almost pinned! why...?

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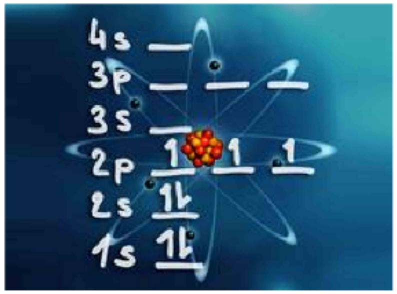
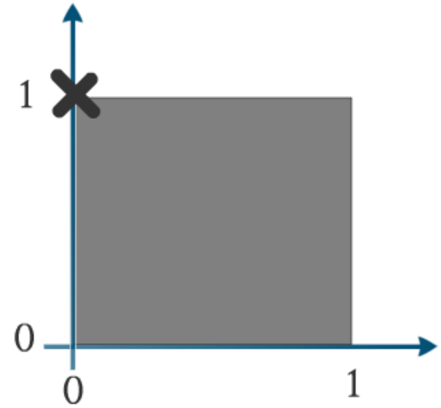


Pauli principle $0 \leq n_i \leq 1$

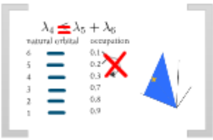
can prevent electrons from falling

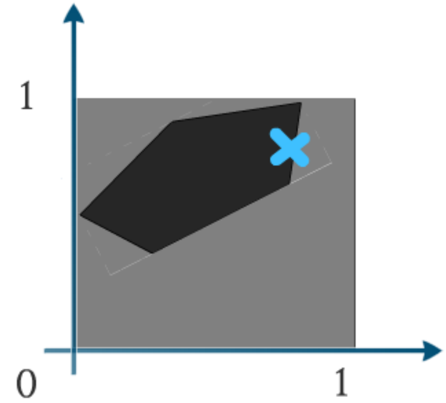


constraints are active $n_i = 0, 1$

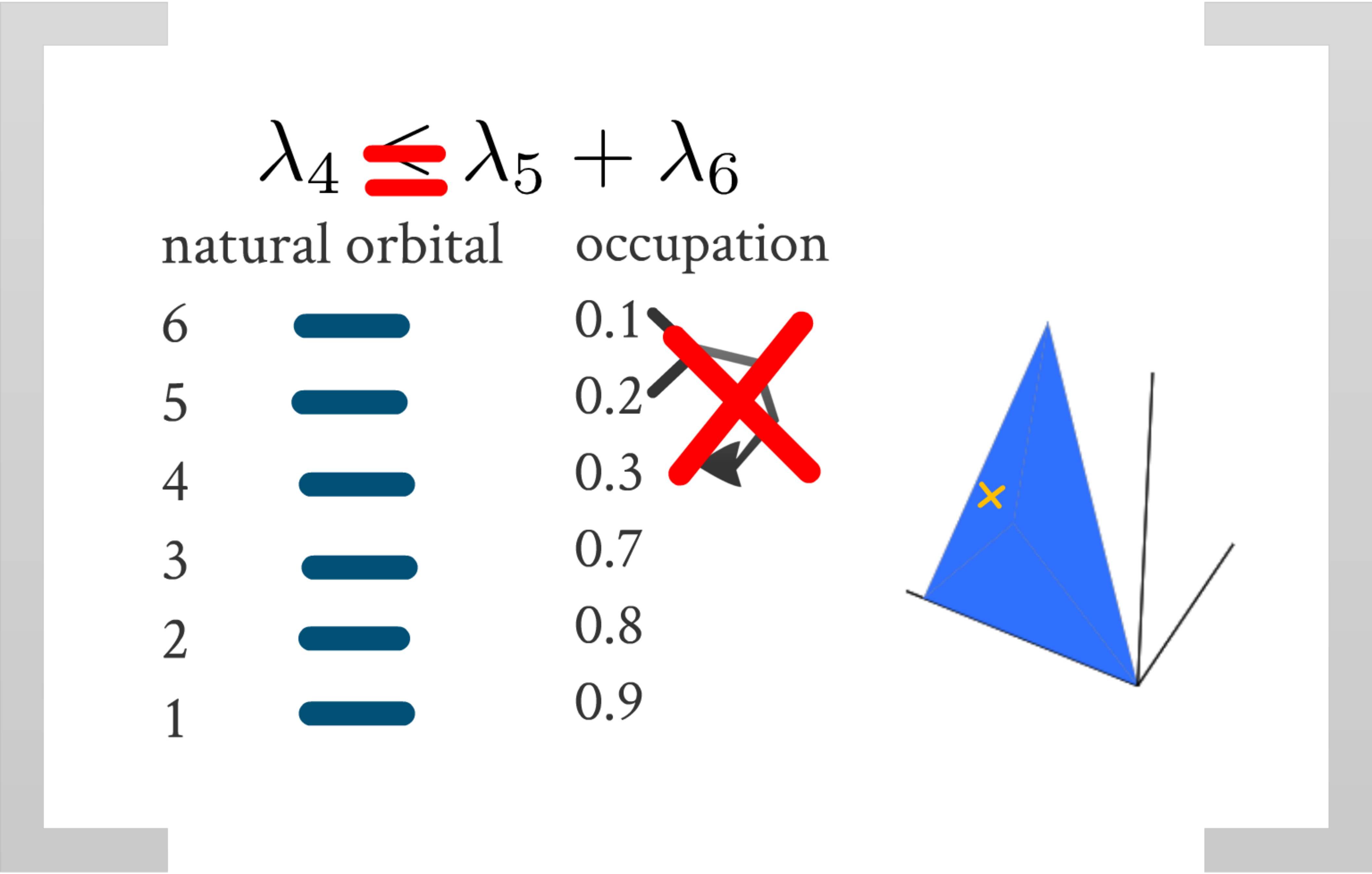
occupation numbers pinned

Are the new constraints active?

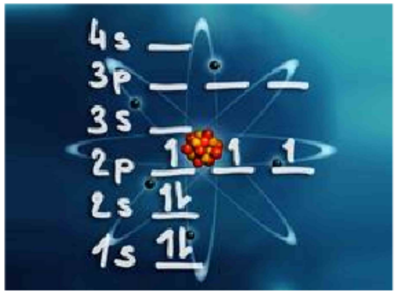
E.g. Dennis-Borland: 



Beryllium Klyachko 2009


$\lambda_4 \leq \lambda_5 + \lambda_6$
natural orbital
occupation
6
5
4
3
2
1
0.1
0.2
0.3
0.7
0.8
0.9

Physical relevance?



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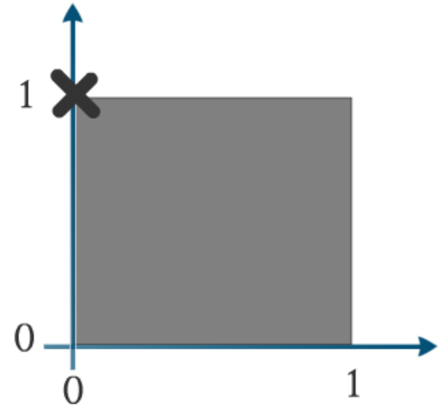

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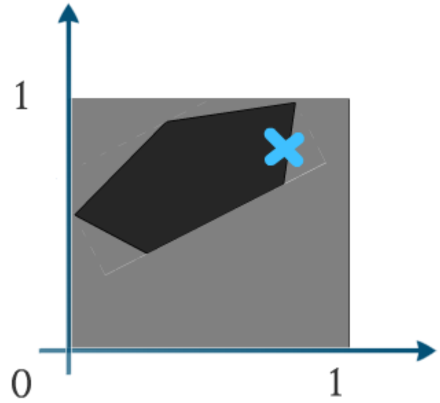

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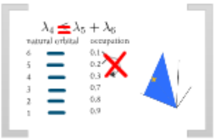
E.g. Dennis-Borland: 

Beryllium Klyachko 2009

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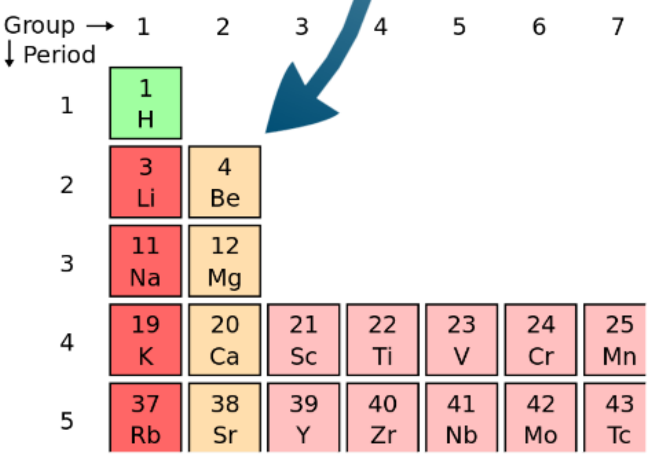
poisonous!



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!

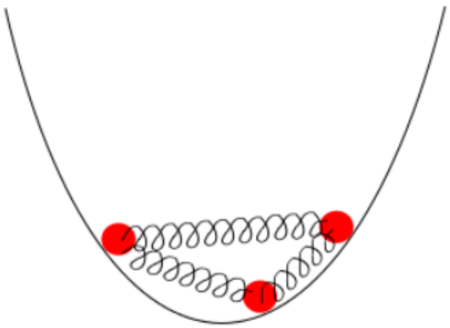
numerics only looks pinned,
exactly pinned?

stronger numerics

exact calculation

new: our analysis suggests no pinning

Model



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

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

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

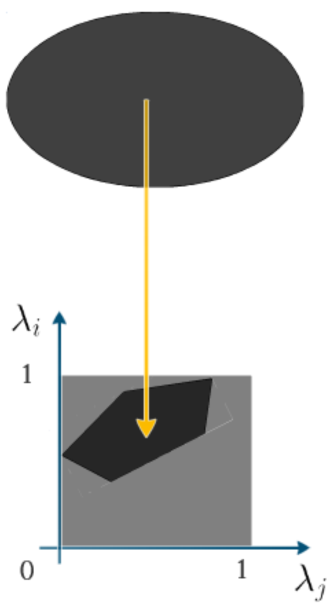
fermionic ground state:

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

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

$N = 3$

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



Pinning Analysis

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

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

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

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

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

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

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

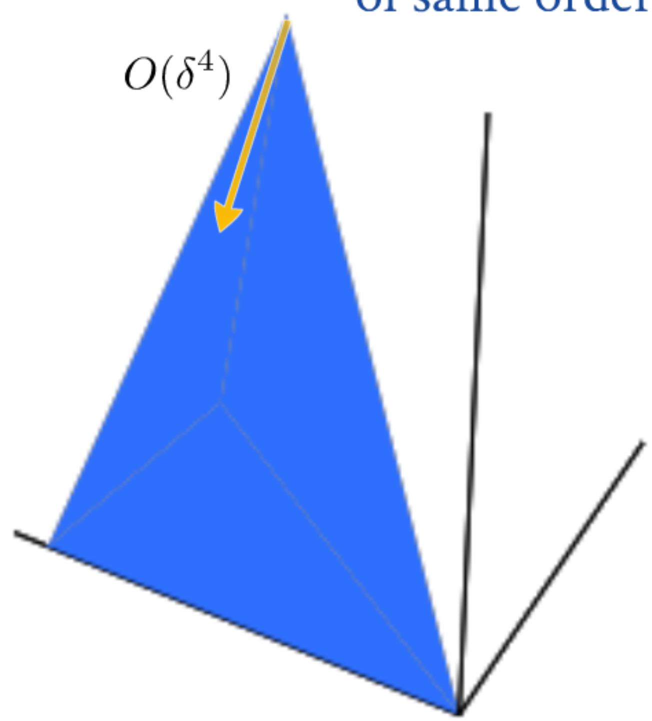
$$\lambda_8 = O(\delta^{10}),$$

$$\vdots \qquad \vdots$$

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?

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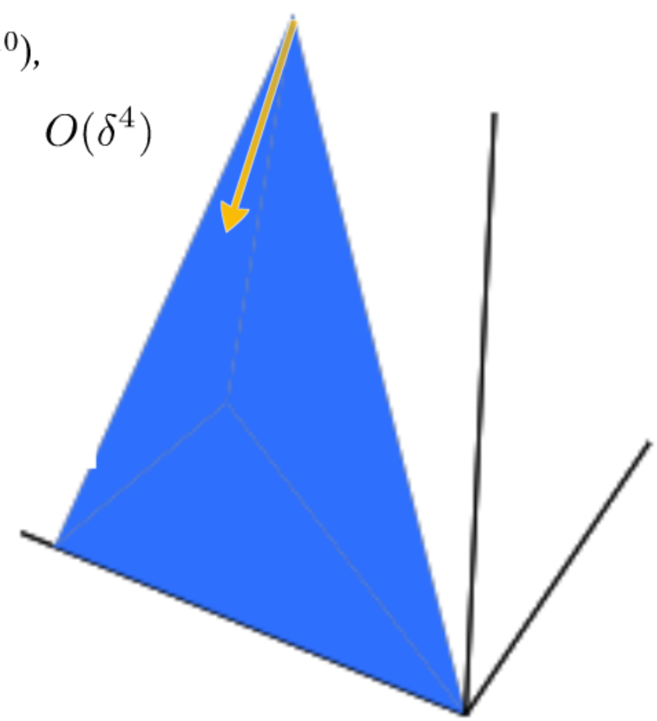
$$\vdots \qquad \vdots$$

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.

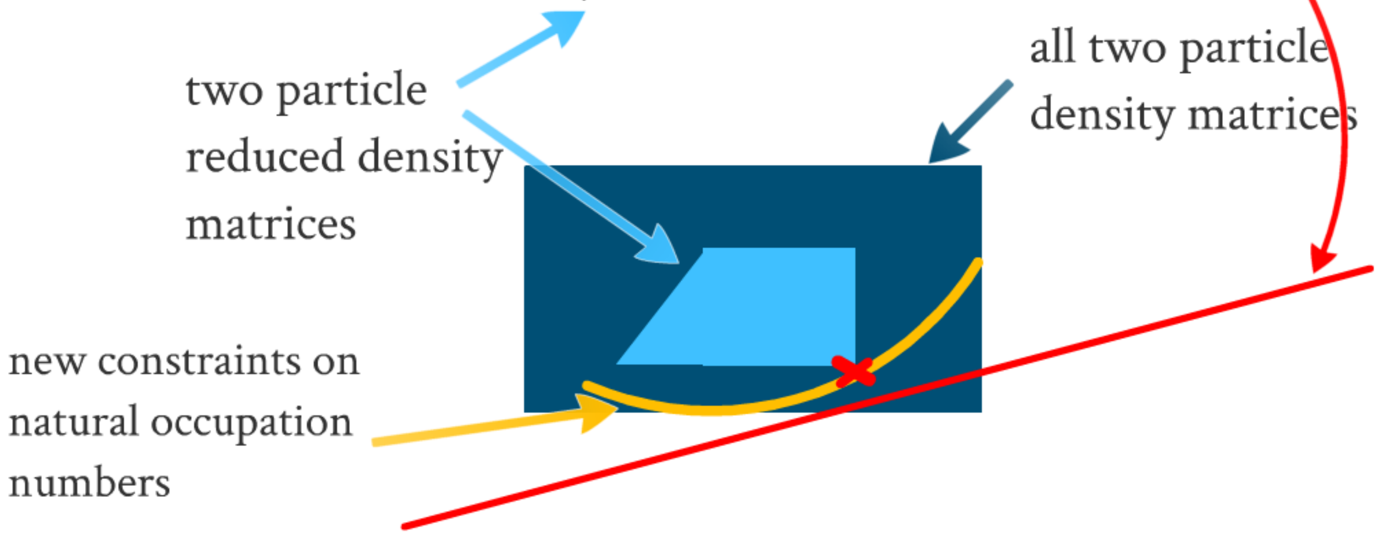
Origin of Pinning?

Klyachko 2009

new constraints in conflict with energy minimisation

kinematical dynamical

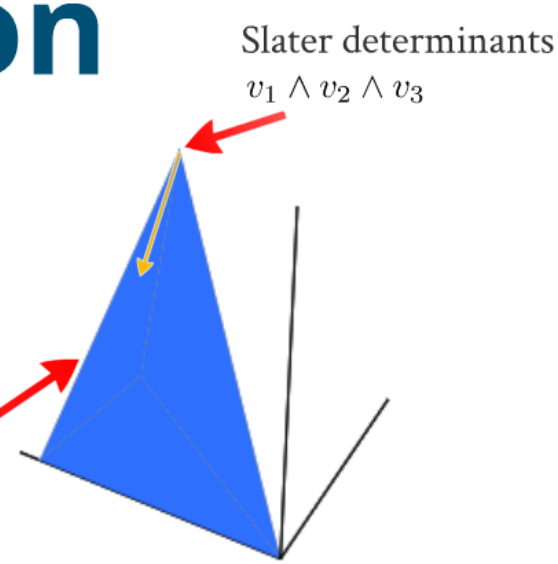
$$E_g = \min_{\Psi_N} \langle \Psi_N | H | \Psi_N \rangle = \min_{\rho^{(2)}} \mathrm{tr}\ h^{(2)} \rho^{(2)}$$



expectation: exactly pinned or not pinned at all!

our findings: almost pinned! why...?

Wave function



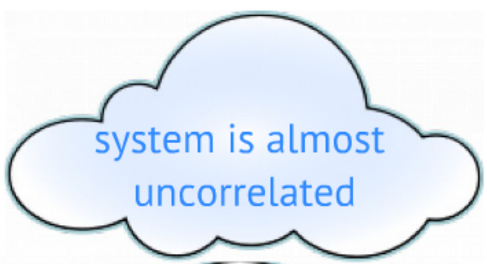
$$\dim \Lambda^3(\mathbb{C}^6) = \binom{6}{3} = 20$$

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

can be written with 8 components
when chosing 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!



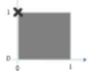
Hartree-Fock method
optimise over Slater determinants

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

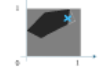
Physical relevance?

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

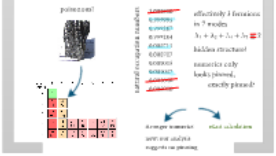
constraints are active $n_i = 0, 1$
occupation numbers pinned



Are the new constraints active?
E.g. Dennis-Borland:



Beryllium



Model

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

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

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

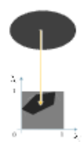
fermionic ground state:

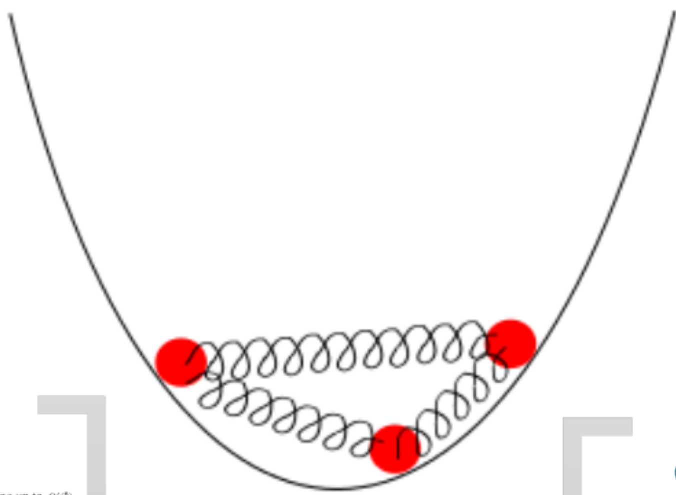
$\Psi_N(\vec{x})$ $|\Psi_N\rangle \in \Lambda^N(\mathcal{H})$

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

$N = 3$

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





Wave function

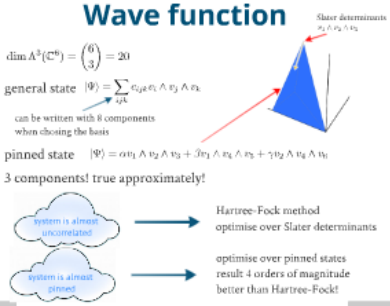
$\dim \Lambda^3(\mathbb{C}^6) = \binom{6}{3} = 20$

general state $|\Psi\rangle = \sum_{ijk} c_{ijk}\, e_i \wedge e_j \wedge e_k$

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!



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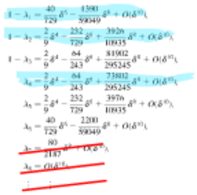
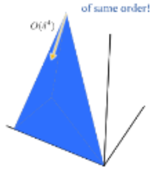
Pinning Analysis



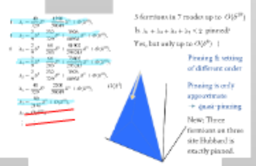
Dennis-Borland setting up to $O(\delta^8)$

Is $\lambda_1 = \lambda_2 + \lambda_4 \le 1$ pinned?

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



Is Pinning Exact?



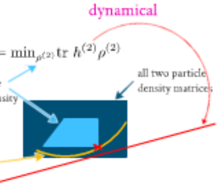
Origin of Pinning?

Klyachko 2009

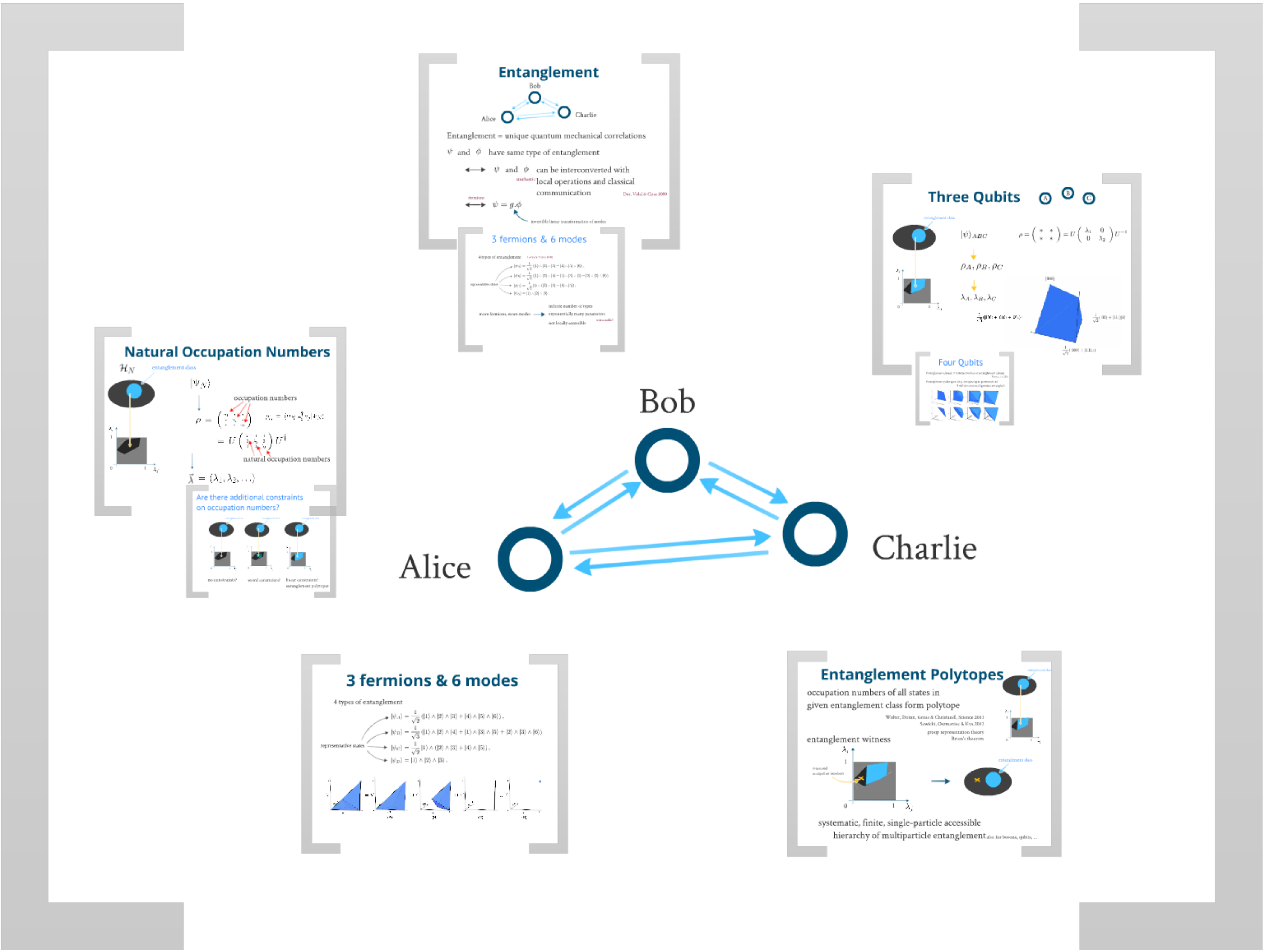
new constraints in conflict with energy minimisation

kinematical dynamical

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

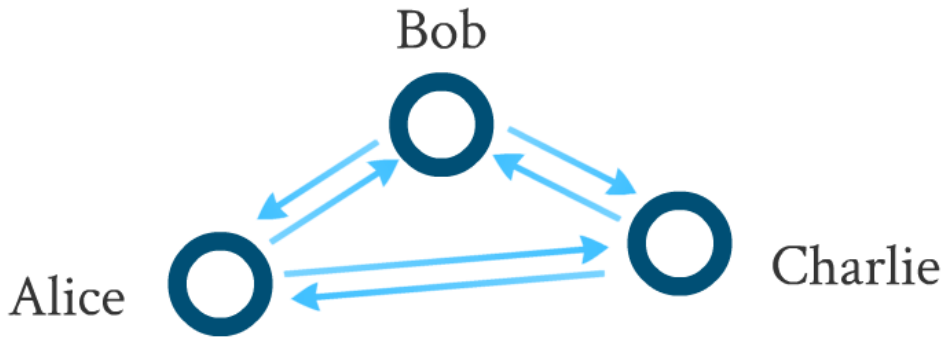


expectation: exactly pinned or not pinned at all!
our findings: almost pinned! why...?



Entanglement
Bob
Alice
Charlie
Entanglement = unique quantum mechanical correlations
ψ and φ have same type of entanglement
ψ and φ can be interconverted with
local operations and classical
communication
ψ = g.φ
3 fermions & 6 modes
Three Qubits
Four Qubits
Natural Occupation Numbers
occupation numbers
natural occupation numbers
Are there additional constraints
on occupation numbers?
Bob
Alice
Charlie
3 fermions & 6 modes
4 types of entanglement
representative states
Entanglement Polytopes
occupation numbers of all states in
given entanglement class form polytope
entanglement witness
systematic, finite, single-particle accessible
hierarchy of multiparticle entanglement

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

$\overset{\text{fermions}}{\longleftrightarrow}$ $\psi = g.\phi$

invertible linear transformation of modes

3 fermions & 6 modes

3 fermions & 6 modes

4 types of entanglement   Levay & Vrana 2008

representative states

$$|\psi_A\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle \wedge |2\rangle \wedge |3\rangle + |4\rangle \wedge |5\rangle \wedge |6\rangle\right),$$

$$|\psi_B\rangle = \frac{1}{\sqrt{3}}\left(|1\rangle \wedge |2\rangle \wedge |4\rangle + |1\rangle \wedge |3\rangle \wedge |5\rangle + |2\rangle \wedge |3\rangle \wedge |6\rangle\right)$$

$$|\psi_C\rangle = \frac{1}{\sqrt{2}}|1\rangle \wedge \left(|2\rangle \wedge |3\rangle + |4\rangle \wedge |5\rangle\right),$$

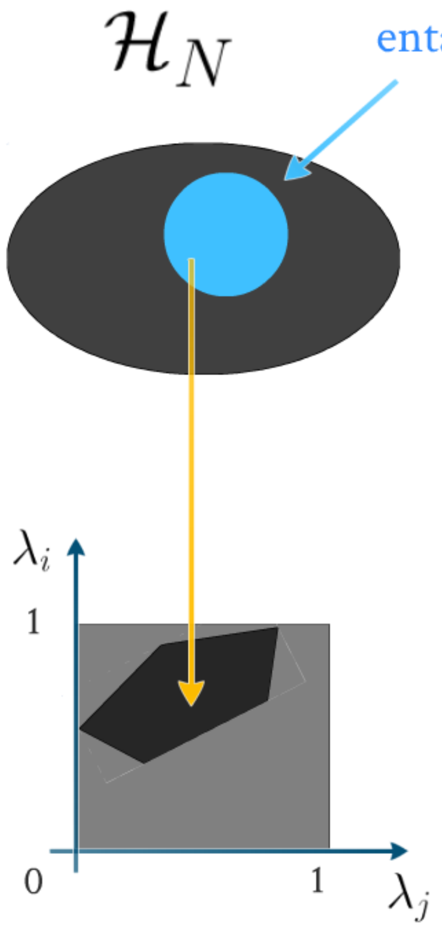
$$|\psi_D\rangle = |1\rangle \wedge |2\rangle \wedge |3\rangle .$$

more fermions, more modes →

- infinite number of types
- exponentially many parameters
- not locally accessible

intractable!

Natural Occupation Numbers



$$|\Psi_N\rangle$$

$$\downarrow$$

occupation numbers

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

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

natural occupation numbers

$$\downarrow$$

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

Are there additional constraints on occupation numbers?

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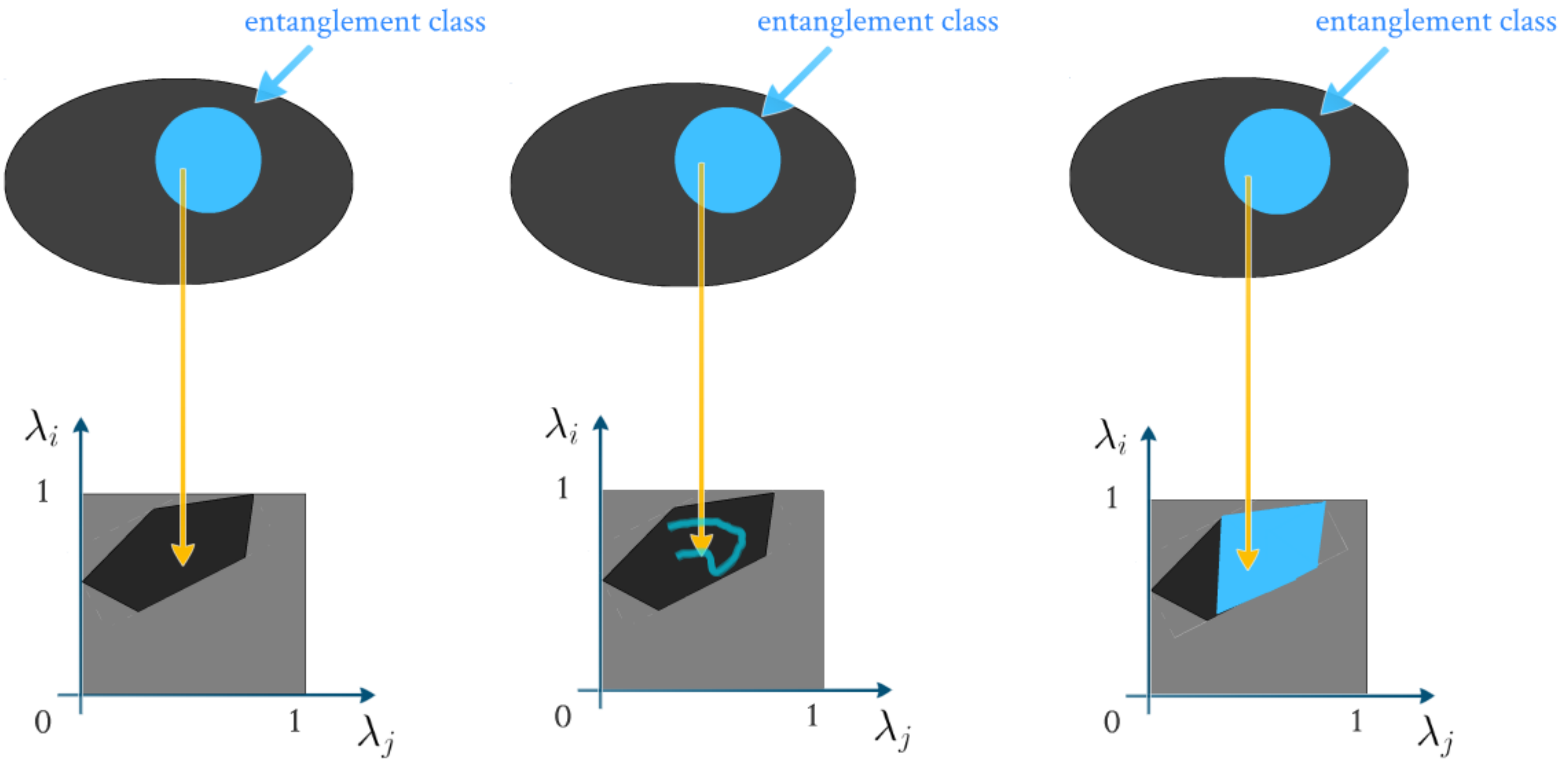

no constraints?

weird constraints?

linear constraints!

entanglement polytopes

3 fermions & 6 modes

4 types of entanglement

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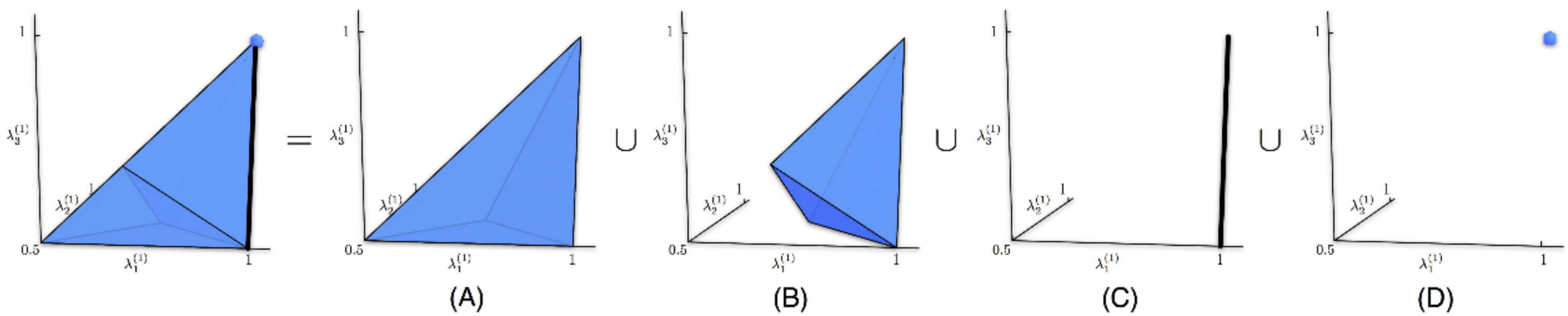
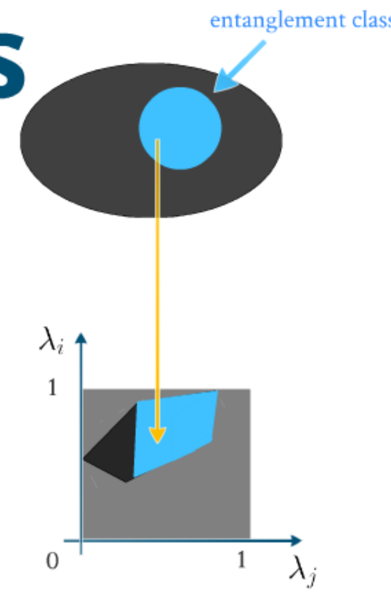


Entanglement Polytopes

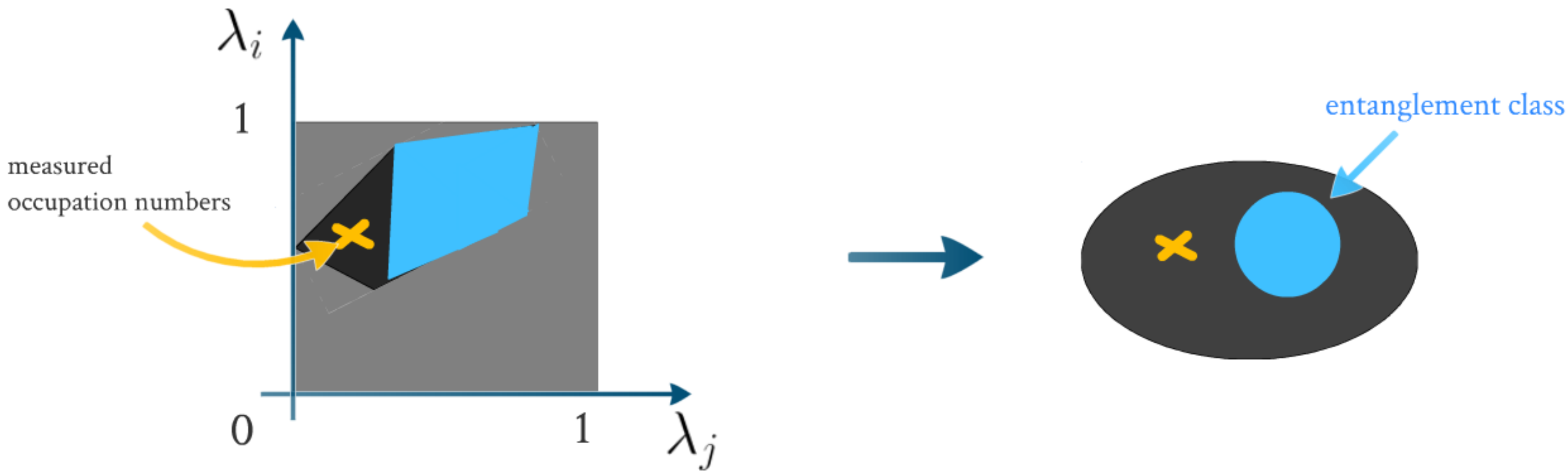


occupation numbers of all states in
given entanglement class form polytope

Walter, Doran, Gross & Christandl, Science 2013
Sawicki, Oszmaniec & Kus 2012

group representation theory
Brion's theorem

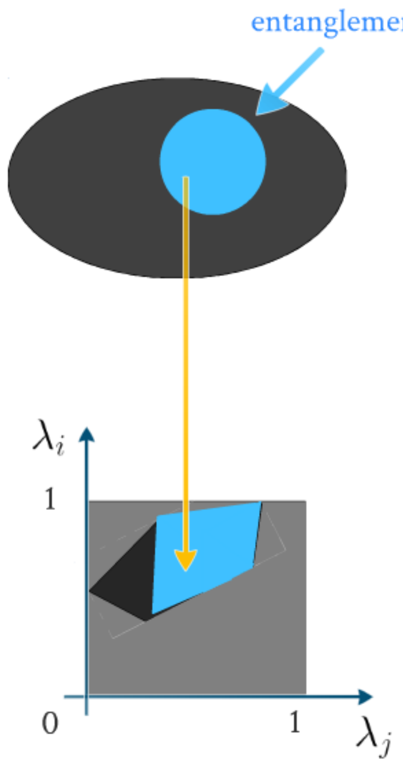
entanglement witness



systematic, finite, single-particle accessible
hierarchy of multiparticle entanglement also for bosons, qubits, ...

Three Qubits

Ⓐ Ⓑ Ⓒ

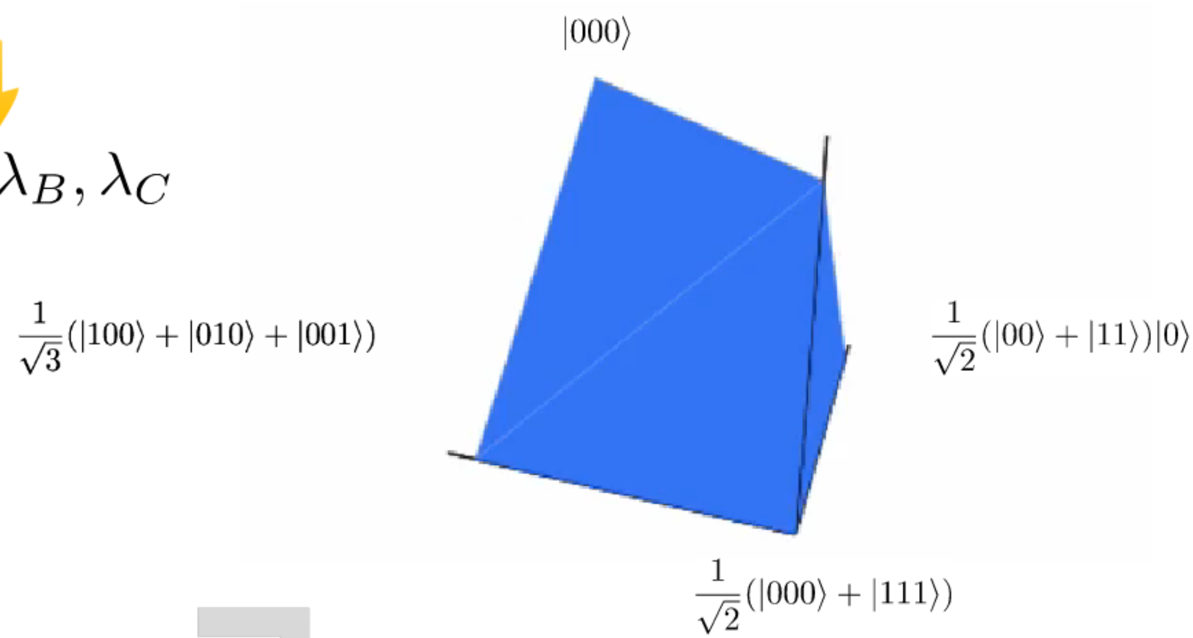


$$|\psi\rangle_{ABC}$$

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

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

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



Four Qubits

Entanglement classes: 9 infinite families of entanglement classes

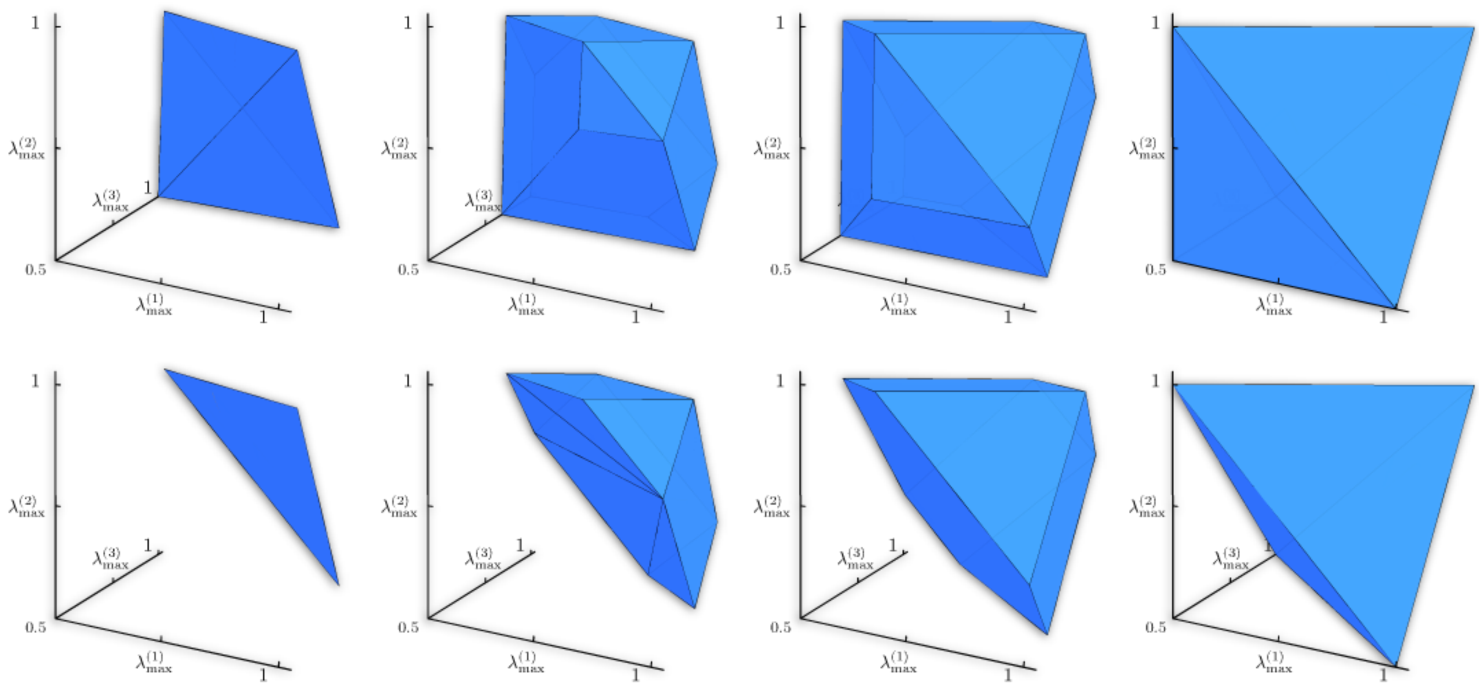
Four Qubits

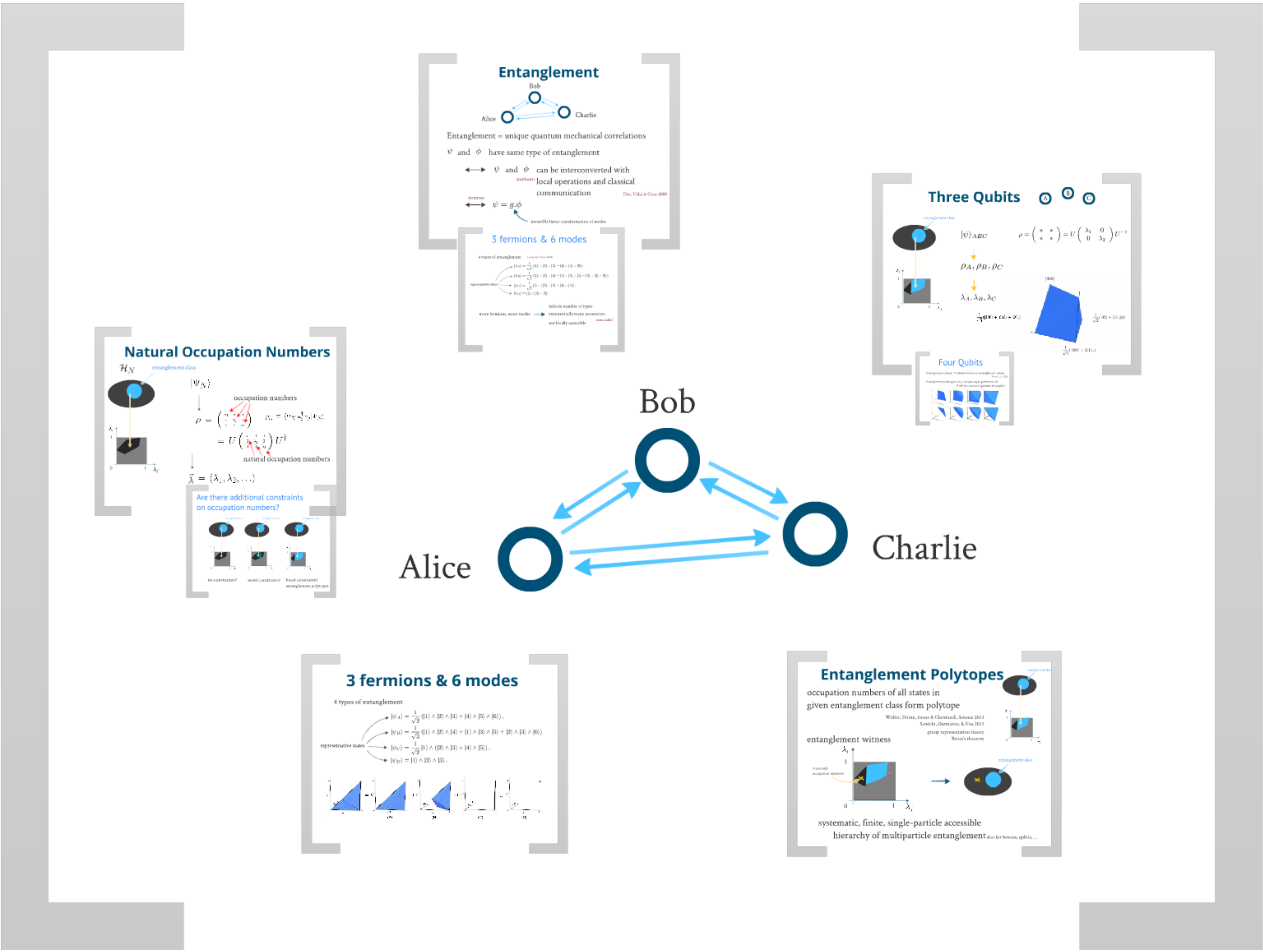
Entanglement classes: 9 infinite families of entanglement classes

Verstraete et al, 2002

Entanglement polytopes: 16 polytopes (up to permutation)

9 full-dimensional (genuine entangled)





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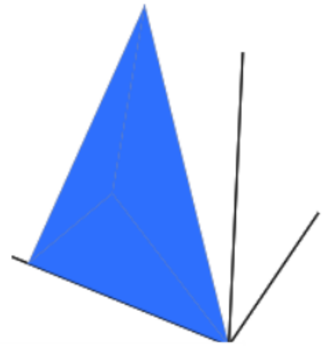
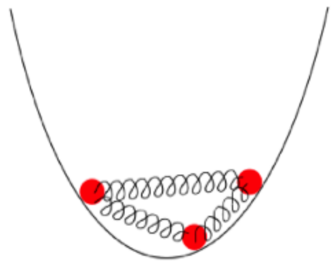
Summary

extended Pauli's principle



physically relevant?



pinned states have simple structure

entanglement polytopes