# Quantum Marginals, Entanglement, and Symmetries

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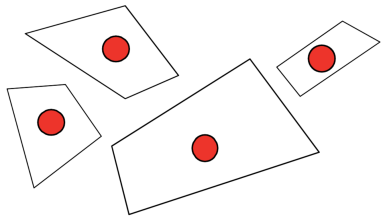
based on joint work with Bürgisser, Franks, Garg, Oliveira, Wigderson
(ITCS'18, FOCS'18, arXiv:1904.xxxxx)

# Summary of Results

Given density matrices $\rho_1$, ..., $\rho_N$, are they compatible with a global pure state $|\Psi\rangle_{1,\ldots,N}$?



Variations:

- bosons and fermions (e.g., Pauli principle: $\langle n_j \rangle \leq 1$)
- restrict to entanglement class (e.g., demand $|\Psi\rangle$ of GHZ type)

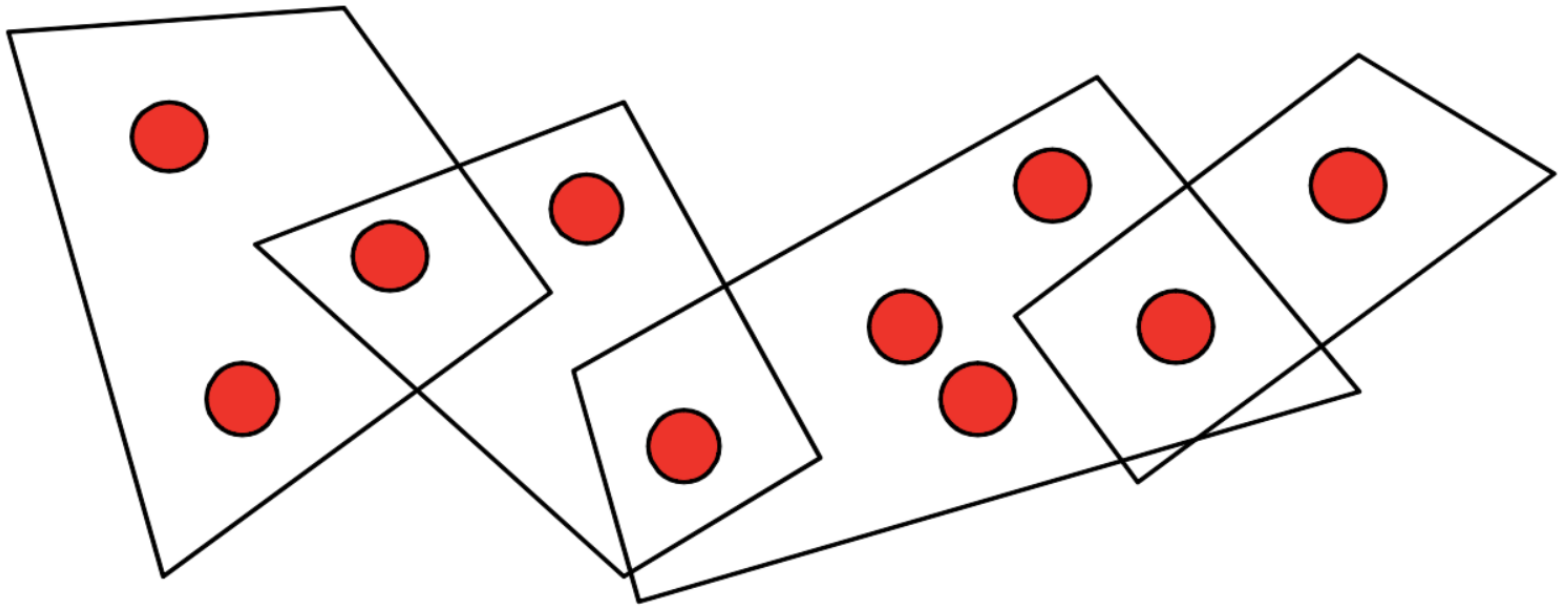
**Result (informal)**

Efficient algorithms to solve all these problems.

- prior to our work, only feasible for very small $d$, $N$

Rest of the talk: Motivation, algorithm, sketch of analysis.

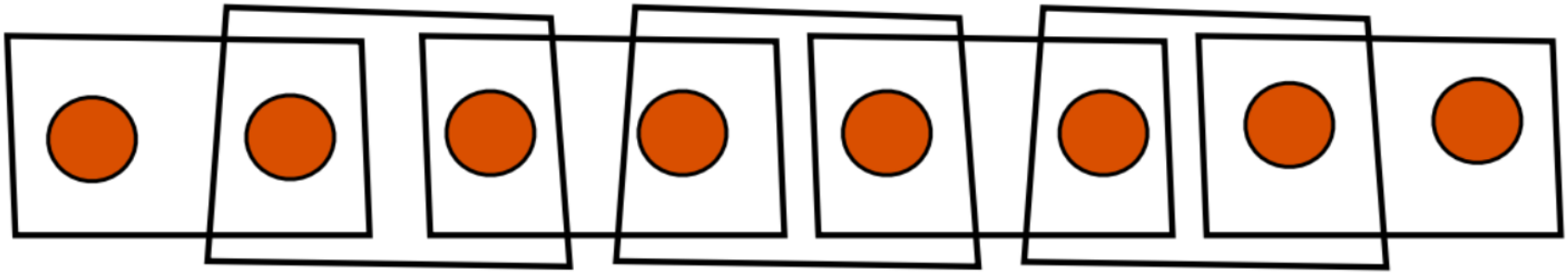
# The Quantum Marginal Problem



Fix subsets of particles $S_k \subseteq \{1,\ldots,N\}$. For each subset, given a density matrix $\rho_{S_k}$. Are they compatible with a global state $\rho_{1,\ldots,N}$?

$$\mathrm{tr}_{S_k^c}\left[\rho_{1,\ldots,N}\right] = \rho_{S_k}$$

# Quantum Marginals and Energy Minimization



Spin chain with nearest-neighbor interactions, $H = \sum_k h_{k,k+1}$:

$$E_0 = \min_{\rho_{1,\ldots,N}} \mathrm{tr}\left[H\rho_{1,\ldots,N}\right] = \min_{\rho_{1,\ldots,N}} \sum_k \mathrm{tr}\left[h_{k,k+1}\rho_{k,k+1}\right]$$

$$= \min_{\text{compatible } \{\rho_{k,k+1}\}} \sum_k \mathrm{tr}\left[h_{k,k+1}\rho_{k,k+1}\right]$$

Reduced minimization from exp. large Hilbert space to polynomially many variables...if we can solve quantum marginal problem!

# Quantum Marginals and Quantum Chemistry

REVIEWS OF MODERN PHYSICS VOLUME 35, NUMBER 3 JULY 1963

## Structure of Fermion Density Matrices

A. J. COLEMAN
*Queen's University, Kingston, Ontario, Canada*

### 1. INTRODUCTION

CAN the wave function be eliminated from quantum mechanics and its role be taken over, in the discussion of physical systems, by reduced density matrices? The author has believed in the affirmative answer to this question for over ten years. In the present paper, he attempts to muster the main current evidence in support of this belief. Prior to the Hylleraas Symposium, the available evidence, probably, would not have convinced the average physicist in the density matrix approach to the $N$-body problem stated, "It has frequently been pointed out that a conventional many-electron wave function tells us more than we need to know. . . . There is an instinctive feeling that matters such as electron correlation should show up in the two-particle density matrix . . . but we still do not know the conditions that must be satisfied by the density matrix. Until these conditions have been elucidated, it is going to be very difficult to make much progress along these lines."

In quantum chemistry, known as the *N*-representability problem:
When does a fermionic density matrix arise from *N*-fermion state?

# The Quantum Marginal Problem

☹ Computational complexity: QMA-complete, thus NP-hard [Liu]

☺ Partial understanding proved to be immensely useful:

- *Entropy inequalities*:

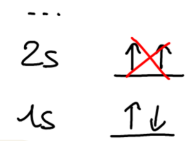
$$S(\rho_{12}) + S(\rho_{23}) \geq S(\rho_{123}) + S(\rho_2) \qquad \text{[Lieb-Ruskai]}$$

- *De Finetti and Monogamy*:

$$\rho_{AB_1} = \ldots = \rho_{AB_N} \overset{N \gg 1}{\Longrightarrow} \rho_{AB_i} \approx \text{unentangled} \qquad \text{[Doherty-Parrilo-Spedialeri]}$$

- *Pauli principle*:

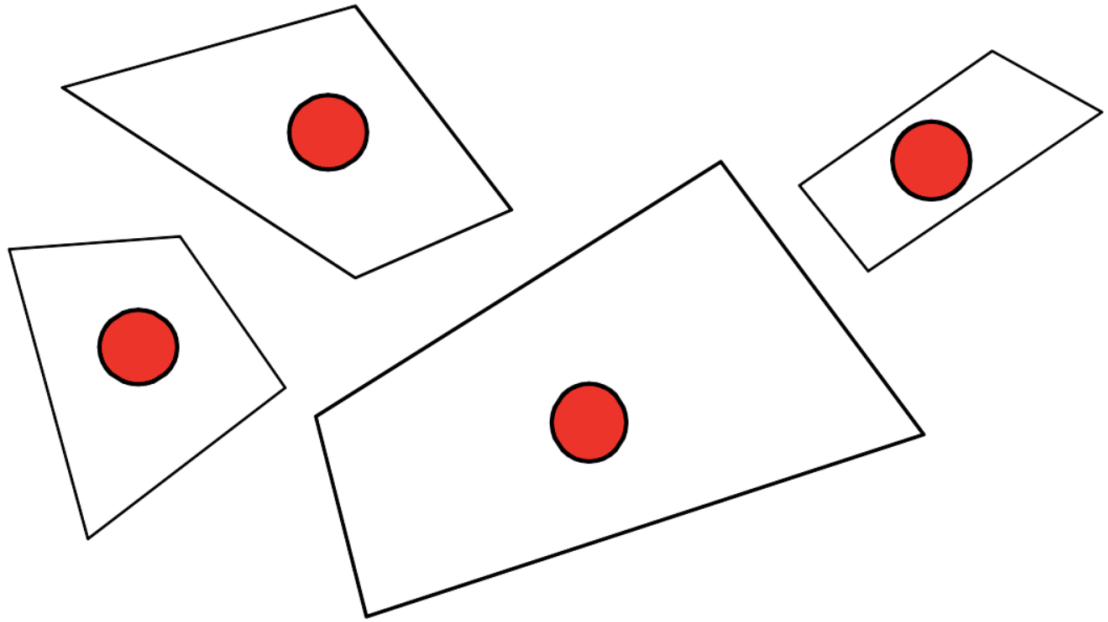
$$\langle n_j \rangle = \langle a_j^\dagger a_j \rangle \leq 1$$




A constraint on the one-body reduced density matrix!
What is the general picture?

Constraints are purely kinematic, arising from structure of q. state space.

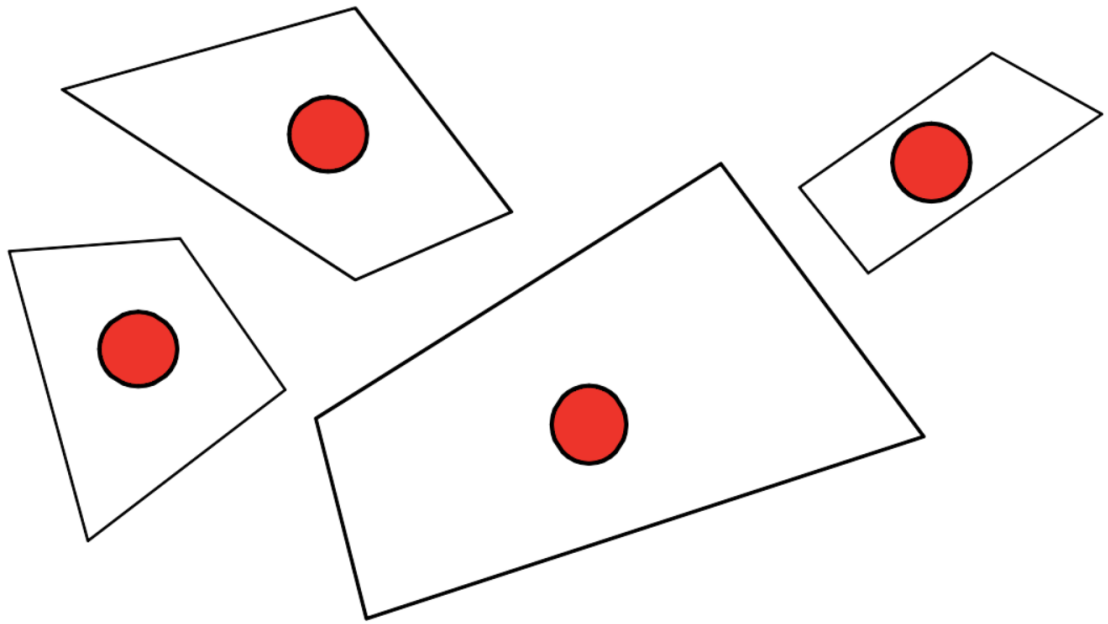
# Towards the One-Body Quantum Marginal Problem



Given density matrices $\rho_1$, ..., $\rho_N$ for each particle. Are they compatible with a global state $\rho_{1,\ldots,N}$?

Of course: $\rho_{1,\ldots,N} = \rho_1 \otimes \ldots \otimes \rho_N$! Also easy for bosons and fermions...

# The One-Body Quantum Marginal Problem



Given density matrices $\rho_1$, ..., $\rho_N$ for each particle. Are they compatible with a global pure state $|\Psi\rangle_{1,\ldots,N}$?

Answer only depends on eigenvalues $\lambda_k = (\lambda_{k,1} \geq \ldots \geq \lambda_{k,d})$ of $\rho_k$.

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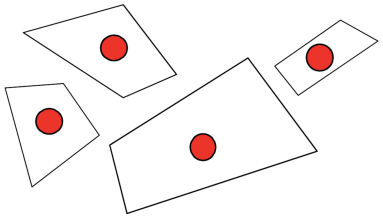
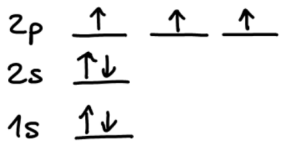
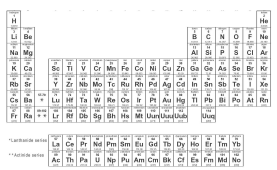


Why relevant? Ground states are pure!

Do they ever 'feel' these constraints? In some cases, yes!

- Pauli principle: $0 \leq \langle n_j \rangle \leq 1 \quad \Leftrightarrow \quad 0 \leq \langle j|\rho_1|j\rangle \leq 1/N$
- assuming $\langle n_j \rangle \approx 0,1$ leads to the *aufbau principle*!



[Wikipedia]

- general picture unclear

cf. recent investigations by Klyachko, Schilling-Christandl-Gross, Benavides-Riveros, ….

But what are the actual constraints?

# Examples

**Two particles:** $\rho_A$ and $\rho_B$ compatible iff same nonzero eigenvalues

- follows from Schmidt decomposition: $|\Psi\rangle_{AB} = \sum_j s_j |e_j\rangle \otimes |f_j\rangle$

**Three particles:**

$$\lambda_{A,\max} + \lambda_{B,\max} \leq \lambda_{C,\max} + 1$$
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- necessary and sufficient for qubits [Higuchi, Sudbery, Szulc]
- follows from variational principle: $\lambda_{A,\max} = \max_{\phi_A} \langle \phi_A | \rho_A | \phi_A \rangle$ etc.

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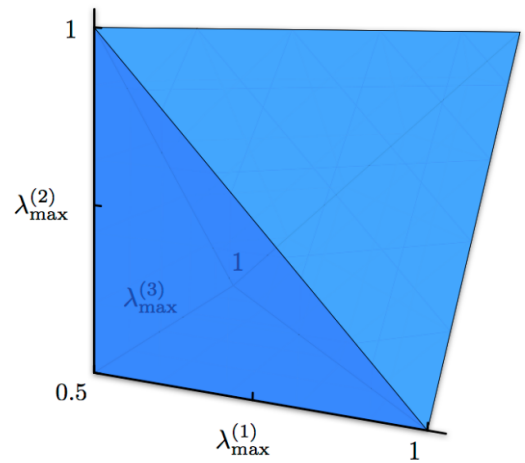


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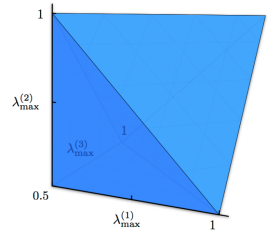
# Solution of the One-Body Quantum Marginal Problem

$$\Delta_{ABC} = \{(\lambda_A, \lambda_B, \lambda_C) \text{ compatible}\}$$



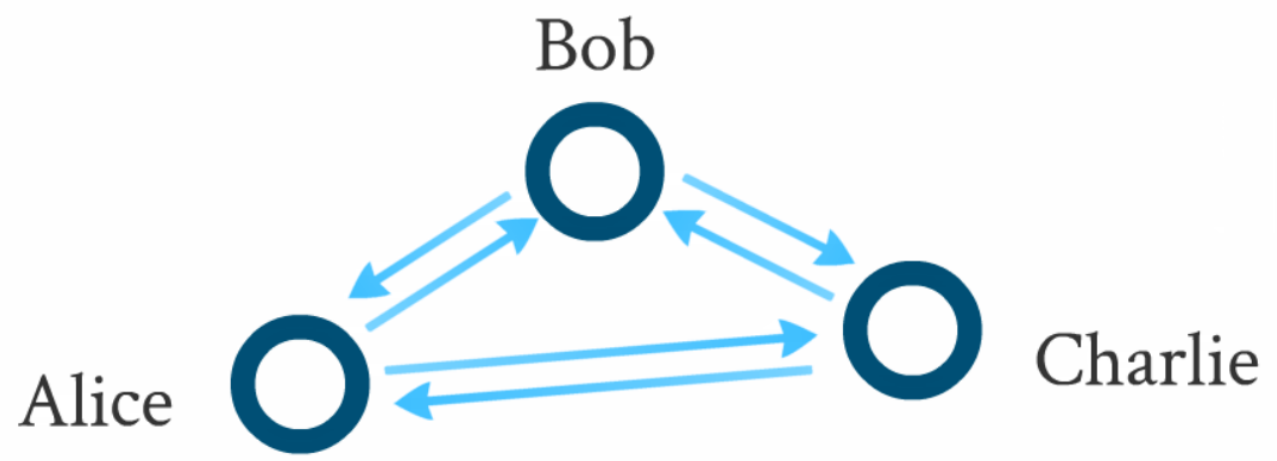

- always convex polytope [Mumford, Kirwan]
- linear inequalities known [Klyachko, Daftuar–Hayden, Berenstein–Sjamaar, Vergne-W]
- representation-theoretic description [Christandl–Mitchison, Mumford, Brion]

Known descriptions intractable beyond very small $N$, $d$. Main obstacle for applications to realistic systems. We provide algorithmic solution:

**Result (informal)**

Efficient algorithm for deciding if $\lambda_A, \lambda_B, \lambda_C$ compatible (i.e., in $\Delta_{ABC}$).

# Multi-Particle Entanglement




$|\Psi\rangle_{ABC}$ is entangled iff $|\Psi\rangle_{ABC} \neq |\psi\rangle_A \otimes |\psi\rangle_B \otimes |\psi\rangle_C$.

Operational approach:

$|\Psi\rangle$ and $|\Phi\rangle$ have same type of entanglement

$\Leftrightarrow$ can be interconverted by some set of operations that do not create entanglement

difficult to handle directly (exp. many continuous parameters)

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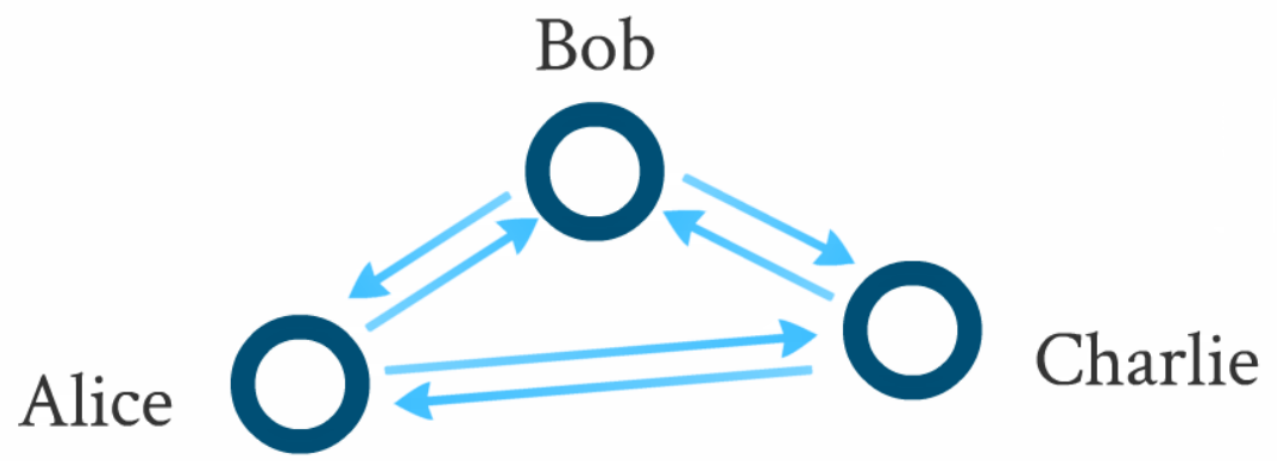


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Operational approach:

$|\Psi\rangle$ and $|\Phi\rangle$ have same type of entanglement

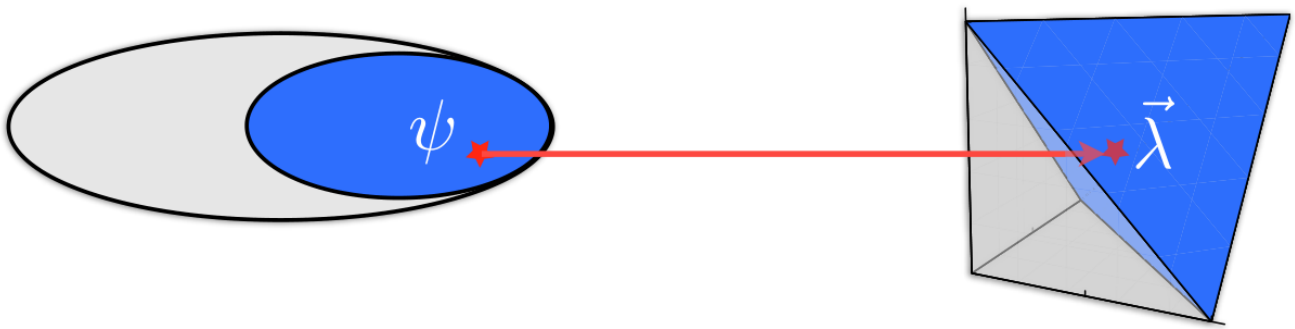
$\Leftrightarrow$ can be interconverted by stochastic local operations and classical communication (SLOCC)

$\Leftrightarrow$ $|\Psi\rangle = (A \otimes B \otimes C)|\Phi\rangle$ for invertible $A$, $B$, $C$ [Dür-Vidal-Cirac]

difficult to handle directly (exp. many continuous parameters)

# Qantum Marginals and Entanglement

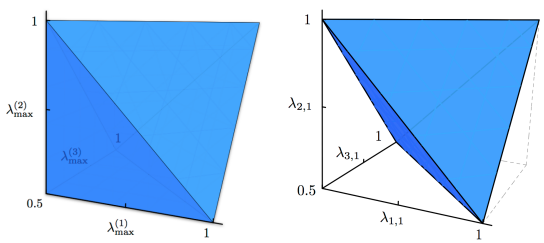
Given density matrices $\rho_1, \ldots, \rho_N$, are they compatible with state in given entanglement class $\mathscr{C}$?



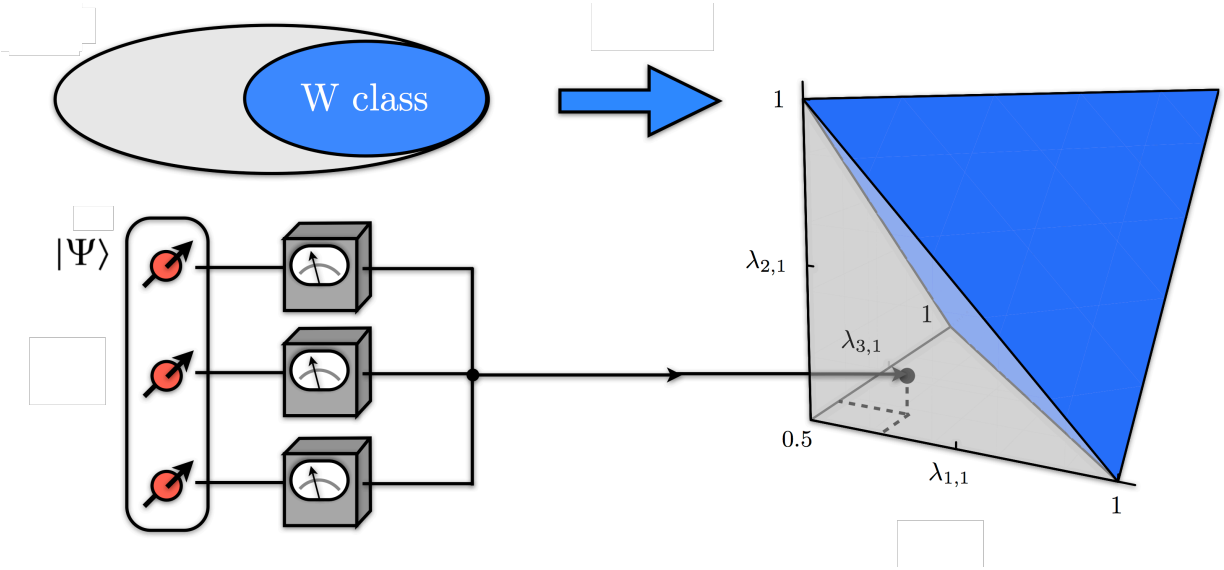

$$\Delta(\mathscr{C}) = \{(\lambda_A, \lambda_B, \lambda_C) \text{ compatible with state in class } \mathscr{C}\}$$

- finite hierarchy of entanglement polytopes [W-Christandl-Doran-Gross]
- contain all local information of global entanglement

*e.g., for three qubits,* $|\mathrm{GHZ}\rangle = |000\rangle + |111\rangle$ *and* $|\mathrm{W}\rangle = |100\rangle + |010\rangle + |001\rangle$*:*



# Inequalities for Multi-Particle Entanglement




$$(\lambda_A, \lambda_B, \lambda_C) \notin \Delta(\mathscr{C}) \Rightarrow \Psi \notin \mathscr{C}$$

- efficient, robust against small noise
- realized in two quantum optics experiments [Aguilar et al, Zhao et al]

Known descriptions of $\Delta(\mathscr{C})$ intractable beyond very small $N$, $d$.

**Result (informal)**

Efficient algorithm for deciding if $\lambda_A, \lambda_B, \lambda_C$ compatible with class.

# The Algorithm

Given $\lambda_A$, $\lambda_B$, $\lambda_C$ and reference state $|\Phi\rangle$, want $|\Psi\rangle = (A \otimes B \otimes C)|\Phi\rangle$ with these marginals. For simplicity, uniform marginals ($\lambda_A \propto 1_A$ etc).

**Algorithm:** Start with $|\Psi\rangle = |\Phi\rangle$. For $t = 1, \ldots, T$:
Compute marginals $\rho_A$, $\rho_B$, $\rho_C$ of $|\Psi\rangle$. If $\varepsilon$-close to uniform, stop.
Otherwise, replace $|\Psi\rangle$ by $e^{-c(\rho_A^o + \rho_B^o + \rho_C^o)}|\Psi\rangle$. *$X^o$ = traceless part*

## Result

Algorithm finds $|\Psi\rangle = (A \otimes B \otimes C)|\Phi\rangle$ with marginals $\varepsilon$-close to uniform within $T = \mathrm{poly}(\frac{1}{\varepsilon}, \text{input size})$ steps.

- also works for bosons, fermions, $N > 3$ subsystems, MPS, ...
- can run on quantum computer
- solve quantum marginal problem by using random $|\Phi\rangle$

cf. algorithm by Verstraete et al (w/o rigorous analysis)

# Why does it work?

"Otherwise, replace $|\Psi\rangle$ by $e^{-c(\rho_A^o+\rho_B^o+\rho_C^o)}|\Psi\rangle$."

This step implements gradient descent for the function

$$F(A,B,C) = \frac{1}{2}\|(A\otimes B\otimes C)|\Psi\rangle\|^2$$

where $A,B,C$ have det=1. Indeed, for traceless $H_A,\dots,H_C$:

$$\partial_{t=0} F(e^{tH_A}, e^{tH_B}, e^{tH_C}) = \mathrm{tr}[\rho_A^o H_A] + \mathrm{tr}[\rho_B^o H_B] + \mathrm{tr}[\rho_C^o H_C]$$

- gradient vanishes iff marginals uniform
- convexity: $\partial_t^2 \geq 0$, so critical points are global minima
- $|\Phi\rangle$ can be transformed to uniform iff $\inf_{\det=1} F(A,B,C) > 0$

'Physics' in the normalization of the wave function! ☺

General fact: $G \to [0,\infty), g \mapsto \frac{1}{2}\|g\cdot v\|^2$ is geodesically (log-)convex. [Kempf-Ness]

# Analysis of Algorithm

To turn this into a rigorous algorithm, show:

- *progress in each step:* $\|e^{-c(\rho_A^o+\rho_B^o+\rho_C^o)}|\Psi\rangle\| \leq (1-c\varepsilon)\|\Psi\|$
- *a priori lower bound:* $\inf_{\det=1}\|(A\otimes B\otimes C)|\Phi\rangle\| \geq Z$

Then, $(1-c\varepsilon)^T \geq Z$ bounds the number of steps $T$.

The first point follows from local convexity bounds.

For the second, use invariant theory: $\inf > 0$ iff exists invariant polynomial $P$ such that $P(\Phi) \neq 0$.

We construct 'explicit' polynomials with 'nice' coefficients to obtain quantitative bound in terms of bitsize of $|\Phi\rangle$.

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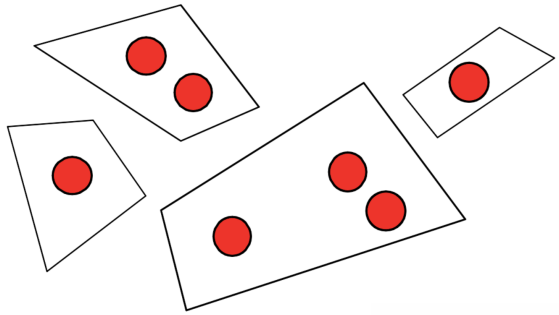
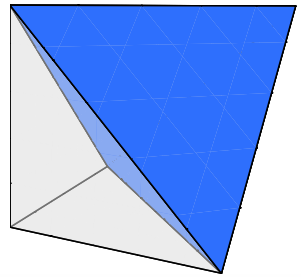
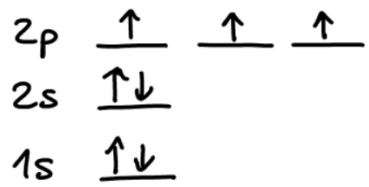
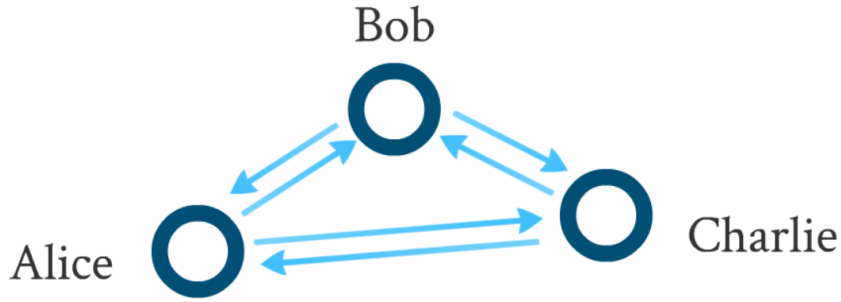
# Summary and Outlook








- efficient algorithms for one-body quantum marginal problem (incl. fermions) and entanglement polytopes
- based on convex optimization and geometric invariant theory
- opens up possibility for numerically studying quantum marginals in many-body systems and larger atoms or molecules

*Thank you for your attention!*