# The Quantum Marginal Problem, Entanglement Polytopes and Pauli's Principle 

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joint work with
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## The Quantum Marginal Problem



Fix subsets of the particles $S_{i} \subseteq\{1, \ldots, N\}$

For each subset, given a density matrix $\rho_{S_{i}}$
Are these compatible? $\exists \rho_{[N]}: \operatorname{tr}_{[N] \backslash S_{i}} \rho_{[N]}=\rho_{S_{i}}$ ?


## The Quantum Marginal Problem

- studied since beginnings of quantum theory
- computionally difficult QMA-complete (Liu, 2006) $\Rightarrow$ NP-hard
- fermionic version, N -representability problem quantum chemistry
QMA-complete (Liu, Ch.\& Verstraete, 2007)
- partial understanding Pauli principle
 Entropy inequalities

$$
S\left(\rho_{12}\right)+S\left(\rho_{23}\right) \geq S\left(\rho_{2}\right)+S\left(\rho_{123}\right)
$$

(Lieb\& Ruskai I973, Pippenger 2003)


Collection of subsets of a set of particles (overlapping)


Collection of subsets of a set of particles (non-overlapping)

Fix subsets of the particles

For each subset, given a density matrix

$$
S_{i} \cap S_{j}=\emptyset
$$

what if required to be pure?

Are these compatible? $\exists \rho_{[N]}: \operatorname{tr}_{[N] \backslash S_{i}} \rho_{[N]}=\rho_{S_{i}}$ ?

## One-Body Quantum Marginal Problem


compatible: $\quad \operatorname{tr}_{[N] \backslash i}|\psi\rangle\langle\psi|=\rho_{i}$
Then $\quad \tilde{\rho}_{i}:=u_{i} \rho_{i} u_{i}^{\dagger}$ compatible: $\quad \operatorname{tr}_{[N] \backslash i}|\tilde{\psi}\rangle\langle\tilde{\psi}|=\tilde{\rho}_{i}$

$$
\left(\widehat{\psi \psi\rangle}:=u_{1} \otimes \cdots \otimes u_{N}|\psi\rangle\right.
$$

$\Rightarrow$ compatibility constraints

$$
\lambda^{(i)}=\left(\lambda_{1}^{\left.\lambda_{1}^{(i)} \geq \lambda_{2}^{(i)} \geq \ldots \geq \lambda_{d}^{(i)}, \ldots, \lambda_{d}^{(i)}\right) \in \mathbb{R}^{d-1}}\right.
$$

Shape of set of admissible $\quad \lambda=\left(\lambda^{(1)}, \cdots, \lambda^{(N)}\right) \in \mathbb{R}^{m}$ ?

## Eigenvalue Polytopes



## Eigenvalue Polytopes

$$
\begin{aligned}
U\left(d_{A}\right) \times U\left(d_{B}\right) \times U\left(d_{C}\right) & \rightarrow U\left(d_{A} d_{B} d_{C}\right) \\
\left(u_{A}, u_{B}, u_{C}\right) & \mapsto u_{A} \otimes u_{B} \otimes u_{C} \\
\mathfrak{u}\left(d_{A}\right) \times \mathfrak{u}\left(d_{B}\right) \times \mathfrak{u}\left(d_{C}\right) & \rightarrow \mathfrak{u}\left(d_{A} d_{B} d_{C}\right)
\end{aligned}
$$



Image of coadjoint orbit restricted to positive Weyl chamber is convex polytope

$$
\left(\lambda_{A}, \lambda_{B}, \lambda_{C}\right) \hookleftarrow\left(\rho_{A}, \rho_{B}, \rho_{C}\right) \leftarrow|\psi\rangle\left\langle\left.\psi\right|_{A B C}\right.
$$

$$
N=2
$$

$$
|\psi\rangle_{A B}=\sum_{j} s_{j}\left|e_{j}\right\rangle_{A}\left|f_{j}\right\rangle_{B}
$$

$$
\left.\Rightarrow \quad \lambda_{j}^{A}=s_{j}^{2}=\lambda_{j}^{B} \xrightarrow\left[{\left.\frac{1}{\sqrt{2}} \right\rvert\, 00+11}\right\rangle\right]{\substack{|00\rangle}} \begin{aligned}
& d=2 \\
& \lambda_{1}^{A} \geq \lambda_{2}^{A} \\
& \lambda_{1}^{A}
\end{aligned}
$$



## $N=3 d=2 \quad$ Higuchi, Sudbery\& Szulc 2003


$\lambda_{1}^{A}+\lambda_{1}^{B} \leq 1+\lambda_{1}^{C} \quad$ and cyclic


3 fermions in 6 modes $\mathcal{H}=\Lambda^{3}\left(\mathbf{C}^{6}\right)$
e.g. electrons hopping on 3 sites
$\lambda_{1} \geq \lambda_{2} \geq \ldots \geq \lambda_{6}$ one-particle eigenvalues $\sum_{i} \lambda_{i}=3$

## Pauli 1924

$\lambda_{1} \leq 1$

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occupation
``` numbers in natural orbitals

Dennis \& Borland 1970
\(\lambda_{1}+\lambda_{6}=1\)
\(\lambda_{2}+\lambda_{5}=1\)
\(\lambda_{3}+\lambda_{4}=1\)
\(\lambda_{5}+\lambda_{6} \geq \lambda_{4}\)


\section*{Entanglement}
state transformations
\[
\psi_{A B C} \mapsto \psi_{A B C}^{\prime}
\]

LOCC: local operations and classical communication
- well-motivated
- complicated definition
- two parties solved (Nielsen majorisation)
- three or more parties: unsolved (MREGS?)

SLOCC: stochastic LOCC
- positive success probability (length doesn't matter)
- easy characterisation
\[
\psi _ { A B C } \mapsto \psi _ { A B C } ^ { \prime } = g _ { a } \longdiv { \otimes g _ { b } \overparen { g _ { c } \psi _ { A B C } } }
\]

\section*{Entanglement}
entanglement class: set of states \(\psi_{A B C} \leftrightarrow \psi_{A B C}^{\prime}\)
entanglement class \(=\) orbit of \(\operatorname{SL}\left(d_{A}\right) \times \operatorname{SL}\left(d_{B}\right) \times \operatorname{SL}\left(d_{C}\right)\)
3 qubits, 6 orbits: fully separable \(|000\rangle\)
\[
\begin{array}{ll}
\text { biseparable } & \frac{1}{\sqrt{2}}|00+11\rangle|0\rangle \\
\text { and permutations }
\end{array}, \begin{aligned}
& \frac{1}{\sqrt{2}}|000+111\rangle \\
& \mathrm{GHZ} \\
& \mathrm{~W}
\end{aligned} \frac{\frac{1}{\sqrt{3}}(|001+010+100\rangle)}{}
\]

4 qubits, infinite number of orbits
n qubits/fermions, \(\exp (\mathrm{O}(\mathrm{n}))\) many parameters intractable!

\section*{Entanglement Polytopes state \(\quad \psi \mapsto \lambda\) local} eigenvalues

convex polytope: entanglement polytope
Brion convexity theorem for moment map
Walter, Doran, Gross, Ch. 2012
subpolytope of quantum marginal polytope
computation using representation theory (difficult)
Entanglement criterion: local eigenvalues not in polytope, implies state is not in corresponding entanglement class

\title{
Entanglement Polytopes
} local state \(\quad \psi \mapsto \lambda\) eigenvalues


Entanglement criterion: local eigenvalues not in polytope, implies state is not in corresponding entanglement class
uses local information only
finite number of polytopes
robust against experimental noise

\section*{Entanglement Polytopes: 3 qubits}

\[
\frac{1}{\sqrt{2}}|000+111\rangle
\]
\[
\frac{1}{\sqrt{3}}|001+010+100\rangle
\]
\[
\begin{aligned}
& \frac{1}{\sqrt{2}}|0\rangle|00+11\rangle \\
& \quad \frac{1}{\sqrt{2}}|00+11\rangle|0\rangle
\end{aligned}
\]
\[
|000\rangle
\]

\section*{Entanglement Polytopes: 3 qubits}

(a)


Entanglement criterion point is not in W polytope (and not in fully or biseparable ones) cannot be in W-class (and not in fully or biseparable ones) must be entangled of GHZ type

\section*{Entanglement Polytopes: 4 qubits}

polytope explorer @ http://polytopes.leetspeak.org/

\section*{Entanglement Polytopes: 3 fermions in 6 modes}


\section*{Summary}
- The Quantum Marginal Problem computationally difficult

- One-Body Quantum Marginal Problem eigenvalue inequalities

- Entanglement Polytopes (arxiv: I 208.0365, Walter et al.)
- Pinning of Fermionic Occupation Numbers (arxiv. 12 I 0.553 I, to appear in PRL, Schilling et al.)

talk to me about relation to entropy inequalities representation theory P vs NP problem
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