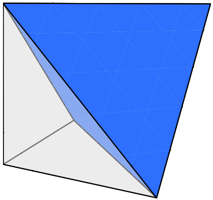
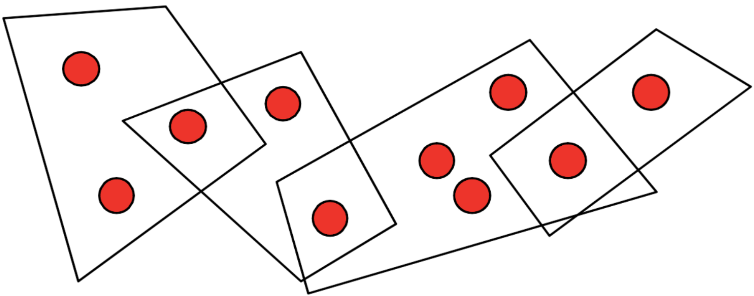


The Quantum Marginal Problem

Michael Walter & Matthias Christandl
(ETH Zürich)

Berlin, March 2014

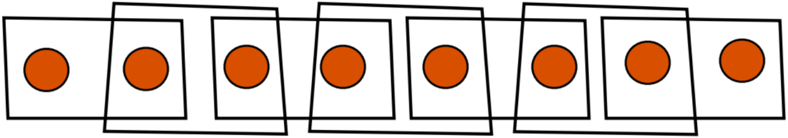
The Quantum Marginal Problem



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

$$\exists \rho_{1,\ldots,N} : \ \operatorname{tr}_{S_k^c} \rho_{1,\ldots,N} = \rho_{S_k}$$

The Quantum Marginal Problem



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

$$E_0 = \min_{\rho_{1,\dots,N}} \operatorname{tr} H \rho_{1,\dots,N} = \min_{\rho_{1,\dots,N}} \sum_k \operatorname{tr} h_{k,k+1} \rho_{k,k+1}$$

$$= \min_{\text{compatible } \{\rho_{k,k+1}\}} \sum_k \operatorname{tr} h_{k,k+1} \rho_{k,k+1}$$

- exponentially large Hilbert space
- reduced optimization to polynomially many variables…
- …if we can solve the Quantum Marginal Problem!

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 physi-

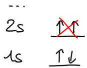
terest in the density matrix approach to the N-body problem stated, "It has frequently been pointed out that a conventional many-electron wave function tells us more than we need to know. . . . There is an instinctive feeling that matters such as electron correlation should show up in the two-particle 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."

The Quantum Marginal Problem

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

- ☺ Partial understanding proved to be immensely useful:
  - Pauli principle:

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



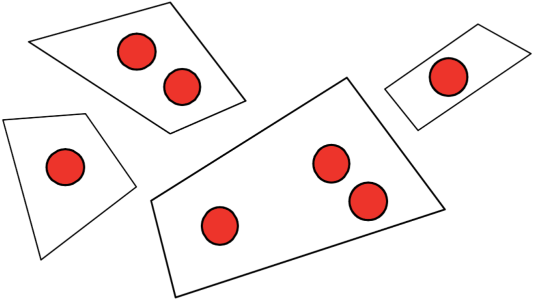
  - Entropy inequalities:

$$S(\rho_{12}) + S(\rho_{23}) \geqslant S(\rho_{123}) + S(\rho_2)$$ [Lieb–Ruskai]

These correlations are purely due to the structure of the state space (kinematic rather than dynamic).

The One-Body Quantum Marginal Problem

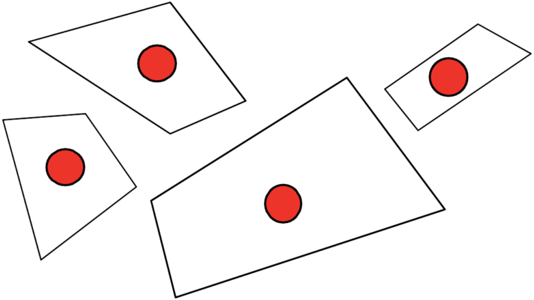
Towards the One-Body Quantum Marginal Problem



- Fix non-overlapping subsets of particles $S_k \cap S_l = \emptyset$.
- For each subset, given a density matrix ρ_{S_k}.
- Are they compatible with a global state?

$$\exists \rho_{1,\dots,N} : \operatorname{tr}_{S_k^c} \rho_{1,\dots,N} = \rho_{S_k}$$

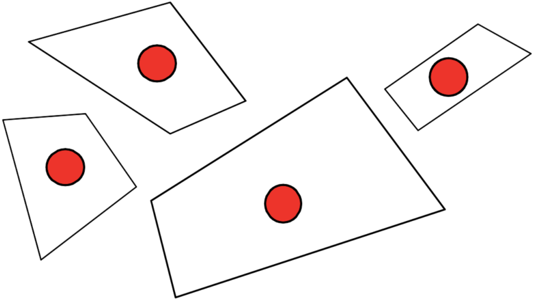
Towards the One-Body Quantum Marginal Problem



- Given density matrices $\rho_1, \ldots, \rho_N$.
- Are they compatible with a global state?

$$\exists \rho_{1,\ldots,N} \colon \operatorname{tr}_{1,\ldots,\check{k},\ldots,N} \rho_{1,\ldots,N} = \rho_k$$

Towards the One-Body Quantum Marginal Problem

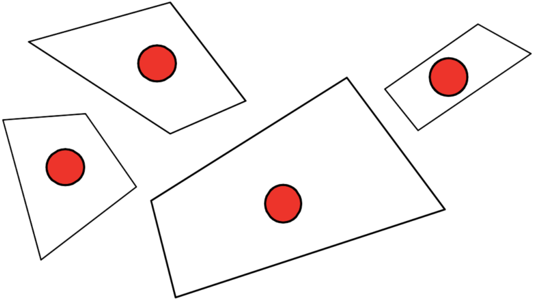


- Given density matrices $\rho_1, \ldots, \rho_N$.
- Are they compatible with a global state?

$$\exists \rho_{1,\ldots,N} : \operatorname{tr}_{1,\ldots,\check{k},\ldots,N} \rho_{1,\ldots,N} = \rho_k$$

- Yes: $\rho_{1,\ldots,N} = \rho_1 \otimes \ldots \otimes \rho_N$!

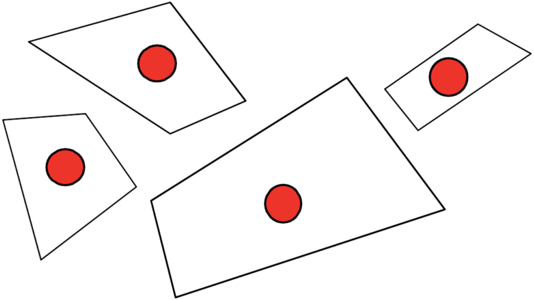
The One-Body Quantum Marginal Problem



- Given density matrices $\rho_1, \ldots, \rho_N$.
- Are they compatible with a global pure state?

$$\exists \, |\psi\rangle_{1,\ldots,N} : \operatorname{tr}_{1,\ldots,\check{k},\ldots,N} \psi_{1,\ldots,N} = \rho_k$$

The One-Body Quantum Marginal Problem



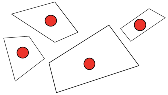
- Given density matrices $\rho_1, \ldots, \rho_N$.
- Are they compatible with a global pure state?

$$\exists\, |\psi\rangle_{1,\ldots,N} : \operatorname{tr}_{1,\ldots,\check{k},\ldots,N} \psi_{1,\ldots,N} = \rho_k$$

- Only depends on eigenvalues $\vec{\lambda}_k = (\lambda_{k,1}, \ldots, \lambda_{k,d})$ of the density matrices ρ_k!

The One-Body Quantum Marginal Problem

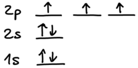
Given density matrices $\rho_1, \ldots, \rho_N$, are they compatible with a global pure state $|\psi\rangle_{1,\ldots,N}$?

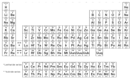


- Energy minimum is attained at global pure state.

But does the ground state ever feel these constraints?
Empirically, yes!

- Pauli principle: $0 \leqslant \langle a_j^\dagger a_j \rangle \leqslant 1 \Leftrightarrow 0 \leqslant \langle j|\rho_1|j\rangle \leqslant 1/N$
- Assuming $\langle a_j^\dagger a_j \rangle \approx 0, 1$ leads to the *Aufbau principle*!





[Wikipedia]

See [Klyachko, Schilling–Christandl–Gross] for more recent investigations.

But what are the actual constraints?

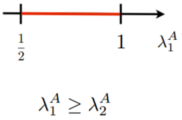
Warmup: Two Particles $N = 2$

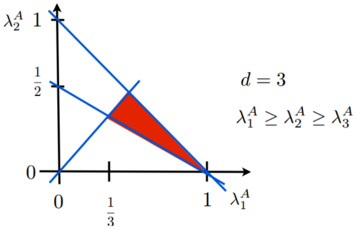
Schmidt decomposition (singular value decomposition):

$$|\psi\rangle_{AB} = \sum_j s_j\, |e_j\rangle \otimes |f_j\rangle$$

$$\Rightarrow \rho_A = \sum_j |s_j|^2\, |e_j\rangle\langle e_j| \quad \text{and} \quad \rho_B = \sum_j |s_j|^2\, |f_j\rangle\langle f_j|$$

Necessary and sufficient: $\vec{\lambda}_A = \vec{\lambda}_B$

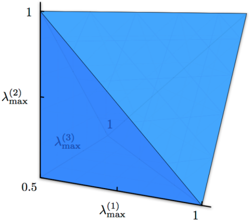




Three Qubits $N = 3,\ d = 2$

Higuchi, Sudbery, Szulc:

$$\lambda_{A,1} + \lambda_{B,1} \leqslant \lambda_{C,1} + 1$$
$$\lambda_{A,1} + \lambda_{C,1} \leqslant \lambda_{B,1} + 1$$
$$\lambda_{B,1} + \lambda_{C,1} \leqslant \lambda_{A,1} + 1$$

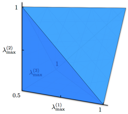


Proof (variational principle, inclusion/exclusion):

$$\begin{aligned}
\lambda_{A,1} + \lambda_{B,1} &= \max_{|\phi\rangle_A, |\phi\rangle_B} \operatorname{tr} \rho_A |\phi\rangle\langle\phi|_A + \operatorname{tr} \rho_B |\phi\rangle\langle\phi|_B \\
&= \max_{|\phi\rangle_A, |\phi\rangle_B} \operatorname{tr} \rho_{AB} \left(|\phi\rangle\langle\phi|_A \otimes I_B + I_A \otimes |\phi\rangle\langle\phi|_B\right) \\
&\leqslant \max_{|\phi\rangle_A, |\phi\rangle_B} \operatorname{tr} \rho_{AB} \left(I_{AB} + |\phi\rangle\langle\phi|_A \otimes |\phi\rangle\langle\phi|_B\right) \\
&\leqslant 1 + \max_{|\phi\rangle_{AB}} \operatorname{tr} \rho_{AB} |\phi\rangle\langle\phi|_{AB} = 1 + \lambda_{AB,1} = 1 + \lambda_{C,1} \qquad \square
\end{aligned}$$

Solution of the One-Body Quantum Marginal Problem

$$\Delta = \left\{ (\vec{\lambda}_A, \vec{\lambda}_B, \vec{\lambda}_C) \text{ compatible} \right\}$$



- Always convex polytope [Kirwan]
- Linear inequalities: [Klyachko, Daftuar–Hayden; Berenstein–Sjamaar]

$$\sum_i a_{\pi(i)} \lambda_{A,i} + \sum_j b_{\tau(j)} \lambda_{B,j} \leqslant \sum_k c_{\sigma(k)} \lambda_{C,k}$$

whenever $[\pi]_a \otimes [\tau]_b \cap \iota^* [\sigma]_c \neq 0 \in H^*$.

algebraic geometry
Schubert calculus

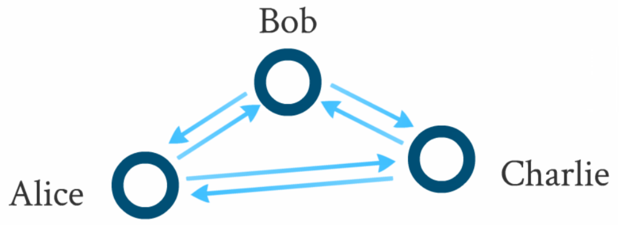
- Representation theory: [Christandl–Mitchison; Mumford, Brion]

$$\Delta_{\mathbb{Q}} = \{ (\alpha, \beta, \gamma)/n : g_{\alpha,\beta,\gamma} \geqslant 0 \}$$

where $g_{\alpha,\beta,\gamma}$ are the Kronecker coefficients.

Quantum Marginals vs. Entanglement

Multi-Particle Entanglement



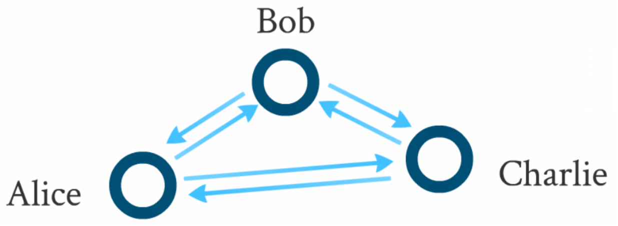
$|\psi\rangle_{ABC}$ is entangled iff $|\psi\rangle_{ABC} \neq |\psi\rangle_A \otimes |\psi\rangle_B \otimes |\psi\rangle_C$.

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

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 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]

Three Qubits $N = 3,\ d = 2$

Six classes of entanglement: [Dür–Vidal–Cirac]

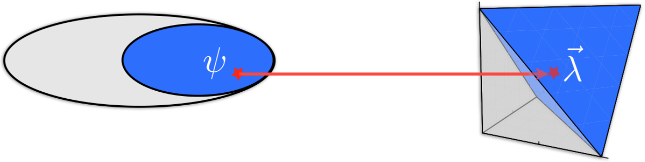
$$|\mathrm{GHZ}\rangle = |000\rangle + |111\rangle$$
$$|\mathrm{W}\rangle = |100\rangle + |010\rangle + |001\rangle$$
$$|\mathrm{B}_1\rangle = |0\rangle \otimes (|00\rangle + |11\rangle), \quad |\mathrm{B}_2\rangle\,, \quad |\mathrm{B}_3\rangle$$
$$|\mathrm{Sep}\rangle = |000\rangle$$

Larger systems:

- infinitely many classes ☹
- exponentially many parameters ☹
- not locally accessible ☹

Quantum Marginals and Entanglement

Given density matrices $\rho_1, \ldots, \rho_N$, are they compatible with a given class of entanglement?



$$\Delta_{\mathcal{C}} = \{(\vec{\lambda}_A, \vec{\lambda}_B, \vec{\lambda}_C) \text{ for } \psi \in \overline{\mathcal{C}}\}$$

Theorem (Walter–Christandl–Doran–Gross)

- *Finite hierarchy of convex polytopes!*
- *Computation via computational invariant theory (difficult)*

Proof using results from algebraic geometry [Mumford, Brion, Kempf–Ness]; cf. [Sawicki–Oszmaniec–Kús]

Three Qubits $N = 3,\ d = 2$

Six classes of entanglement: [Dür–Vidal–Cirac]

$$
\begin{aligned}
|\mathrm{GHZ}\rangle &= |000\rangle + |111\rangle \\
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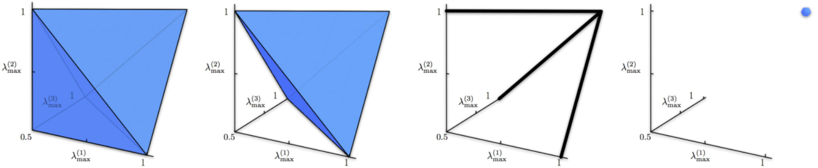
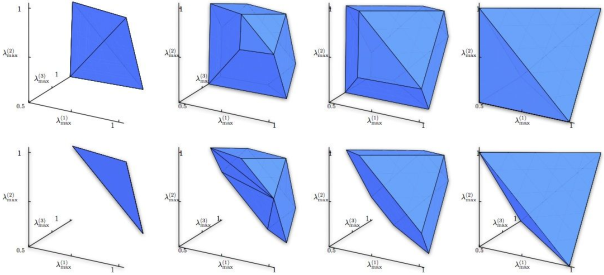
|\mathrm{Sep}\rangle &= |000\rangle
\end{aligned}
$$

Entanglement polytopes:



Further Examples

- Four qubits: six non-trivial polytopes



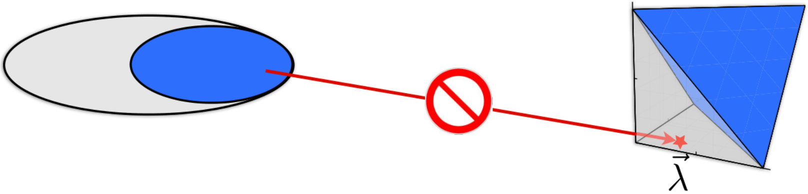
- Bosonic and fermionic systems

  `http://www.entanglement-polytopes.org`

- Genuine multi-particle entanglement:

$$\Delta \supsetneq \bigcup_{S:S^c} \Delta_S \times \Delta_{S^c}$$

Entanglement Criterion



$$(\vec{\lambda}_A, \vec{\lambda}_B, \vec{\lambda}_C) \notin \Delta_{\mathcal{C}} \quad \Rightarrow \quad \psi \notin \mathcal{C}$$

- efficient, requires only linearly many measurements
- robust against small noise, $\psi \approx$ pure

Cf. geometric complexity theory approach to VP vs. VNP.

Geometric Invariant Theory

Suppose that P is a G-invariant homogeneous polynomial on $\mathcal{H}$ with $P(|\psi\rangle) \neq 0$.

$$\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d \otimes \mathbb{C}^d$$
$$G = \mathrm{SL}(d) \times \mathrm{SL}(d) \times \mathrm{SL}(d)$$

Geometric Invariant Theory

Suppose that P is a G-invariant homogeneous polynomial on $\mathcal{H}$ with $P(|\psi\rangle) \neq 0$.

$$\Rightarrow \overline{G \cdot |\psi\rangle} \not\ni 0$$

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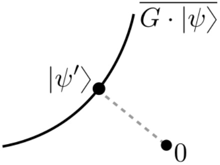

Let $|\psi'\rangle$ be a vector of minimal length.

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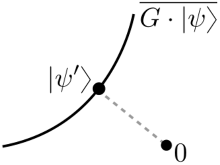

$$\Rightarrow \overline{G \cdot |\psi\rangle} \not\ni 0$$

Let $|\psi'\rangle$ be a vector of minimal length. Then

$$0 = \frac{d}{dt}\Big|_{=0} \| e^{tX} \cdot |\psi'\rangle \|^2 = 2 \langle \psi' | X | \psi' \rangle$$

for all traceless local observables $X \in \mathfrak{g}$.

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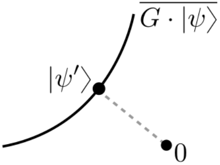

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Thus $|\psi'\rangle$ is locally maximally mixed: $\vec{\lambda}_A = \vec{\lambda}_B = \vec{\lambda}_C \equiv 1/d$

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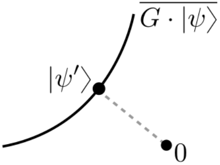

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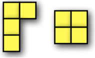
Invariant Theory $\Leftrightarrow$ Local Eigenvalues [Kempf–Ness, Klyachko]

Computing Entanglement Polytopes

Covariant: G-equivariant homogeneous polynomial

$$\Phi \colon \mathcal{H} \to V_\lambda$$

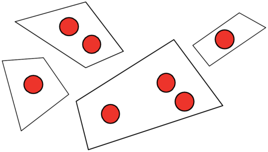


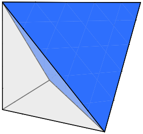
where V_λ is an G-irrep with highest weight λ.

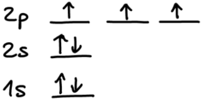
- Find a finite set of generators Φ_i with highest weights λ_i and degree d_i.
- Then the entanglement polytope of a class $\mathcal{C}_\psi$ is given by

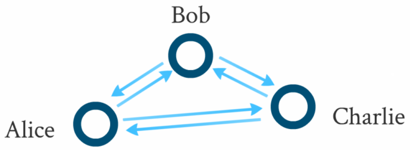
$$\Delta_\psi = \operatorname{conv} \left\{ \vec{\lambda}_i / d_i : \Phi_i(\psi) \neq 0 \right\}.$$

Simultaneously coarser and finer than polynomial invariants!









Thanks for your attention!

Walter, Doran, Gross, Christandl, *Entanglement Polytopes*, Science **340** (6137), 1205–1208 (2013)