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 $\rho_1, \ldots, \rho_N$, 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 $\rho_{1,\ldots,N}$?

\[ \text{tr}_{S_k^c}[\rho_{1,\ldots,N}] = \rho_{S_k} \]
Quantum Marginals and Energy Minimization

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

$$E_0 = \min_{\rho_1,\ldots,N} \operatorname{tr}[H\rho_1,\ldots,N] = \min_{\rho_1,\ldots,N} \sum_k \operatorname{tr}[h_{k,k+1}\rho_{k,k+1}]$$

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

Reduced minimization from exp. large Hilbert space to polynomially many variables...if we can solve quantum marginal problem!
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:**
  \[ S(ρ_{12}) + S(ρ_{23}) \geq S(ρ_{123}) + S(ρ_{2}) \]  
  [Lieb–Ruskai]

- **De Finetti and Monogamy:**
  \[ ρ_{AB_1} = \ldots = ρ_{AB_N} \xrightarrow{N \gg 1} ρ_{AB_i} \approx \text{unentangled} \]  
  [Doherty–Parrilo–Spedalieri]

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

Answer only depends on eigenvalues $\lambda_k = (\lambda_{k,1} \geq \cdots \geq \lambda_{k,d})$ of $\rho_k$. 
The One-Body Quantum Marginal Problem

Given density matrices $\rho_1, \ldots, \rho_N$, are they compatible with a global pure state $|\Psi\rangle_1, \ldots, N$?

Why relevant? **Ground states** are pure!

Do they ever ‘feel’ these constraints? **In some cases, yes!**

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

  ![Aufbau principle diagram](https://example.com/aufbau.png)

- 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:

\[
\begin{align*}
\lambda_{A,\max} + \lambda_{B,\max} &\leq \lambda_{C,\max} + 1 \\
\lambda_{A,\max} + \lambda_{C,\max} &\leq \lambda_{B,\max} + 1 \\
\lambda_{B,\max} + \lambda_{C,\max} &\leq \lambda_{A,\max} + 1
\end{align*}
\]

- necessary and sufficient for qubits
- follows from variational principle: $\lambda_{A,\max} = \max_{\phi_A} \langle \phi_A | \rho_A | \phi_A \rangle$ etc. [Higuchi, Sudbery, Szulc]
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[Higuchi, Sudbery, Szulc]
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)
Multi-Particle Entanglement

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

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]

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 \( \mathcal{C} \)?

\[
\Delta(\mathcal{C}) = \{ (\lambda_A, \lambda_B, \lambda_C) \text{ compatible with state in class } \mathcal{C} \}
\]

- finite hierarchy of entanglement polytopes  
  - contain all local information of global entanglement

\textit{e.g., for three qubits}, \( |\text{GHZ}\rangle = |000\rangle + |111\rangle \)  
\textit{and} \( |\text{W}\rangle = |100\rangle + |010\rangle + |001\rangle \):
Inequalities for Multi-Particle Entanglement

- efficient, robust against small noise
- realized in two quantum optics experiments

Known descriptions of $\Delta(C)$ 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 $\epsilon$-close to uniform, stop.

Otherwise, replace $|\Psi\rangle$ by $e^{-c(\rho_A^o + \rho_B^o + \rho_C^o)}|\Psi\rangle$. $X^o = \text{traceless part}$

**Result**

Algorithm finds $|\Psi\rangle = (A \otimes B \otimes C)|\Phi\rangle$ with marginals $\epsilon$-close to uniform within $T = \text{poly}(\frac{1}{\epsilon}, \text{input size})$ 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 $e^{-c(\rho_A^0+\rho_B^0+\rho_C^0)}|\Psi\rangle$.”

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 $H_A, \ldots, H_C$:

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

- gradient vanishes iff marginals uniform
- convexity: $\partial^2_t \geq 0$, 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: $G \rightarrow [0, \infty), g \mapsto \frac{1}{2} \| g \cdot v \|^2$ is geodesically (log-)convex. [Kempf-Ness]
Analysis of Algorithm

To turn this into a rigorous algorithm, show:

- **progress in each step:** \[ \| e^{-c(\rho_A^0 + \rho_B^0 + \rho_C^0)} |\Psi\rangle \| \leq (1 - c\epsilon) \| \Psi \| \]
- **a priori lower bound:** \[ \inf_{\det = 1} \| (A \otimes B \otimes C) |\Phi\rangle \| \geq Z \]

Then, \((1 - c\epsilon)^T \geq Z\) 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!