# The Quantum Marginals Problem

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# Overview

# Big Picture

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- Originally appeared with application to quantum chemistry[1]
- Consider a state of $N$-fermions $|\psi\rangle \in \bigwedge^N \mathcal{H}$
- and any $2$-local Hamiltonian

$$H = \sum_{1 \le i \le N} h_i + \sum_{1 \le i < j \le N} h_{ij}$$

- Energetics of a state $|\psi\rangle\langle\psi|$ only depend on reduced densities

$$\mathrm{Tr}(H\,|\psi\rangle\langle\psi|) = \sum_{1 \le i < j \le N} \mathrm{Tr}\left(\tilde{h}_{ij}\rho_{ij}\right)$$

> The advantage of (8.2) is that it does not involve the $N$-particle wave function but only the 2 matrix $\sigma(12;1'2')$, it is exact, and unlike approximations to the energy in terms of the 1 matrix, it is *linear* in the density matrix and occupation numbers. One could, therefore, hope to obtain the ground-state energy of an $N$-particle system merely by choosing $\sigma$ to minimize (8.2). It was while he enjoyed the hospitality of the Summer Research Institute of the Canadian Mathematical Congress in 1951 that this possibility first occurred to the present author. He proceeded to calculate the energy of the ground state of Li and was somewhat surprised to obtain a value about 30% *too low!* This shook his naive and unexamined faith in Ritz and Rayleigh but aroused his interest. In that first attempt $\sigma$ had been varied over too large a class of functions. The restriction to $N$-representable $\sigma$ had not been imposed. If the
>
> — A. J. Coleman, 1963

- The $N$-*representability problem* aims to characterize the space of $2$-body density operators which can be realized as the reduced states of an $N$-body fermionic pure state

[1] A John Coleman. "Structure of fermion density matrices". In: *Reviews of modern Physics* 35.3 (1963), p. 668.

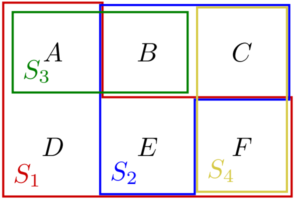
> *"We make no apology for the consideration of such a special case. The general $N$-representability problem for one and two body reduced density matrices is so difficult and yet so fundamental to many branches of science that each concrete result is useful in shedding light on the nature of the solution of the more general problem."*[2]
> — B. E. Borland, K. Dennis

- The $N$-representability problem is QMA-complete[3].

[2] RE Borland and K Dennis. "The conditions on the one-matrix for three-body fermion wavefunctions with one-rank equal to six". In: *Journal of Physics B: Atomic and Molecular Physics* 5.1 (1972), p. 7.

[3] Yi-Kai Liu, Matthias Christandl, and Frank Verstraete. "Quantum computational complexity of the N-representability problem: QMA complete". In: *Physical review letters* 98.11 (2007), p. 110503.

# Terminology




$$\mathcal{T} = \{A, B, C, D, E, F\}$$
$$S_1 = \{A, D, E, F\}$$
$$S_2 = \{B, C, E\}$$
$$S_3 = \{A, B\}$$
$$S_4 = \{C, F\}$$

### Definition

A **quantum marginals problem (QMP)** can be identified by a family of subsystems $\{S_1, S_2, \ldots, S_m\} \in 2^{\mathcal{T}}$ of some total system $\mathcal{T}$.
The objective is to characterize the space of families of density operators $\{\rho_{S_1}, \rho_{S_2}, \ldots, \rho_{S_m}\}$ with $\rho_{S_j} \in \mathcal{B}(\mathcal{H}_{S_j})$ for which

$$\text{there exists} \quad \rho_{\mathcal{T}} \in \mathcal{B}(\mathcal{H}_{\mathcal{T}}) \quad \text{such that} \quad \forall j : \mathrm{Tr}_{\mathcal{T} \setminus S_j}(\rho_{\mathcal{T}}) = \rho_{S_j}$$

# Variations of the Quantum Marginals Problem

- *pure* QMP : joint density operator $\rho_{\mathcal{T}} = |\psi_{\mathcal{T}}\rangle \langle\psi_{\mathcal{T}}|$ is pure
- *disjoint/univariate* QMP : the subsystems do not overlap $S_i \cap S_j = \delta_{ij} S_i$
- *spectral* QMP : characterize the space of specta $\lambda_j = \mathrm{spec}(\rho_{S_j})$
- *fermionic* QMP : the joint density operator is $\rho_{\mathcal{T}} \in \mathcal{B}(\bigwedge^{|\mathcal{T}|} \mathcal{H})$
- *Gaussian* QMP : the marginal $\rho_{S_j}$ and joint density operators are Gaussian states
- and many more

# Results About the Disjoint Spectral QMP

**Theorem (Higuchi-Sudbery-Szulc, 2003[4])**

*For $N$ qubits $\otimes_{i=1}^{N}\mathcal{H}_i$ $(\dim(\mathcal{H}_i) = 2)$, all constraints on the margins $\{\rho_i\}_{i=1}^{n}$ of a pure state are given by*

$$\lambda_i \leq \sum_{j\neq i} \lambda_i$$

*where $\lambda_i$ is the minimal eigenvalue of $\rho_i$.*

[4] Atsushi Higuchi, Anthony Sudbery, and Jason Szulc. "One-qubit reduced states of a pure many-qubit state: polygon inequalities". In: *Physical review letters* 90.10 (2003), p. 107902.

**Theorem (Bravyi, 2003[5])**

*For 2 qubits $\mathcal{H}_A \otimes \mathcal{H}_B$, the spectral marginal problem for $\{A, B, AB\}$ is solved by*

$$\begin{aligned} \min(\lambda_A, \lambda_B) &\geq \lambda_3^{AB} + \lambda_4^{AB}, \\ \lambda_A + \lambda_B &\geq \lambda_2^{AB} + \lambda_3^{AB} + 2\lambda_4^{AB}, \\ |\lambda_A - \lambda_B| &\leq \min(\lambda_1^{AB} - \lambda_3^{AB}, \lambda_2^{AB} - \lambda_4^{AB}), \end{aligned}$$

*where $\lambda_A, \lambda_B$ are minimal eigenvalues of $\rho_A, \rho_B$ and $\lambda_1^{AB} \geq \lambda_2^{AB} \geq \lambda_3^{AB} \geq \lambda_4^{AB}$ is the spectrum of $\rho_{AB}$.*

[5] Sergey Bravyi. "Requirements for compatibility between local and multipartite quantum states". In: *arXiv preprint quant-ph/0301014* (2003).

# Pure Spectral Marginal Problem for 3 Qutrits

## Theorem (Higuchi, 2003[6])

*For* $3$ *qutrits* $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ $(\dim(\mathcal{H}_i) = 3)$*, a necessary and sufficient condition on the nine spectral values* $0 \leq \lambda_1^{(a)} \leq \lambda_2^{(a)} \leq \lambda_3^{(a)}$ *and* $\lambda_1^{(a)} + \lambda_2^{(a)} + \lambda_3^{(a)} = 1$ *for* $a = 1, 2, 3$ *to be the reduced spectra of a pure three-qutrit quantum state is given by the following:*

$$
\begin{aligned}
\lambda_2^{(a)} + \lambda_1^{(a)} &\leq \lambda_2^{(b)} + \lambda_1^{(b)} + \lambda_2^{(c)} + \lambda_1^{(c)}, \\
\lambda_3^{(a)} + \lambda_1^{(a)} &\leq \lambda_2^{(b)} + \lambda_1^{(b)} + \lambda_3^{(c)} + \lambda_1^{(c)}, \\
\lambda_2^{(a)} + \lambda_3^{(a)} &\leq \lambda_2^{(b)} + \lambda_1^{(b)} + \lambda_2^{(c)} + \lambda_3^{(c)}, \\
2\lambda_2^{(a)} + \lambda_1^{(a)} &\leq 2\lambda_2^{(b)} + \lambda_1^{(b)} + 2\lambda_2^{(c)} + \lambda_1^{(c)}, \\
2\lambda_1^{(a)} + \lambda_2^{(a)} &\leq 2\lambda_2^{(b)} + \lambda_1^{(b)} + 2\lambda_1^{(c)} + \lambda_2^{(c)}, \\
2\lambda_2^{(a)} + \lambda_3^{(a)} &\leq 2\lambda_2^{(b)} + \lambda_1^{(b)} + 2\lambda_2^{(c)} + \lambda_3^{(c)}, \\
2\lambda_2^{(a)} + \lambda_3^{(a)} &\leq 2\lambda_1^{(b)} + \lambda_2^{(b)} + 2\lambda_3^{(c)} + \lambda_2^{(c)},
\end{aligned}
$$

*where* $(abc)$ *are any permutations of* $(123)$*.*

[6] Atsushi Higuchi. "On the one-particle reduced density matrices of a pure three-qutrit quantum state". In: *arXiv preprint quant-ph/0309186* (2003).

# Klyachko Shows Us the Light

## Gravitational Marginal Problem

# Notable PhD Theses

- Schilling's thesis[7]:
  - Greatly elaborates and expands upon the mathematical formalism behind Klyachko's approach
  - Ephasizes the importance of variational principles (Ky-Fan, Hersch-Zwahlen)
  - Develops the physical inuition behind Klyachko's solution to the fermionic $N$-representability in terms of *generalized Pauli constraints* and *(quasi-)pinning*.
- Klassen's thesis[8]:
  - Investigates the extent to which aspects of the global quantum state can be uniquely determined by its marginals.

[7] Christian Schilling. "The quantum marginal problem". In: *Mathematical Results in Quantum Mechanics: Proceedings of the QMath12 Conference*. World Scientific. 2015, pp. 165–176.

[8] Joel David Klassen. "Existence and Uniqueness in the Quantum Marginal Problem". PhD thesis. 2017.

# Connections to the Representation Theory of $S_k$

- Keyl and Werner[9] interested in indirect *measurement* of the spectra of a $d$-level system $\rho$
- Find a sequence projections $P_k$ over possible spectra $\Sigma$

$$\Sigma = \{s \in \mathbb{R}^d \mid \sum_{j=1}^{d} s_j = 1, \forall j : s_j \geq s_{j+1} \geq 0\}$$

- So that if $\Delta$ is the *complement* of a neighborhood around $r = \mathrm{spec}(\rho) \in \Sigma$, the error

$$E_k(\Delta) = \mathrm{Tr}\left(P_k(\Delta)\rho^{\otimes k}\right)$$

  vanishes as $k \to \infty$
- Main idea: exploit the symmetry of $\rho^{\otimes k}$

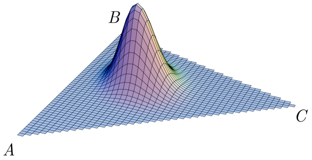



FIG. 1. Probability distribution $\mathrm{tr}(\rho^{\otimes N} P_Y)$ for $d = 3$, $N = 120$ and $r = (0.6, 0.3, 0.1)$. The set $\Sigma$ is the triangle with corners $A = (1,0,0)$, $B = (1/2, 1/2, 0)$, $C = (1/3, 1/3, 1/3)$.

[9] Michael Keyl and Reinhard F Werner. "Estimating the spectrum of a density operator". In: *Asymptotic Theory Of Quantum Statistical Inference: Selected Papers*. World Scientific, 2005, pp. 458–467.

# Spectral Estimation Using Representation Theory

- Elegant proof by Christandl and Mitchison[10]
- Spectra of $\rho^{\otimes k}$ is *invariant* under both the action of $SU(d)$ and of $S_k$
- Utilize Weyl-Schur duality indexed by partitions of $\lambda \in \mathcal{Y}_k$

$$(\mathbb{C}^d)^{\otimes k} = \bigoplus_{\lambda \in \mathcal{Y}_k} \mathcal{U}_\lambda \otimes \mathcal{V}_\lambda$$

  where $\mathcal{U}_\lambda$ and $\mathcal{V}_\lambda$ are irreps of $S_k$ and $SU(d)$ respectively
- Young diagrams $\mathcal{Y}_k$ describe partitions of $k$

$$\mathcal{Y}_1 = \{\ydiagram{1}\}, \qquad \mathcal{Y}_2 = \{\ydiagram{2}, \ydiagram{1,1}\},$$

$$\mathcal{Y}_3 = \{\ydiagram{3}, \ydiagram{2,1}, \ydiagram{1,1,1}\} \qquad \mathcal{Y}_4 = \{\ydiagram{4}, \ydiagram{3,1}, \ydiagram{2,2}, \ydiagram{2,1,1}, \ydiagram{1,1,1,1}\}, \ldots$$

- The eigenvectors of $\rho^{\otimes k}$ which are "sufficiently symmetric" are annihilated by the Young projection $P_\lambda$ onto the subspace $\mathcal{U}_\lambda \otimes \mathcal{V}_\lambda \subset (\mathbb{C}^d)^{\otimes k}$

[10] Matthias Christandl and Graeme Mitchison. "The spectra of quantum states and the Kronecker coefficients of the symmetric group". In: *Communications in mathematical physics* 261.3 (2006), pp. 789–797.

## How to Survive a Young Projector

- Eigen-decomposition of $\rho = \sum_{j=1}^{d} r_j \left|v_j\right\rangle \left\langle v_j\right|$
- Eigen-vectors of $\rho^{\otimes k}$ are then of the form

$$\left|V_J\right\rangle := \left|V_{(j_1,\ldots,j_k)}\right\rangle := \left|v_{j_1}\right\rangle \otimes \left|v_{j_2}\right\rangle \otimes \cdots \otimes \left|v_{j_k}\right\rangle \qquad J \in \{1,\ldots,d\}^k$$

- Example for $1 \leq i,j \leq d$ and $k=3$ with $\lambda = [1,1,1] \simeq \ydiagram{1,1,1}$:

$$P_{\ydiagram{1,1,1}} \left|V_{(i,i,j)}\right\rangle \propto \left|V_{(i,i,j)}\right\rangle - \left|V_{(i,i,j)}\right\rangle + \left|V_{(i,j,i)}\right\rangle - \left|V_{(i,j,i)}\right\rangle + \left|V_{(j,i,i)}\right\rangle - \left|V_{(j,i,i)}\right\rangle = 0$$

- Similar example for $1 \leq i,j \leq d$ and $k=4$ with $\lambda = [2,1,1] \simeq \ydiagram{2,1,1}$:

$$P_{\ydiagram{2,1,1}} \left|V_{(i,i,j,j)}\right\rangle \propto \left|V_{(i,i,j,j)}\right\rangle - \left|V_{(i,i,j,j)}\right\rangle + \cdots = 0$$

- Eigenvectors of $\rho^{\otimes k}$ which are "too symmetric" are annihilated!

# How to Survive a Yound Projector, Cont'd

- For $J \in \{1, \ldots, d\}^k$ define the *multiplicity partition* $\mu(J) \in \mathcal{Y}_k$ in the obvious way:

$$\mu((1,1,2,4,4,4)) = [3,2,1] \simeq$$ 

**Theorem**

*Let* $|V_J\rangle$ *be an eigenvector of* $\rho^{\otimes k}$ *with multiplicity partition* $\mu(J) \in \mathcal{Y}_k$. *Then*

$$\mathrm{Tr}(P_\lambda |V_J\rangle \langle V_J|) = \begin{cases} 0 & \mu(J) \preceq \lambda \\ 1 & \textit{otherwise} \end{cases}$$

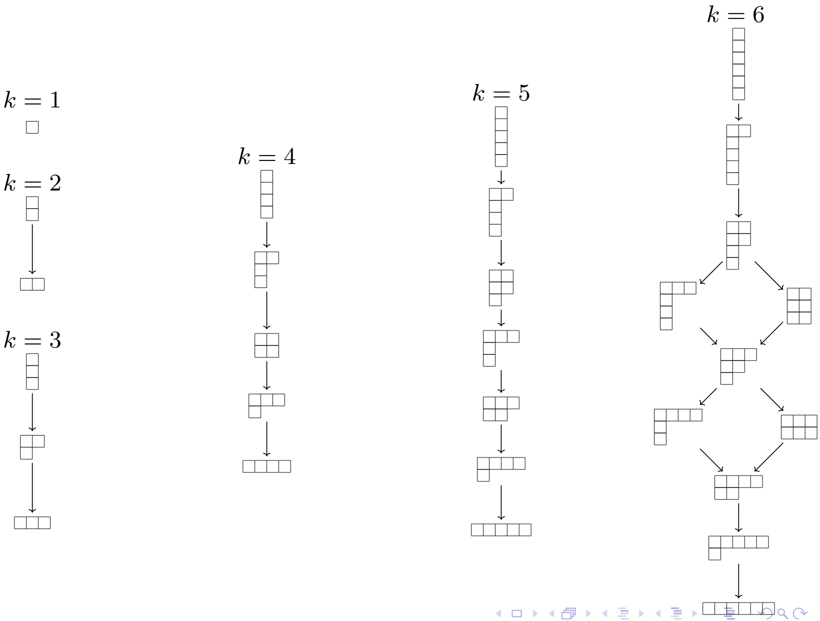
- Where $\preceq$ is the *majorization preorder* defined on partitions of $k$ as

$$\mu \preceq \lambda \iff \begin{cases} \sum_{i=1}^m \mu_i \leq \sum_{i=1}^m \lambda_i & \forall m \leq k-1, \\ \sum_{i=1}^k \mu_i = \sum_{i=1}^k \lambda_i \end{cases}$$

  where $\mu_1 \geq \mu_2 \geq \cdots \geq 0$ and $\lambda_1 \geq \lambda_2 \geq \cdots \geq 0$.

- As a corollary, eigenvalues of $P_\lambda \rho^{\otimes k} P_\lambda$ will be upper bounded by $\prod_i r_i^{\lambda_i}$ (which is largest for $\lambda_i / k \sim r_i$)

# Hasse Diagrams for the Majorization Preorder of Partitions



**Theorem (Christandl and Mitchison 2006)**

*Let $\rho$ be a density operator with spectrum $r = \mathrm{spec}(\rho)$ and let $P_\lambda$ be the projection onto $\mathcal{U}_\lambda \otimes \mathcal{V}_\lambda$ for $\lambda \in \mathcal{Y}_k$. Then*

$$\mathrm{Tr}\left(P_\lambda \rho^{\otimes k}\right) \leq (k+1)^{d(d-1)/2} \exp\left(-kD(\bar{\lambda}||r)\right)$$

*where $\bar{\lambda} = \lambda/k$.*

**Definition (KL Divergence)**

The Kullback-Liebler divergence $D(p||q)$ between two normalized probability distributions $p$ and $q$ is

$$D(p||q) = \sum_i p_i(\log p_i - \log q_i).$$

## Definition

The *Kronecker coefficients* dictate the irreps of $S_k$ which are sub-representations of products of irreps of $S_k$:

$$\mathcal{U}_\mu \otimes \mathcal{U}_\nu = \bigoplus_{\lambda \in \mathcal{Y}_k} g_{\lambda\mu\nu} U_\lambda$$

## Theorem (Christandl and Mitchison 2006)

*For every density operator $\rho_{AB}$, there is a sequence $(\lambda_j, \mu_j, \nu_j)$ of partitions with $j \in \mathbb{N}_+$ of $k_j = |\lambda_j| = |\mu_j| = |\nu_j|$ such that*

$$g_{\lambda_j \mu_j \nu_j} \neq 0 \quad \textit{i.e.} \quad \mathcal{U}_{\lambda_j} \subset \mathcal{U}_{\mu_j} \otimes \mathcal{U}_{\nu_j}$$

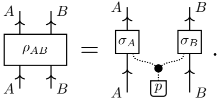
$$\lim_{j\to\infty} \bar{\lambda}_j = \operatorname{spec}(\rho_{AB}), \qquad \lim_{j\to\infty} \bar{\mu}_j = \operatorname{spec}(\rho_A), \qquad \lim_{j\to\infty} \bar{\nu}_j = \operatorname{spec}(\rho_B).$$

*"Calculation of the Kronecker coefficients is a tricky problem, arguably considered as '... the last major problem in ordinary representation theory of $S_k$' – Yoav Dvir."*

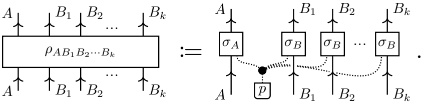
— A. Klyachko

# Results about Overlapping QMP

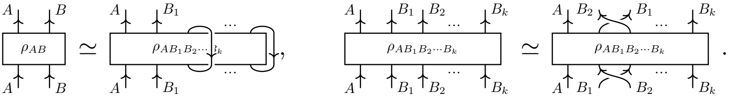
- The separability of a bipartite state $\rho_{AB} = \sum_j p_j \sigma_A^{(j)} \otimes \sigma_B^{(j)}$ can encoded as quantum marginals problem




- Assuming separability, there must exist a new state $\rho_{AB_1B_2\cdots B_k}$ called the *$k$-symmetric extension* of $\rho_{AB}$ defined by




- The $k$-symmetric extension has $\rho_{AB_i}$ marginals equal to $\rho_{AB}$ for all $i$:



# A Complete Hierarchy of Separability Tests

**Theorem (Doherty-Parrilo-Spedalieri, 2004)**

*A bipartite mixed state $\rho$ on $\mathcal{H}_A \otimes \mathcal{H}_B$ is separable if and only if $\rho$ has a symmetric extension to $k$ copies for any and all $k$.*

**Theorem (Chen-Ji-Kribs-Lütkenhaus-Zeng, 2014)**

*A bipartite qubit mixed state $\rho$ on $\mathcal{H}_A \otimes \mathcal{H}_B$ admits of a $k = 2$ symmetric extension if and only if*

$$\mathrm{Tr}\left(\rho_B^2\right) \geq \mathrm{Tr}\left(\rho_{AB}^2\right) - 4\sqrt{\det(\rho_{AB})}.$$

- Serves as first analytic complete solution to an overlapping quantum marginals problem (as far as I know).
- Can be written entirely in terms of spectra:

$$\sum_j (\lambda_j^B)^2 \geq \sum_i (\lambda_i^{AB})^2 - 4\left(\prod_i \lambda_i^{AB}\right)^{1/2}.$$

[10] Andrew C Doherty, Pablo A Parrilo, and Federico M Spedalieri. "Complete family of separability criteria". In: *Physical Review A* 69.2 (2004), p. 022308.

[10] Jianxin Chen et al. "Symmetric extension of two-qubit states". In: *Physical Review A* 90.3 (2014), p. 032318.

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