The Quantum Marginals Problem

XXX
TC Fraser

Quantum Foundations Group Meeting

March 6th, 2019

Overview

Big Picture

Big Picture

Origins of the Problem

- 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

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

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

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

> 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 σ 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 σ had been varied over too large a class of functions. The restriction to N-representable σ 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

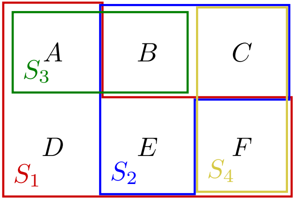
- The N-representability problem is QMA-complete[3].

[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

The Quantum Marginals Problem: 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

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

- *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 ρ_{S_j} and joint density operators are Gaussian states
- and many more

Results About the Disjoint Spectral QMP

Pure Marginal Problem for N Qubits

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 λ_i is the minimal eigenvalue of ρ_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.

Mixed Spectral Marginal Problem for 2 Qubits

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 λ_A, λ_B are minimal eigenvalues of ρ_A, ρ_B and $\lambda_1^{AB} \geq \lambda_2^{AB} \geq \lambda_3^{AB} \geq \lambda_4^{AB}$ is the spectrum of ρ_{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

Estimating the Spectra of a Density Operator

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

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

- So that if Δ 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 $\rho^{\otimes k}$

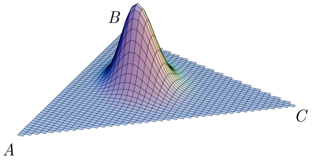


FIG. 1. Probability distribution $\mathrm{tr}(\rho^{\otimes N} P_Y)$ for $d = 3$, $N = 120$ and $r = (0.6, 0.3, 0.1)$. The set Σ is the triangle with corners $A = (1, 0, 0)$, $B = (1/2, 1/2, 0)$, $C = (1/3, 1/3, 1/3)$.

[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.

- 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_λ 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!

- 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*

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

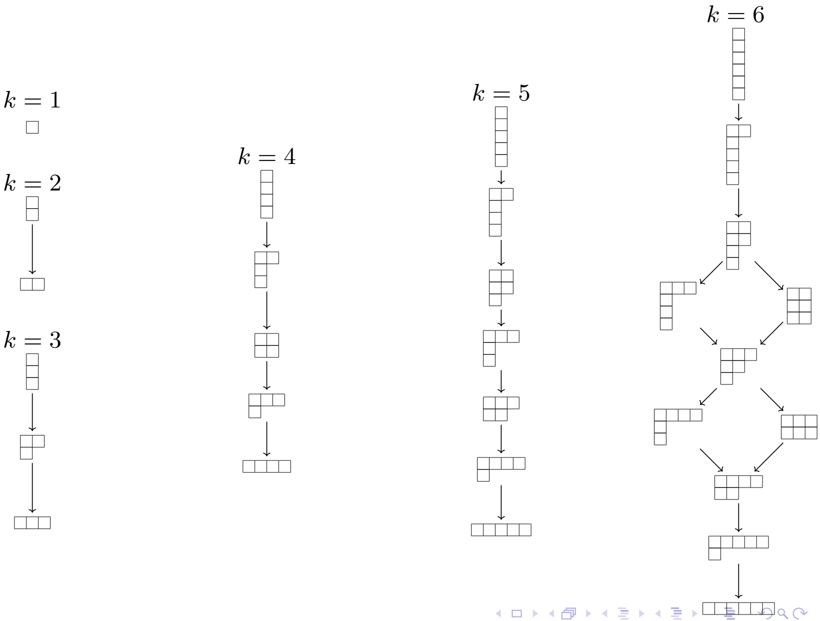
- Where $\preceq$ is the *majorization preorder* defined on partitions of k as

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

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

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

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 ρ_{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

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

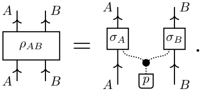
$$\lim_{j\to\infty} \bar{\lambda}_j = \mathrm{spec}(\rho_{AB}), \qquad \lim_{j\to\infty} \bar{\mu}_j = \mathrm{spec}(\rho_A), \qquad \lim_{j\to\infty} \bar{\nu}_j = \mathrm{spec}(\rho_B).$$

"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."

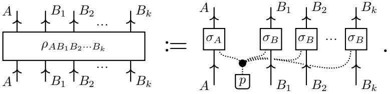
— A. Klyachko

Results about Overlapping QMP

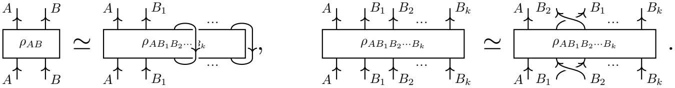
- The separability of a bipartite state $\rho_{AB} = \sum_j p_j \sigma_A^{(j)} \otimes \sigma_B^{(j)}$ can encoded as quantum marginals problem



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



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



A Complete Hierarchy of Separability Tests

Theorem (Doherty-Parrilo-Spedalieri, 2004)

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

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

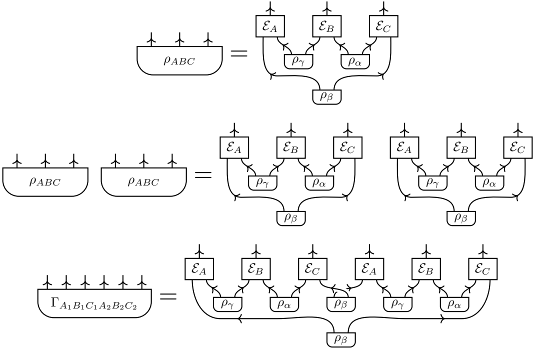
A bipartite qubit mixed state ρ on $\mathcal{H}_A \otimes \mathcal{H}_B$ admits of a $k = 2$ symmetric extension if and only if

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

- 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:

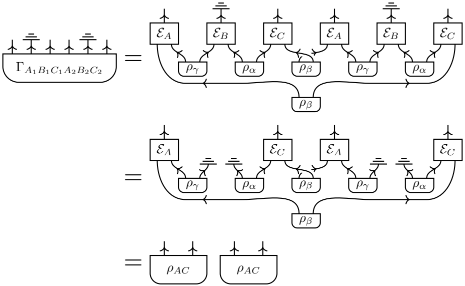
$$\sum_j (\lambda_j^B)^2 \geq \sum_i (\lambda_i^{AB})^2 - 4\left(\prod_i \lambda_i^{AB}\right)^{1/2}.$$

[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.



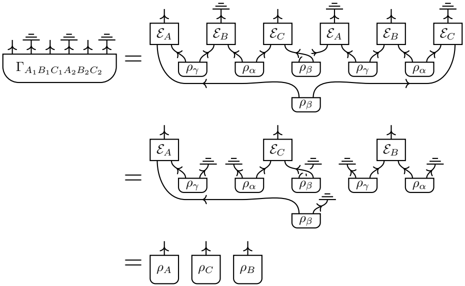
$$\Gamma_{A_1B_1C_1A_2B_2C_2} = \Gamma_{A_2B_2C_2A_1B_1C_1}$$

A QMP for Triangle Network Compatibility, Cont'd



$$\mathrm{Tr}_{B_1B_2}(\Gamma_{A_1B_1C_1A_2B_2C_2}) = \rho_{AC} \otimes \rho_{AC}$$
$$\mathrm{Tr}_{A_1A_2}(\Gamma_{A_1B_1C_1A_2B_2C_2}) = \rho_{BC} \otimes \rho_{BC}$$
$$\mathrm{Tr}_{C_1C_2}(\Gamma_{A_1B_1C_1A_2B_2C_2}) = \rho_{AB} \otimes \rho_{AB}$$

A QMP for Triangle Network Compatibility, Cont'd



$$\mathrm{Tr}_{B_1 A_2 C_2}(\Gamma_{A_1 B_1 C_1 A_2 B_2 C_2}) = \rho_A \otimes \rho_B \otimes \rho_C$$
$$\mathrm{Tr}_{A_1 C_1 B_2}(\Gamma_{A_1 B_1 C_1 A_2 B_2 C_2}) = \rho_B \otimes \rho_A \otimes \rho_C$$

References I

Aloy, Albert, Matteo Fadel, and Jordi Tura. "The quantum marginal problem for symmetric states: applications to variational optimization, nonlocality and self-testing". In: *arXiv preprint arXiv:2001.04440* (2020).

Berenstein, Arkady and Reyer Sjamaar. "Coadjoint orbits, moment polytopes, and the Hilbert-Mumford criterion". In: *Journal of the American Mathematical Society* 13.2 (2000), pp. 433–466.

Borland, RE 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.

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

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

Christandl, Matthias 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.

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

Daftuar, Sumit and Patrick Hayden. "Quantum state transformations and the Schubert calculus". In: *Annals of Physics* 315.1 (2005), pp. 80–122.

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

Dvir, Yoav. "On the Kronecker product of Sn characters". In: *Journal of Algebra* 154.1 (1993), pp. 125–140.

Eisert, Jens et al. “Gaussian quantum marginal problem”. In: *Communications in mathematical physics* 280.1 (2008), pp. 263–280.

Fritz, Tobias and Rafael Chaves. “Entropic inequalities and marginal problems”. In: *IEEE transactions on information theory* 59.2 (2012), pp. 803–817.

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

Higuchi, Atsushi, 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.

Keyl, Michael 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.

Klassen, Joel David. “Existence and Uniqueness in the Quantum Marginal Problem”. PhD thesis. 2017.

Klyachko, Alexander. “Quantum marginal problem and representations of the symmetric group”. In: *arXiv preprint quant-ph/0409113* (2004).

Klyachko, Alexander A. “Quantum marginal problem and N-representability”. In: *Journal of Physics: Conference Series*. Vol. 36. 1. IOP Publishing. 2006, p. 72.

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

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

References III

Walter, Michael et al. “Entanglement polytopes: multiparticle entanglement from single-particle information”. In: *Science* 340.6137 (2013), pp. 1205–1208.

Wolfe, Elie et al. “Quantum inflation: a general approach to quantum causal compatibility”. In: *arXiv preprint arXiv:1909.10519* (2019).