Calculation of Generalized Pauli Constraints

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April, 2016

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ρ is a non-negative ($\rho \geq 0$) Hermitian operator with $\mathrm{Tr}\rho = 1$, called Density matrix.

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implies that the state space of composite system AB splits into tensor product of its components A and B

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Density Matrix of Composite Systems

Density matrix of composite system can be written as linear combination

$$\rho_{AB} = \sum_{\alpha} a_\alpha L_A^\alpha \otimes L_B^\alpha$$

where L_A^α, L_B^α are linear operators on $\mathcal{H}_A$, $\mathcal{H}_B$, respectively.

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they are called one-particle reduced density matrices.

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  which implies that the state space of N electrons shrinks to $\wedge^N \mathcal{H} \subset \mathcal{H}^{\otimes N}$.
- This implies the original Pauli principle, because $\psi \wedge \psi = 0$.

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Mixed N-representability

More generally we have mixed N-representability problem:
"What are the constraints on the spectra of a mixed state and its reduced matrix?"

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- Similar results hold for two-hole system.

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Borland-Dennis system

- For the system $\wedge^3\mathcal{H}_6$ of three electrons of rank 6, the N-representability conditions are given by the following (in)equalities:

$$\lambda_1 + \lambda_6 = \lambda_2 + \lambda_5 = \lambda_3 + \lambda_4 = 1, \quad \lambda_4 \leq \lambda_5 + \lambda_6,$$

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- Sufficiency proved by Borland-Dennis (1972)
- Necessity proved by Ruskai (2007)

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Main Theorem. Let $\rho^N : \wedge^N \mathcal{H}_r$ $(\mathrm{Tr}\rho^N = 1)$ be mixed state and $\rho : \mathcal{H}_r$ $(\mathrm{Tr}\rho = N)$ be its particle density matrix.

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$$\sum_i a_i \lambda_{v(i)} \leq \sum_k (\wedge^N a)_k \mu_{w(k)} \qquad (a, v, w)$$

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$$\sum_i a_i \lambda_{v(i)} \leq \sum_k (\wedge^N a)_k \mu_{w(k)} \qquad (a, v, w)$$

Here, $\wedge^N a$ consists of all sums $a_{i_1} + a_{i_2} + \cdots + a_{i_N}$, $1 \leq i_1 < i_2 < \cdots < i_N \leq r$ arranged in decreasing order, $v \in S_r$ and $w \in S_R$ subject to topological condition $c_v^w(a) \neq 0$ explained soon.

Remark

Solution of Pure N-representability

Solution of pure N-representability problem can be deduced from the above theorem by specialization $\mu_i = 0$ for $i \neq 1$, because pure states corresponds projector operators $|\psi\rangle\langle\psi|$.

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In this case all costraints together with ordering ineqaulities and normalization condition describe a convex polytope, called Moment Polytope.

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and morphism

$$\begin{array}{rcl} \varphi_a : \mathcal{F}_a(\mathcal{H}_r) & \to & \mathcal{F}_{\wedge^N a}(\wedge^N \mathcal{H}_r) \\ X & \mapsto & X^{(N)} \end{array}$$

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Here, $X^{(N)} : \psi_1 \wedge \psi_2 \wedge \ldots \wedge \psi_N \mapsto \sum_i \psi_1 \wedge \psi_2 \wedge \ldots \wedge X\psi_i \wedge \ldots \wedge \psi_N$.

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written in the basis of Schubert cocycles σ_w.

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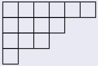
It splits into irreducible components H_λ, parameterized by Young diagrams $\lambda =$  of size $N.m$, with multiplicity m_λ

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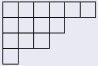
It splits into irreducible components H_λ, parameterized by Young diagrams $\lambda =$  of size $N.m$, with multiplicity m_λ

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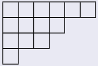
It splits into irreducible components H_λ, parameterized by Young diagrams $\lambda =$  of size $N.m$, with multiplicity m_λ

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Surprisingly solution of this problem coincides with that of pure N-representability problem.

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Representation theoretical solution

Theorem. Every $\widetilde{\lambda}$ obtained from irreducible component $\mathcal{H}_\lambda \subset S^m(\wedge^N \mathcal{H}_r)$ is a spectrum of one point reduced matrix ρ of a pure state $\psi \in \wedge^N \mathcal{H}_r$.

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- Increase M and continue until $\mathcal{P}_M^{\mathrm{in}} = \mathcal{P}_M^{\mathrm{out}}$.

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m	λ
1	$[1, 1, 1, 0, 0, 0]$
2	$[2, 2, 2, 0, 0, 0]$, $[2, 1, 1, 1, 1, 0]$
3	$[2, 2, 2, 1, 1, 1]$, $[3, 3, 3, 0, 0, 0]$, $[3, 2, 2, 1, 1, 0]$
4	$[2, 2, 2, 2, 2, 2]$, $[3, 3, 3, 1, 1, 1]$, $[4, 4, 4, 0, 0, 0]$, $[3, 3, 2, 2, 1, 1]$, $[4, 3, 3, 1, 1, 0]$, $[4, 2, 2, 2, 2, 0]$

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4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$, $[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$, $[1, 1, 1, 0, 0, 0]$, $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$, $[1, \frac{3}{4}, \frac{3}{4}, \frac{1}{4}, \frac{1}{4}, 0]$, $[1, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0]$

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3	$[\frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{1}{3}, \frac{1}{3}]$, $[1, 1, 1, 0, 0, 0]$, $[1, \frac{2}{3}, \frac{2}{3}, \frac{1}{3}, \frac{1}{3}, 0]$
4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$, $[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$, $[1, 1, 1, 0, 0, 0]$, $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$, $[1, \frac{3}{4}, \frac{3}{4}, \frac{1}{4}, \frac{1}{4}, 0]$, $[1, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0]$

Taking convex hull of these spectra we obtain the full moment polytope which is described by 3 equalities and 1 inequality.

Borland-Dennis System ($N = 3,\ r = 6$)

After the normalization we obtain the spectra $\widetilde{\lambda}$

m	$\widetilde{\lambda}$
1	$[1,1,1,0,0,0]$
2	$[1,1,1,0,0,0]$, $[1,\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},0]$
3	$[\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{1}{3},\frac{1}{3}]$, $[1,1,1,0,0,0]$, $[1,\frac{2}{3},\frac{2}{3},\frac{1}{3},\frac{1}{3},0]$
4	$[\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}]$, $[\frac{3}{4},\frac{3}{4},\frac{3}{4},\frac{1}{4},\frac{1}{4},\frac{1}{4}]$, $[1,1,1,0,0,0]$, $[\frac{3}{4},\frac{3}{4},\frac{1}{2},\frac{1}{2},\frac{1}{4},\frac{1}{4}]$, $[1,\frac{3}{4},\frac{3}{4},\frac{1}{4},\frac{1}{4},0]$, $[1,\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},0]$

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$N = 3,\ r = 7$

$M = 8$.

How it works?

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$N = 3,\ r = 7$

$M = 8$.

$N = 4,\ r = 8$

$M = 10$.

How it works?

$N = 3,\ r = 8$

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Thus the polytope is the genuine moment polytope for $\wedge^3\mathcal{H}_8$ which is given by 31 independent inequalities.

Number of Constraints for systems of rank ≤ 10

r	N	Number of constraints
7	3	4
8	3	31
8	4	15
9	3	52
9	4	60
10	3	93
10	4	125
10	5	161

Thank You for your attention!!!