

# Quantum marginal problem

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# Quantum marginal problem

The **Quantum Marginal Problem** came into focus about 2003 in connection with QI applications. In its simplest form the problem is about constraints on reduced states  $\rho_A, \rho_B, \rho_C$  of a pure state  $\psi \in \mathcal{H}_{ABC} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ . Clearly the compatibility depends only on spectra

$$\lambda_A = \text{Spec}(\rho_A), \lambda_B = \text{Spec}(\rho_B), \lambda_C = \text{Spec}(\rho_C).$$

Its **mixed version** looking for constraints on spectra  $\lambda_{AB}, \lambda_A, \lambda_B$  of a mixed state  $\rho_{AB}$  of two component system  $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$  and its reduced states  $\rho_A, \rho_B$ . It can be reduced to pure one for system  $\mathcal{H}_{AB} \otimes \mathcal{H}_A \otimes \mathcal{H}_B$ .

**Warning:** I'll consider below only **disjoint margins**, where the classical MP is trivial. For overlapping margins like  $\rho_{AB}, \rho_{BC}, \rho_{CA}$  the problem is beyond the scope of the current approach.

# Examples

Higuchi, Sudbery, Szulc, PRL, 90, 107902 (2003)

For array of qubits  $\bigotimes_{i=1}^n \mathcal{H}_i$ ,  $\dim \mathcal{H}_i = 2$  the compatibility conditions for pure QMP are given by *polygonal inequalities*

$$\lambda_i \leq \sum_{j(\neq i)} \lambda_j$$

for minimal eigenvalues  $\lambda_i$  of the marginal states  $\rho_i$ .

For two qubits  $\mathcal{H}_A \otimes \mathcal{H}_B$  solution of the *mixed QMP* is given by *Bravyi inequalities*

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

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

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## Outline of the talk

The above inequalities look miraculous. Even linearity is puzzling. In this lecture I'll focus on a rather nontrivial mathematical origin of general quantum marginal constraints and provide a way for their efficient calculation.

# Quantum logic

Every binary observable  $X : \mathcal{H} \rightarrow \mathcal{H}$  assuming values 0, 1 is a projection operator onto a subspace  $F \subset \mathcal{H}$ . This fact led von Neumann and Birkhoff (1936) to the notion of **quantum logic** understood as algebra of subspaces in  $\mathcal{H}$  with respect to operations  $F \cap E$  and  $F + E$  modeling conjunction and disjunction of the classical logic.

This brings into focus **geometry of linear configurations** of subspaces  $F_\alpha \subset \mathcal{H}$  possibly subject to certain constraints stated in terms of the above “logical” operations.

You might enjoy this kind of geometry of points, lines, planes, etc. in high school, and QM gives us a chance to revisit this beautiful world with a new perspective.

# Plücker coordinates

$d$ -subspace  $F = \langle f_1, f_2, \dots, f_d \rangle$  is uniquely determined by decomposable skew symmetric tensor

$$\varphi = f_1 \wedge f_2 \wedge \dots \wedge f_d \in \wedge^d \mathcal{H}$$

also known as **Slater determinant**. Applying this construction to every space  $F_\alpha \subset \mathcal{H}$  of a configuration we can describe it by a single tensor

$$\Phi = \bigotimes_\alpha \varphi_\alpha \in \bigotimes_\alpha \wedge^{d_\alpha} \mathcal{H}, \quad d_\alpha = \dim F_\alpha$$

called **Plücker vector** of the configuration. Its components are said to be **Plücker coordinates**.

# Stability of a configuration

As Klein taught us, to extract geometrical gist from a mess of coordinate calculations we have to use invariant notions and quantities. In particular, geometry of a configuration should be described in terms of **invariant polynomials**

$$f(\Phi) = f(g\Phi), \quad \forall g \in \mathrm{SL}(\mathcal{H})$$

evaluated at the corresponding Plücker vector  $\Phi \in \bigotimes_{\alpha} \wedge^{d_{\alpha}} \mathcal{H}$ .



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A drawback of this approach is that the invariants can characterize only **closed orbits**  $\mathrm{SL}(\mathcal{H})\Phi \subset \bigotimes_{\alpha} \wedge^{d_{\alpha}} \mathcal{H}$ . In this case the Plücker vector  $\Phi$  and the configuration are said to be **stable**. Vectors  $\Phi$  which can't be separated from zero by invariants should be discarded. They are termed **unstable** vectors and configurations. The remaining vectors and configurations are called **semistable**.

# Example: Points in Riemann sphere

$n$  points in  $\mathbb{P}^1$  can be seen as roots of a homogeneous polynomial  $f_n(x, y)$  of degree  $n$ . Suppose the polynomial has a root, say  $x = 0$ , of a big multiplicity  $m > n/2$ . Write  $f_n(x, y) = x^m f_{n-m}(x, y)$ ,  $m > n - m$ . Then for  $SL(2)$  transformation  $(x : y) \mapsto (\varepsilon x : \varepsilon^{-1} y)$  we have

$$\lim_{\varepsilon \rightarrow 0} f_n(\varepsilon x, \varepsilon^{-1} y) = \lim_{\varepsilon \rightarrow 0} \varepsilon^m x^m f_{n-m}(\varepsilon x, \varepsilon^{-1} y) = 0,$$

i.e. a configuration in which more than half of the points coincide is unstable. One can check that if the maximal multiplicity of a point  $m = n/2$ , then the configuration is semistable, and for  $m < n/2$  it is stable.

[Majorana interpretation of spin  $s$  states as a configuration of  $2s$  points in  $\mathbb{P}^1$ . A complete description of invariants is known only for  $n \leq 8$ .]

# Mumford's criterion

By a similar limiting argument, going back to Hilbert, Mumford (1962) derived a general

## Geometric stability criterion

A configuration of subspaces  $F_\alpha \subset \mathcal{H}$  is **semistable** iff for every proper subspace  $E \subset \mathcal{H}$  the following inequality holds

$$\frac{1}{\dim E} \sum_{\alpha} \dim(E \cap F_{\alpha}) \leq \frac{1}{\dim \mathcal{H}} \sum_{\alpha} \dim F_{\alpha}. \quad (1)$$

Moreover, for **strict** inequalities the configuration is **stable**.

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Recall that this condition separates configurations that admit an **invariant description** from those that can't be treated in invariant terms and, in a sense, are **conceptually intractable**.

# Example

## Configuration of points in $\mathbb{P}^n$ (Mumford-Tate)

For a configuration of one-dimensional subspaces  $F_\alpha \in \mathcal{H}$ , i.e. points  $f_\alpha \in \mathbb{P}(\mathcal{H})$ , the stability criterion just tells that for any subspace  $E \subset \mathcal{H}$

$$\frac{\#\{F_\alpha \subset E\}}{\dim E} \leq \frac{\#\{F_\alpha \subset \mathcal{H}\}}{\dim \mathcal{H}}.$$

For Riemann sphere  $\mathbb{P}^1$  this just tells that in a semistable configuration no more than half of the points coincide.

# Metric properties of stable configurations

The concept of stability is purely logical and independent of the metric in complex space  $\mathcal{H}$  and therefore may look irrelevant to QM which heavily relies on the metric. The point is that stable configurations have indeed very peculiar metric properties.

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## Kempf-Ness unitary trick (1978)

The following conditions are equivalent

- Vector  $\Phi$  is stable,
- its orbit contains a vector  $\Phi_0 = g_0\Phi$ ,  $g_0 \in SL(\mathcal{H})$  of minimal length  $|\Phi_0| \leq |g\Phi|, \forall g \in SL(\mathcal{H})$ .

Moreover, the minimal vector  $\Phi_0$  is unique up to a unitary rotation  $\Phi_0 \mapsto u\Phi_0$ ,  $u \in U(\mathcal{H})$ . **To put this in other way:** Stable vector  $\Phi$  defines unique up to proportionality metric in which  $\Phi$  is the minimal vector  $|\Phi| \leq |g\Phi|, \forall g \in SL(\mathcal{H})$ .

# Metric properties of stable configurations

The minimality of length  $|\Phi|$  amounts to the infinitesimal equation

$$\langle \Phi | X | \Phi \rangle = 0, \quad \forall X \in \mathfrak{sl}(\mathcal{H}),$$

which in terms of configurations reads as follows.



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## Metric characterization of stable configurations

A configuration of subspaces  $F_\alpha \subset \mathcal{H}$  is stable iff there exists a Hermitean metric in  $\mathcal{H}$  s.t.

$$\sum_{\alpha} P_{\alpha} = \text{scalar},$$

where  $P_{\alpha}$  = orthogonal projector onto  $F_{\alpha}$  in the above metric.

## Exercise

Let  $z_\alpha \in \mathbb{C} \cup \infty = \mathbb{P}^1$  be a configuration of points in the extended complex plane, and  $\ell_\alpha \in \mathbb{S}^2 \subset \mathbb{E}^3$  be stereographic projections of  $z_\alpha$  into the unit Riemann sphere. Then the configuration is stable iff there exists a linear fractional transform  $z \mapsto \tilde{z} = \frac{az+b}{cz+d}$  such that  $\sum_\alpha \tilde{\ell}_\alpha = 0$ .

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## Solution in physical terms

$\mathbb{P}^1 = \mathbb{P}(\mathcal{H})$ , where  $\mathcal{H}$  is spin 1/2 space,  $F_\alpha \subset \mathcal{H}$  is a subspace spanned by state  $|1/2\rangle_{\ell_\alpha}$  with spin projection 1/2 onto direction  $\ell_\alpha$ , and  $P_\alpha = S_{\ell_\alpha} + 1/2 = \text{projector into } F_\alpha$ . The metric defined by a stable configuration is characterized by equation  $\sum_\alpha P_\alpha = \text{scalar}$ , which for traceless spin projector operators  $S_\ell$  amounts to  $\sum_\alpha S_{\ell_\alpha} = 0$ . In terms of Pauli matrices  $S_\ell = \ell_x \sigma_x + \ell_y \sigma_y + \ell_z \sigma_z$ , whence  $\sum_\alpha \ell_\alpha = 0$ .

## Summary

The geometric stability condition

$$\frac{1}{\dim E} \sum_{\alpha} \dim(E \cap F_{\alpha}) \leq \frac{1}{\dim \mathcal{H}} \sum_{\alpha} \dim F_{\alpha}, \quad E \subset \mathcal{H} \quad (2)$$

for any practical end is equivalent to existence of a metric in  $\mathcal{H}$  such that

$$\sum_{\alpha} P_{\alpha} = \text{scalar}, \quad (3)$$

where  $P_{\alpha}$ =orthogonal projector onto  $F_{\alpha}$ . **More precisely:**  
(3)  $\Rightarrow$  (2) and (2) with **strict** inequalities implies (3).

# From Quantum logic to Quantum observables

Logic, quantum or classical, is essentially content free and in itself solves no problem. Instead, it provides the simplest basic elements sufficient for dealing with objects of unlimited complexity. As an example I consider below description of **quantum observables**  $X_\alpha : \mathcal{H}$  in terms of the projector operators, named by von Neumann and Birkhoff **quantum questions**.

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Logic, quantum or classical, is essentially content free and in itself solves no problem. Instead, it provides the simplest basic elements sufficient for dealing with objects of unlimited complexity. As an example I consider below description of **quantum observables**  $X_\alpha : \mathcal{H}$  in terms of the projector operators, named by von Neumann and Birkhoff **quantum questions**.

To this end we first of all need a **holomorphic** metric independent substitution for Hermitean operator  $X_\alpha$ , which would play the same role as subspace  $F_\alpha = \text{Im}(P_\alpha)$  used for projector  $P_\alpha$ . Such a substitution is known in operator theory as **spectral filtration**.

## Spectral filtration

$$F_\alpha(s) = \left\{ \text{sum of eigenspaces of } X_\alpha \text{ with eigenvalues } \geq s \right\}, \quad s \in \mathbb{R}.$$

This is a piecewise constant decreasing family of subspaces with drops at eigenvalues  $\lambda_1 > \lambda_2 > \dots > \lambda_k$  of  $X_\alpha$ .

Geometrically it can be represented by a **flag of subspaces**

$$0 \subset F_\alpha(\lambda_1) \subset F_\alpha(\lambda_2) \subset \dots \subset F_\alpha(\lambda_k) = \mathcal{H} \quad (4)$$

labeled by the eigenvalues  $\lambda_i$ . To avoid technicalities I'll consider below only **non-negative operators**  $X_\alpha \geq 0$ .

## Recovery of the operator

The operator  $X_\alpha \geq 0$  can be recovered from its spectral filtration using **projector operators**  $P_\alpha(s)$  onto subspaces  $F_\alpha(s)$

$$X_\alpha = \int_0^\infty P_\alpha(s) ds = \quad (5)$$
$$(\lambda_1^\alpha - \lambda_2^\alpha)P_\alpha(\lambda_1^\alpha) + (\lambda_2^\alpha - \lambda_3^\alpha)P_\alpha(\lambda_2^\alpha) + \dots$$

The spectrum of  $X_\alpha$  depends only on the **labels** of the flag (4), but not the flag itself, i.e. it is essentially a **free parameter**.



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## Reduction to quantum logic

Treating filtrations  $F_\alpha(s)$  as a system of subspaces  $F_\alpha(\lambda_i^\alpha)$  each taken with multiplicity  $m_i^\alpha = \lambda_i^\alpha - \lambda_{i+1}^\alpha$  we get the standard package of a **geometric stability criterion** together with a **metric characterization** of stable systems of filtrations.

# The standard package for filtrations

## Geometric stability criterion

A system of filtrations  $F_\alpha(s)$  is **semistable** iff  $\forall$  proper  $E \subset \mathcal{H}$

$$\frac{1}{\dim E} \sum_{\alpha} \int_0^{\infty} \dim(F_\alpha(s) \cap E) ds \leq \frac{1}{\dim \mathcal{H}} \sum_{\alpha} \int_0^{\infty} \dim F_\alpha(s) ds. \quad (6)$$

Moreover, for **strict** inequalities the system is **stable**.

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## Metric characterization of stable filtrations

A system of filtrations  $F_\alpha(s)$  is stable iff there exists a metric such that sum of the corresponding operators is a scalar

$$\sum X_\alpha = \text{scalar}. \quad (7)$$

Here  $X_\alpha = \int_0^{\infty} P_\alpha(s) ds$ , and  $P_\alpha(s) =$  projector onto  $F_\alpha(s)$ .

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This isn't an extension, but **specialization** of the QLogic result!

## A closer look at the integrals

Suppose the operators  $X_\alpha$  have simple spectra. Then

$$\int_0^\infty \dim(F_\alpha(s) \cap E) ds = - \int_0^\infty s d \dim(F_\alpha(s) \cap E) = \sum_{i \in I} \lambda_i^\alpha := \lambda_I^\alpha, \quad (8)$$

where  $I = I_\alpha$  consists of those indices  $i$  where the dimension drops:  $\dim(F_\alpha(\lambda_i^\alpha) \cap E) > \dim(F_\alpha(\lambda_i^\alpha + 0) \cap E)$ . Clearly  $|I| = \dim E := d$ . Subspaces  $E \subset \mathcal{H}$  with a fixed drop set  $I$  form a **Schubert cell**  $s_I$  in Grassmanian  $G_d(\mathcal{H})$ . Observe that  $E \in \bigcap_\alpha s_{I_\alpha} \neq \emptyset$ . For filtrations in general position this means that the product of the cohomological classes  $\sigma_{I_\alpha} = [\overline{s_{I_\alpha}}]$  in  $H^*(G_d(\mathcal{H}))$  is nonzero:  $\prod_\alpha \sigma_{I_\alpha} \neq 0$ .

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## Summary

The geometric stability criterion (6) imposes linear inequalities on spectra

$$\frac{1}{\dim E} \sum_\alpha \lambda_{I_\alpha}^\alpha \leq \frac{1}{\dim \mathcal{H}} \sum_\alpha \text{Tr } X_\alpha$$

with indices  $I_\alpha$  subject to the geometrical  $\bigcap_\alpha s_{I_\alpha} \neq \emptyset$  or the topological  $\prod_\alpha \sigma_{I_\alpha} \neq 0$  constraints. Here is a typical example.

# Weyl's additive spectral problem

Klyachko (1998), see also talk at ICM, Beijing (2002)

The following conditions are equivalent

- There exist Hermitian operators  $L, M, N = L + M$  with given spectra  $\lambda, \mu, \nu$ ;
- The spectra satisfy the inequality

$$\sum_{i \in I} \lambda_i + \sum_{j \in J} \mu_j \geq \sum_{k \in K} \nu_k \quad (\text{IJK})$$

each time  $|I| = |J| = |K|$  and Schubert cocycle  $\sigma_K$  enters into decomposition of  $\sigma_I \cdot \sigma_J$  with a nonzero coefficient.

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## Hermit-Einstein metric

S.K.Donaldson Proc. London Math. Soc., 59, 1-26 (1985); Duke Math. J., 54, 231-247 (1987); M.S.Narasimhan, C.S.Seshadri, Annals of Math., 82, 540-564 (1965).



# Passing to a subgroup

Geometric stability criterion (6) can be restated in terms of **test filtrations**  $E(t)$ , rather than test subspaces  $E \subset \mathcal{H}$ ,

$$\sum_{\alpha} \iint \left[ \dim(F_{\alpha}(s) \cap E(t)) - \frac{\dim F_{\alpha}(s) \dim E(t)}{\dim \mathcal{H}} \right] ds dt \leq 0, \quad (9)$$

where the integration is over the whole  $(s, t)$  plane. This extension is redundant for the full group  $SU(\mathcal{H})$ , but can be essential for its subgroups.

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$G \subset SU(\mathcal{H})$  – connected Lie subgroup;

$\mathfrak{g} \subset \mathfrak{su}(\mathcal{H})$  – its Lie algebra considered as algebra of **Hermitean** operators with Lie bracket  $[X, Y] = i(XY - YX)$ ;

$\mathfrak{su}(\mathcal{H})$  – Lie algebra of traceless **Hermitean** operators in  $\mathcal{H}$ .

$G^c \subset SL(\mathcal{H})$  – complexification of  $G$ ;

$G^c$ -**stable**, -**semistable**, and -**unstable** configurations are defined as above 7 by formal substitution  $SL(\mathcal{H}) \mapsto G^c$ .

# The standard package for a subgroup

## Geometric stability criterion

A system of filtrations  $F_\alpha(s)$  is  $G^c$ -semistable iff for every nonzero operator  $x \in \mathfrak{g} : \mathcal{H}$  with spectral filtration  $E_x(t)$  the following inequality holds

$$\sum_{\alpha} \iint \left[ \dim(F_\alpha(s) \cap E_x(t)) - \frac{\dim F_\alpha(s) \dim E_x(t)}{\dim \mathcal{H}} \right] ds dt \leq 0, \quad (10)$$

Moreover, for strict inequalities the system is  $G^c$ -stable.

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Moreover, for strict inequalities the system is  $G^c$ -stable.

## Metric characterization of stability

A system of filtrations  $F_\alpha(s)$  is  $G^c$ -stable iff there exists a metric such that

$$\sum_{\alpha} X_{\alpha} \in \mathfrak{g}^{\perp} \quad [= \text{scalars for } \mathfrak{g} = \mathfrak{su}(\mathcal{H})]. \quad (11)$$

Here  $X_{\alpha} = \int_0^{\infty} P_{\alpha}(s) ds$ ,  $P_{\alpha}(s)$  = projector onto  $F_{\alpha}(s)$ , and  $\mathfrak{g}^{\perp}$  is orthogonal complement to  $\mathfrak{g}$  in the space of all Hermitean operators with trace form  $(X, Y) = \text{Tr}(XY)$ .

## A closer look at the integrals

Let  $F(s)$  and  $E(t)$  be **complete** filtrations, meaning the spaces  $F(s)/F(s+0)$  and  $E(t)/E(t+0)$  have dimension  $\leq 1$ . Then

$$\begin{aligned} \iint \dim(F(s) \cap E(t)) ds dt &= \int t d_t \left( \int s ds [\dim(F(s) \cap E(t))] \right) = \\ \int t d_t \left( - \sum_s s \dim \frac{F(s) \cap E(t)}{F(s+0) \cap E(t)} \right) &= \\ \int t d_t \left( - \sum_s s \dim \frac{F(s) \cap E(t) + F(s+0)}{F(s+0)} \right) &= \\ \sum_{s,t} ts \dim \frac{F(s) \cap E(t) + F(s+0)}{F(s) \cap E(t+0) + F(s+0)} &= \sum_i t_i s_{w(i)} \end{aligned} \quad (12)$$

where  $s_i, t_j$  are discontinuity points of the filtrations [= eigenvalues of the respective operators] arranged in decreasing order;  $w$  is a permutation describing **relative position** of the respective flags.

Flags in position  $w$  with respect to a reference flag form a Schubert cell  $s_w$ . In the geometric criterion setting (10)  $E_x \in \bigcap_{\alpha} s_{w_{\alpha}} \neq \emptyset$ . For generic filtrations this amounts to the topological constraint on the respective Schubert cocycles  $\sigma_w = [\overline{s_w}]$ :  $\prod_{\alpha} \varphi_x^* \sigma_{w_{\alpha}} \neq 0$ , where  $\varphi_x : \mathcal{F}_x(\mathfrak{g}) \rightarrow \mathcal{F}_x(\mathcal{H})$  is the natural inclusion of flag varieties (= adjoint orbits) of type  $x$  in  $\mathfrak{g}$  and  $\mathfrak{su}(\mathcal{H})$  respectively.

Flags in position  $w$  with respect to a reference flag form a **Shubert cell**  $s_w$ . In the geometric criterion setting (10)  $E_x \in \bigcap_{\alpha} s_{w_{\alpha}} \neq \emptyset$ . For generic filtrations this amounts to the topological constraint on the respective **Schubert cocycles**  $\sigma_w = [\overline{s_w}]$ :  $\prod_{\alpha} \varphi_x^* \sigma_{w_{\alpha}} \neq 0$ , where  $\varphi_x : \mathcal{F}_x(\mathfrak{g}) \rightarrow \mathcal{F}_x(\mathcal{H})$  is the natural inclusion of flag varieties (= adjoint orbits) of type  $x$  in  $\mathfrak{g}$  and  $\mathfrak{su}(\mathcal{H})$  respectively.

Let now turn to the simplest case of two operators  $X : \mathcal{H}$  and its projection  $X_{\mathfrak{g}}$  into  $\mathfrak{g}$ , so that  $X_{\mathfrak{g}} - X \in \mathfrak{g}^{\perp}$  and stability condition (10), enhanced by (12), give all constraints on spectra of  $X$  and  $X_{\mathfrak{g}}$ . To simplify notations suppose  $\mathfrak{g}$  to be a sum of  $\mathfrak{su}$ , so that the notions of spectrum and flag has the usual meaning. Let  $\varphi : \mathfrak{g} \hookrightarrow \mathfrak{su}(\mathcal{H})$ , and for a given  $x \in \mathfrak{g}$  put  $a = \text{Spec } x$  and  $a^{\varphi} = \text{Spec } \varphi(x)$ . We also need flag varieties  $\mathcal{F}_a$  and  $\mathcal{F}_{a^{\varphi}}$  consisting of operators in  $\mathfrak{g}$  and  $\mathfrak{su}(\mathcal{H})$  of spectra  $a$  and  $a^{\varphi}$  respectively, together with natural morphism  $\varphi_a : \mathcal{F}_a \rightarrow \mathcal{F}_{a^{\varphi}}, x \mapsto \varphi(x)$  and its cohomological counterpart  $\varphi_a^* : H^*(\mathcal{F}_{a^{\varphi}}) \rightarrow H^*(\mathcal{F}_a)$ .

## Notations

$\varphi : \mathfrak{g} \hookrightarrow \mathfrak{su}(\mathcal{H})$ ,  $X_{\mathfrak{g}}$  = projection of  $X \in \mathfrak{su}(\mathcal{H})$  into  $\mathfrak{g}$ . For a given  $x \in \mathfrak{g}$  with spectrum  $a = \text{Spec } x$  put  $a^{\varphi} = \text{Spec } \varphi(x)$ . We also need flag varieties  $\mathcal{F}_a$  and  $\mathcal{F}_{a^{\varphi}}$  consisting of operators in  $\mathfrak{g}$  and  $\mathfrak{su}(\mathcal{H})$  of spectra  $a$  and  $a^{\varphi}$  respectively, together with natural morphism  $\varphi_a : \mathcal{F}_a \rightarrow \mathcal{F}_{a^{\varphi}}$ ,  $x \mapsto \varphi(x)$  and its cohomological counterpart  $\varphi_a^* : H^*(\mathcal{F}_{a^{\varphi}}) \rightarrow H^*(\mathcal{F}_a)$ .

## A version of Berenstein-Sjamaar Thm

In the above notations all constraints on spectra  $\lambda = \text{Spec } X$  and  $\mu = \text{Spec } X^{\mathfrak{g}}$  are given by inequalities

$$\sum_i a_i \mu_{\nu(i)} \leq \sum_j a_j^{\varphi} \lambda_{w(j)} \quad (\text{vwa})$$

for all test spectra  $a = \text{Spec } x$ ,  $x \in \mathfrak{g}$  and permutations  $\nu, w$  s.t. Schubert cocycle  $\sigma_{\nu}$  enters into  $\varphi_a^*(\sigma_w)$  with a nonzero coefficient  $c_w^{\nu}(a)$ . [ $c_w^{\nu}(a) = 1$  are enough, Ressayre (2007)]



# Application to QMP

## Two component system

Consider two-component system  $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$  with local unitaries  $G = \mathrm{SU}(\mathcal{H}_A) \times \mathrm{SU}(\mathcal{H}_B)$  as the structure group with Lie algebra  $\mathfrak{g} = \mathfrak{su}(\mathcal{H}_A) \otimes I + I \otimes \mathfrak{su}(\mathcal{H}_B)$ . Recall, that reduced states of  $\rho_A, \rho_B$  are defined by equations

$$\mathrm{Tr}_{AB}(X_A \rho_{AB}) = \mathrm{Tr}_A(X_A \rho_A), \quad X_A \in \mathfrak{su}(\mathcal{H}_A),$$

$$\mathrm{Tr}_{AB}(X_B \rho_{AB}) = \mathrm{Tr}_B(X_B \rho_B), \quad X_B \in \mathfrak{su}(\mathcal{H}_B),$$

which just tell that  $\rho_{AB} - \rho_A \otimes I - I \otimes \rho_B \in \mathfrak{g}^\perp$ , i.e.

$\rho_A \otimes I - I \otimes \rho_B$  is the projection of  $\rho^{AB}$  into  $\mathfrak{g}$ . Then (vwa) gives all constraints on the density spectra  $\lambda^{AB}, \lambda^A, \lambda^B$ . For a precise statement we need a case specific notations.

## Notations

For a given spectra  $a : a_1 \geq a_2 \geq \dots \geq a_m$ ,  $b : b_1 \geq b_2 \geq \dots \geq b_n$  define **flag varieties**

$$\mathcal{F}_a(\mathcal{H}_A) := \{X_A | \text{Spec}(X_A) = a\}, \quad \mathcal{F}_b(\mathcal{H}_B) := \{X_B | \text{Spec}(X_B) = b\},$$

natural morphism

$$\begin{aligned} \varphi_{ab} : \mathcal{F}_a(\mathcal{H}_A) \times \mathcal{F}_b(\mathcal{H}_B) &\rightarrow \mathcal{F}_{a+b}(\mathcal{H}_A \otimes \mathcal{H}_B), \\ X_A \times X_B &\mapsto X_A \otimes 1 + 1 \otimes X_B, \end{aligned} \quad (13)$$

and its cohomological counterpart

$$\varphi_{ab}^* : H^*(\mathcal{F}_{a+b}(\mathcal{H}_{AB})) \rightarrow H^*(\mathcal{F}_a(\mathcal{H}_A)) \otimes H^*(\mathcal{F}_b(\mathcal{H}_B)) \quad (14)$$

given in the basis of **Schubert cocycles**  $\sigma_w$  by equation

$$\varphi_{ab}^* : \sigma_w \mapsto \sum_{u,v} c_w^{uv}(a, b) \sigma_u \otimes \sigma_v. \quad (15)$$

# Mixed Quantum MP

A. Klyachko, quant-ph/040913.

The following conditions are equivalent

- There exist mixed state  $\rho_{AB}$  of  $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$  with margins  $\rho_A, \rho_B$  and spectra  $\lambda^{AB}, \lambda^A, \lambda^B$ .
- The spectra satisfy the inequality

$$\sum_i a_i \lambda_{u(i)}^A + \sum_j b_j \lambda_{v(j)}^B \leq \sum_k (a + b)_k^\downarrow \lambda_{w(k)}^{AB}, \quad (\text{uvw})$$

for traceless test spectra  $a : a_1 \geq a_2 \geq \dots \geq a_m$ ,  
 $b : b_1 \geq b_2 \geq \dots \geq b_n$ ,  $\sum a_i = \sum b_j = 0$  each time the  
coefficient  $c_w^{uv}(a, b) \neq 0$ .

Here  $(a + b)^\downarrow$  denotes the sequence terms  $a_i + b_j$  arranged in  
non-increasing order. [special case of (vwa) ].

## A closer look at the coefficients $c_w^{uv}(a, b)$

### Künneth formula

Let  $F_A(s)$  and  $F_B(t)$  be filtrations in  $\mathcal{H}_A$  and  $\mathcal{H}_B$ . Define their tensor product  $F_{AB} := F_A \otimes F_B$  as a filtration of  $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$  given by equation

$$F_{AB}(r) = \sum_{r=s+t} F_A(s) \otimes F_B(t).$$

For spectral filtrations of operators  $X_A, X_B$ , the construction amounts to spectral filtration of  $X_A \otimes I + I \otimes X_B$  cf. (13). **Künneth formula** gives composition factors  $[F](s) := F(s)/F(s+0)$  of the tensor product

$$[F_{AB}](r) = \bigoplus_{r=s+t} [F_A](s) \otimes [F_B](t). \quad (16)$$

When all composition factors have dimension  $\leq 1$  the formula amounts to unique nonzero term

$$[F_{AB}](r_k) = [F_A](s_i) \otimes [F_B](t_j), \text{ for } r_k = s_i + t_j,$$

where  $r_k, s_i, t_j$  are discontinuity points of the filtrations  $F_{AB}, F_A, F_B$  arranged in decreasing order [= spectra of the respective operators].

## The cohomology morphism and Chern classes

Returning to flag varieties, observe that eigenspaces of  $X_A \in \mathcal{F}_a(\mathcal{H}_A)$  of given eigenvalue  $a_i$  form an **eigenbundle**  $\mathcal{E}_i^A$  on  $\mathcal{F}_a(\mathcal{H}_A)$ . Alternatively,  $\mathcal{E}_i^A$  can be described as  $i$ -th composition factor of the spectral filtration  $F_A$  of  $X_A$ . This allows to evaluate pull back of the eigenbundle  $\mathcal{E}_k^{AB}$  on  $\mathcal{F}(\mathcal{H}_{AB})$  w.r. to the natural morphism

$$\begin{aligned} \varphi_{ab} : \mathcal{F}_a(\mathcal{H}_A) \times \mathcal{F}_b(\mathcal{H}_B) &\rightarrow \mathcal{F}_{a+b}(\mathcal{H}_A \otimes \mathcal{H}_B) \\ X_A \times X_B &\mapsto X_A \otimes I + I \otimes X_B \end{aligned}$$

using Künneth formula (16) which for simple spectra reads

$$\varphi_{ab}^*(\mathcal{E}_k^{AB}) = \mathcal{E}_i^A \boxtimes \mathcal{E}_j^B, \text{ for } (a+b)_k^\downarrow = a_i + b_j.$$

This gives the cohomology morphism (14) in terms of Chern classes  $x_k^{AB} = c_1(\mathcal{E}_k^{AB})$

$$\varphi_{ab}^* : x_k^{AB} \mapsto x_i^A + x_j^B, \text{ for } (a+b)_k^\downarrow = a_i + b_j. \quad (17)$$

However, it is not easy to express  $\varphi_{ab}^*$  directly in terms of  $\sigma_w$ .

## Back to Schubert cocycles

An explicit formula for Schubert cocycle  $\sigma_w$  in terms of the characteristic classes is given by [Schubert polynomial](#)

$$\sigma_w = S_w(x_1, x_2, \dots) = \partial_{w^{-1}w_0}(x_1^{n-1}x_2^{n-2} \cdots x_{n-1}),$$

where  $w_0 = (n, n-1, \dots, 2, 1)$  is the longest permutation, and operator  $\partial_w = \partial_{i_1} \partial_{i_2} \cdots \partial_{i_\ell}$  is defined via BGG operators

$$\partial_i f = \frac{f(\dots, x_i, x_{i+1}, \dots) - f(\dots, x_{i+1}, x_i, \dots)}{x_i - x_{i+1}}.$$

with indices taken from a decomposition  $w = s_{i_1} s_{i_2} \cdots s_{i_\ell}$ , into product of transpositions  $s_i = (i, i+1)$  of minimal length  $\ell = \ell(w)$ .

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with indices taken from a decomposition  $w = s_{i_1} s_{i_2} \cdots s_{i_\ell}$ , into product of transpositions  $s_i = (i, i+1)$  of minimal length  $\ell = \ell(w)$ .

## Computational formula

Adding everything together we end up with explicit formula

$$c_w^{uv}(a, b) = \partial_u^A \partial_v^B S_w(x^{AB}) \Big|_{x_k^{AB} = x_i^A + x_j^B}$$

where  $(a+b)_k^\downarrow = a_i + b_j$  and  $\ell(w) = \ell(u) + \ell(v)$ .

## Finiteness of the constraints

The coefficient  $c_w^{uv}(a, b)$  depends only on the order in which quantities  $a_i + b_j$  appear in the spectrum  $(a + b)^\downarrow$ . The order changes when the pair  $(a, b)$  crosses a hyperplane

$$H_{ij|kl} : a_i + b_j = a_k + b_\ell.$$

The hyperplanes cut the set of all pairs  $(a, b)$  into finite number of pieces called *cubicles*. For each cubicle one have to check inequality  $(uvw)$  only for its *extremal edges*. Hence the marginal constraints amounts to a *finite system* of inequalities, but the total number of extremal edges increases rapidly:

# qubits	2	3	4	5	6
# edges	2	4	12	125	>11344



## Some examples and numerology

Unfortunately for most systems **mixed** marginal constraints are too numerous to be reproduced here.

System	Rank	Inequalities
$2 \times 2$	2	7[4]
$2 \times 2 \times 2$	3	40[38]
$2 \times 3$	3	41
$2 \times 4$	4	234
$3 \times 3$	4	387
$2 \times 2 \times 3$	4	442
$2 \times 2 \times 2 \times 2$	4	805

*Pure* QMP is understandably more simple, [3,82].

## Basic inequalities

Clearly  $c_w^{uv}(a, b) = 1$  for identical permutations  $u, v, w$ . Hence the inequality

$$\sum_i a_i \lambda_i^A + \sum_j b_j \lambda_j^B \leq \sum_k (a + b)_k \lambda_k^{AB}$$

holds for all test spectra  $(a, b)$ . This amounts to a *finite* system of constraints for  $k \leq m = \dim \mathcal{H}_A, \ell \leq n = \dim \mathcal{H}_B$ :

$$\begin{aligned} \lambda_1^A + \lambda_2^A + \cdots + \lambda_k^A &\leq \lambda_1^{AB} + \lambda_2^{AB} + \cdots + \lambda_{kn}^{AB}, \\ \lambda_1^B + \lambda_2^B + \cdots + \lambda_\ell^B &\leq \lambda_1^{AB} + \lambda_2^{AB} + \cdots + \lambda_{m\ell}^{AB}, \end{aligned}$$

discovered independently by

Han Y-J , Zhang Y-Sh and Guo G-C [quant-ph/0403151](#)  
along with some inequalities from Knutson lecture.

Let  $\rho$  be a mixed state of  $n$  qubit system  $\mathcal{H}^{\otimes n}$ ,  $\dim \mathcal{H} = 2$ , and  $\rho^{(i)}$  be the reduced state of  $i$ -th component. A multicomponent version of the above solution QMP tells that all constraints on spectra  $\lambda = \text{Spec } \rho$  and  $\lambda^{(i)} = \text{Spec } \rho^{(i)}$  are given by inequalities

$$\sum_i (-1)^{u_i} a_i (\lambda_1^{(i)} - \lambda_2^{(i)}) \leq \sum_{\pm} (\pm a_1 \pm a_2 \pm \dots \pm a_n)_k^{\downarrow} \lambda_{w(k)} \quad (18)$$

for all test spectra  $\pm a_i$ , and all permutations  $u_i \in S_2$ ,  $w \in S_{2^n}$  subject to the topological condition  $c_w^{u_1 u_2 \dots u_n}(a_1, a_2, \dots, a_n) \neq 0$ . Here  $c_w^{u_1 u_2 \dots u_n}(a)$  is a coefficient at  $x_1^{u_1} x_2^{u_2} \dots x_n^{u_n}$  in the specialization of the Schubert polynomial [cf. (17)]

$$S_w(z_1, z_2, \dots, z_{2^n})|_{z_k = \pm x_1 \pm x_2 \pm \dots \pm x_n}, \quad (19)$$

where the signs are taken from  $k$ -th term of the sequence  $(\pm a_1 \pm a_2 \pm \dots \pm a_n)^{\downarrow}$ . Here  $u_i \in S_2 \simeq \mathbb{Z}_2$  is identified with binary variable  $u_i = 0, 1$ ;  $z_j$  are generators of  $H^*(\mathcal{F}(\mathcal{H}^{\otimes n}))$ , and  $x_j$  is the generator of cohomology of flag variety of  $j$ -th qubit  $\simeq \mathbb{P}^1$ .

The Ressayre condition “ $c = 1$ ” allows us to focus on **odd** coefficients and perform all the calculations modulo 2, in which case the specialization (19) takes form

$$S_w(1, 1, \dots, 1)(x_1 + x_2 + \dots + x_n)^{\ell(w)} \pmod{2} \quad (20)$$

It contains a monomial  $x_1^{u_1} x_1^{u_2} \dots x_1^{u_n}$  with  $u_i = 0, 1$  only for  $\ell(w) = 0, 1$ . This leaves us with two possibilities:

- $w$  and  $u_i$  are identical permutations. This returns us the **basic inequality**

$$\sum_i a_i (\lambda_1^{(i)} - \lambda_2^{(i)}) \leq \sum_{\pm} (\pm a_1 \pm a_2 \pm \dots \pm a_n)_k^{\downarrow} \lambda_k.$$

- $w = (k, k + 1)$  is a transposition and all  $u_i$  except one are identical permutations.

The Schubert polynomial for a transposition is well known  $S_{(k, k+1)}(z) = z_1 + z_2 + \dots + z_k$ . Hence for even  $k$  specialization (20) vanishes.

## Mixed QMP Ansatz for an array of qubits

For an array of qubits all marginal constraints can be obtained from the basic inequality

$$\sum_i a_i (\lambda_1^{(i)} - \lambda_2^{(i)}) \leq \sum_{\pm} (\pm a_1 \pm a_2 \pm \cdots \pm a_n)_k^{\downarrow} \lambda_k$$

by a transposition  $\lambda_k \leftrightarrow \lambda_{k+1}$  for an **odd**  $k$  in its RHS combined with sign change  $a_i \mapsto -a_i$  of a term in LHS.

## Mixed 3-qubit constraints

$$\Delta_3 \leq \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 - \lambda_5 - \lambda_6 - \lambda_7 - \lambda_8.$$

$$\Delta_2 + \Delta_3 \leq 2\lambda_1 + 2\lambda_2 - 2\lambda_7 - 2\lambda_8.$$

$$\Delta_1 + \Delta_2 + \Delta_3 \leq 3\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 - \lambda_5 - \lambda_6 - \lambda_7 - 3\lambda_8,$$

$$-\Delta_1 + \Delta_2 + \Delta_3 \leq 3\lambda_2 + \lambda_1 + \lambda_3 + \lambda_4 - \lambda_5 - \lambda_6 - \lambda_7 - 3\lambda_8,$$

$$-\Delta_1 + \Delta_2 + \Delta_3 \leq 3\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 - \lambda_5 - \lambda_6 - \lambda_8 - 3\lambda_7.$$

$$\Delta_1 + \Delta_2 + 2\Delta_3 \leq 4\lambda_1 + 2\lambda_2 + 2\lambda_3 - 2\lambda_6 - 2\lambda_7 - 4\lambda_8,$$

$$-\Delta_1 + \Delta_2 + 2\Delta_3 \leq 4\lambda_2 + 2\lambda_1 + 2\lambda_3 - 2\lambda_6 - 2\lambda_7 - 4\lambda_8,$$

$$-\Delta_1 + \Delta_2 + 2\Delta_3 \leq 4\lambda_1 + 2\lambda_2 + 2\lambda_4 - 2\lambda_6 - 2\lambda_7 - 4\lambda_8,$$

$$-\Delta_1 + \Delta_2 + 2\Delta_3 \leq 4\lambda_1 + 2\lambda_2 + 2\lambda_3 - 2\lambda_5 - 2\lambda_7 - 4\lambda_8,$$

$$-\Delta_1 + \Delta_2 + 2\Delta_3 \leq 4\lambda_1 + 2\lambda_2 + 2\lambda_3 - 2\lambda_6 - 2\lambda_8 - 4\lambda_7,$$

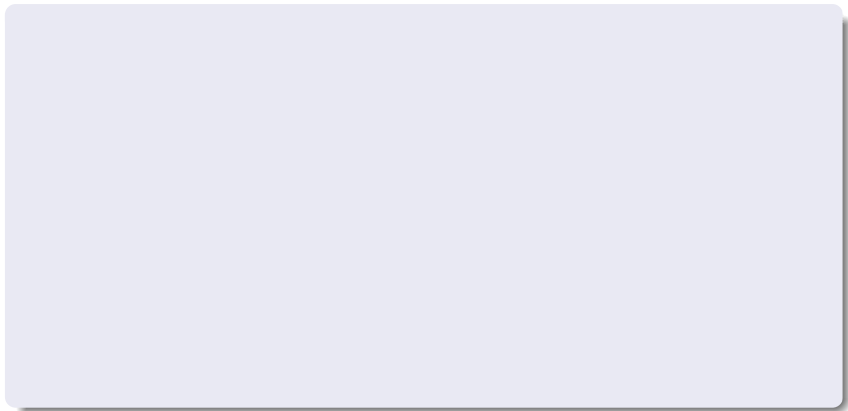
where  $\Delta_i = \lambda_1^{(i)} - \lambda_2^{(i)}$ ,  $\Delta_1 \leq \Delta_2 \leq \Delta_3$ . The transposed eigenvalues and added signs are shown in color.

# The Pauli exclusion principle and beyond

*“Symmetry principles underpin the elegant quantum mechanical description in an abstract picture in which statics and dynamics are paradoxically conflated in a way which often leave us hovering between abstract mathematical understanding and literal physical misunderstanding.”*

Sir Harold Kroto, Nobel Lecture 1996

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$$\langle \psi | \rho | \psi \rangle \leq 1, \quad (\text{PEP})$$

for any one-electron state  $\psi$ . Here  $\rho = \langle \Psi | a_i^\dagger a_j | \Psi \rangle$  is Dirac's density matrix of a multi-electron state  $\Psi$ , normalized to  $\text{Tr } \rho = N$ .

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- Or in terms of its eigenvalues:  $\text{Spec } \rho \leq 1$ .

# Heisenberg refinement

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- **Heisenberg (1926):** The multi-electron state  $\Psi$  is skew symmetric with respect to permutations of particles

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- The impact of this replacement on the density matrix  $\rho$  goes far beyond the original Pauli exclusion principle and leads to numerous *extended Pauli constraints* independent of (PEP). These constraints and their physical manifestations are the main subject of this talk. For more details see Altunbulak and Klyachko, Commun. Math. Phys. **292**, 287 (2008); A. Klyachko, arXiv:0904.2009v1 [quant-ph].

## Explicit form of the extended Pauli constraints

Let  $\rho^N$  be a mixed state of a system  $\wedge^N \mathcal{H}_r$  and  $\rho$  its density matrix. Then all constraints on spectra  $\mu = \text{Spec } \rho^N$  and  $\lambda = \text{Spec } \rho$  are of the form

$$\sum_i a_i \lambda_{v(i)} \leq \sum_j (\wedge^N a)_j \mu_{w(j)}, \quad (\text{avw})$$

for all “test spectra”  $a : a_1 \geq a_2 \geq \cdots \geq a_r, \sum a_i = 0$ . Here  $\wedge^N a = \{a_{i_1} + a_{i_2} + \cdots + a_{i_N}\}^\downarrow$  and  $v$  and  $w$  are permutations, subject to a **topological constraint**  $c_w^v(a) \neq 0$  coming from (vwa).

The test spectrum  $a$  defines the *flag variety*

$\mathcal{F}_a(\mathcal{H}) = \{X : \mathcal{H} \rightarrow \mathcal{H} \mid \text{Spec } X = a\}$  and morphism  
 $\varphi_a : \mathcal{F}_a(\mathcal{H}) \rightarrow \mathcal{F}_{\wedge^N a}(\wedge^N \mathcal{H}), \quad X \mapsto X^{(N)}$

$$X^{(N)} : x \wedge y \wedge \cdots \mapsto Xx \wedge y \wedge \cdots + x \wedge Xy \wedge \cdots$$

The coefficients  $c_w^\vee(\alpha)$  are determined by the induced morphism of cohomology

$$\varphi_a^* : H^*(\mathcal{F}_{\wedge^N a}(\wedge^N \mathcal{H})) \rightarrow H^*(\mathcal{F}_a(\mathcal{H}))$$

written in the basis of *Schubert cocycles*  $\sigma_w$

$$\varphi_a^* : \sigma_w \mapsto \sum_v c_w^\vee(a) \sigma_v.$$



# Application

## Application

- Riemann curvature tensor  $R : \wedge^2 \mathcal{T} \rightarrow \wedge^2 \mathcal{T}$  can be considered as a selfadjoint operator on 2-forms (or 2-vectors) in tangent space  $\mathcal{T}$  of a Riemann manifold  $\mathcal{M}$ .

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- It determines the characteristic classes and shapes the topology of the manifold  $\mathcal{M}$ .
- Contraction of the Riemann tensor  $Ric : \mathcal{T} \rightarrow \mathcal{T}$  is known as Ricci curvature. The latter via **trace reversed** Einstein equation  $Ric = 8\pi(T - \frac{1}{2} \text{Tr } T)$  is determined by matter, i.e. by the stress-energy-momentum tensor  $T$ .

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- While in dimension 5 there are **460** constraints.

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where  $\nu^t =$  transpose diagram,  $\mathcal{H}_\ell^\nu =$  irrep. of  $U(\mathcal{H}_\ell)$ ,  $\mathcal{H}_s^{\nu^t} =$  irrep. of  $U(\mathcal{H}_s)$  with Young diagrams  $\nu, \nu^t$ .



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- Similar constraints hold for spin resolved **bosonic** state  $\Psi \in \mathcal{H}_\ell^\nu \otimes \mathcal{H}_s^\nu$ , where reference to Pauli is irrelevant.
- **Example.** Consider three electrons in  $d$ -shell ( $\dim \mathcal{H}_\ell = 5$ ) in low spin configuration  $\nu = \begin{array}{|c|c|} \hline & \\ \hline \end{array}$  where the constraints are as follows

$$\begin{aligned}\lambda_1 + \frac{1}{2}(\lambda_4 + \lambda_5) &\leq 2, \\ \mu &\leq 3 - 2(\lambda_1 - \lambda_2), \quad \mu \leq 3 - 2(\lambda_2 - \lambda_3), \\ \mu &\geq 2(\lambda_1 - \lambda_3) - 3, \quad \mu \geq 4\lambda_1 - 2\lambda_2 + 2\lambda_4 - 7.\end{aligned}$$

Here  $\mu = \mu_1 - \mu_2$  is spin magnetic moment in Bohr magnetons  $\mu_B$ .

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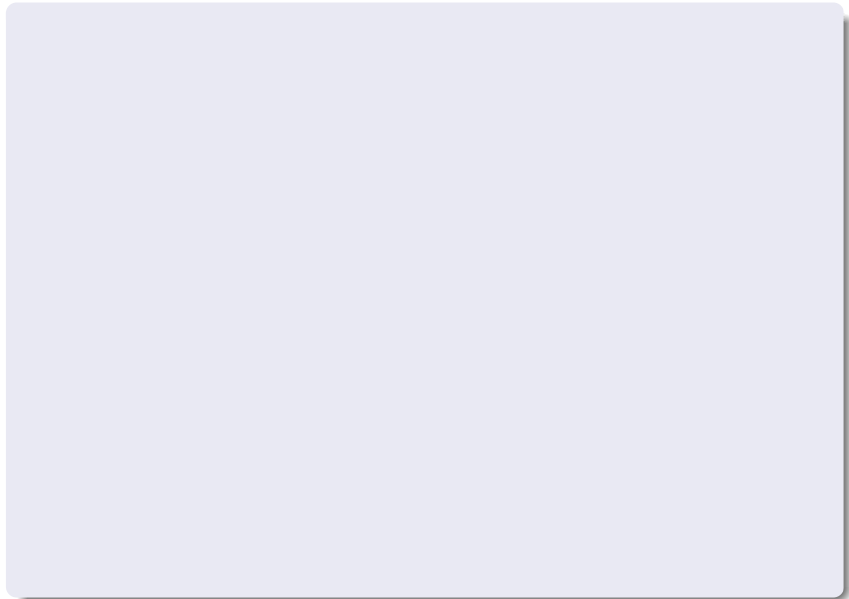
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- A pinned system is essentially a new physical entity with its own dynamics and kinematics.

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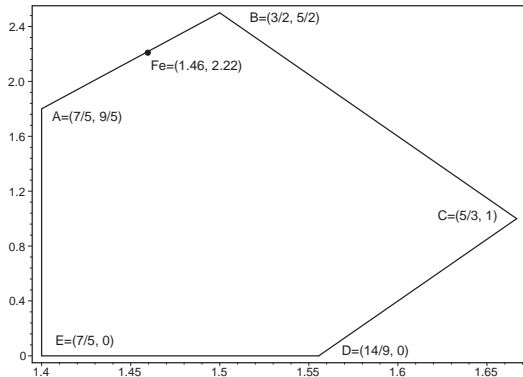
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- Hence orbital occupation numbers  $\lambda = (n_t, n_t, n_t, n_e, n_e)$ ,  $3n_t + 2n_e = 7$ ,  $n_t \geq n_e$  depend only on one parameter  $n_t$ .

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- The occupation number for iron  $n_t = 1.46$  was found by W.Jauch&M.Reehuis, Phys. Rev. B, **76**, 235121 (2007).





**Figure:** Pauli constraints on spin magnetic moment ( $\mu_B$ ) for 7 electrons in  $d$ -shell in cubic crystal field versus the occupation number  $n_t$  of a  $t_{2g}$  orbital. All points within the pentagon  $ABCDE$  are admissible. A black dot represents experimental data for iron.

QMP includes as a special case *quasiclassical MP* about relations between spectra of Hermitean matrices  $H_A$ ,  $H_B$ , and

$$H_{AB} = \left[ \begin{array}{c|c} H_A & * \\ \hline * & H_B \end{array} \right], \quad (22)$$

which may be seen as Hamiltonians of mechanical systems  $A$ ,  $B$  and their coupling  $AB$ . For another approach see C.-K. Li and Y.-T. Poon, *Linear and Multilinear Algebra*, **51** (2003), no. 2, 199–208.

# Entanglement and GIT

A driving force of these results is *Geometric Invariant Theory*, which fairly can be called a *mathematical theory of entanglement*, see

[A. Klyachko, quant-ph/0206012](#).

*“The basic principles of quantum mechanics seem to require the postulation of Lie algebra of observables and a representation of this algebra by skew Hermitean operators in a Hilbert space.”* [R. Hartman](#)

$\mathcal{L}$  – the Lie algebra of *essential* observables,

$G = \exp(\mathcal{L})$  – dynamic symmetry group,

$G_{\mathbb{C}} = \exp(\mathcal{L} \otimes \mathbb{C})$  – its complexification,

$G : \mathcal{H}$  – quantum dynamic system.

## Example

For two component system  $\mathcal{H}_A \otimes \mathcal{H}_B$  with full access to local degrees of freedom

$$\mathcal{L} = \{X_A \otimes 1 + 1 \otimes X_B\}, \quad G = \mathrm{SU}(\mathcal{H}_A) \times \mathrm{SU}(\mathcal{H}_B),$$

and complexified group  $G_{\mathbb{C}} = \mathrm{SL}(\mathcal{H}_A) \times \mathrm{SL}(\mathcal{H}_B)$  can be interpreted as group of invertible SLOCC transformations, see [F. Verstrate, J. Dehaene, and B. De Moor, quant-ph/0105090](#).

An important invariant of dynamic system  $G : \mathcal{H}$  is the *total variance* of state  $\psi \in \mathcal{H}$

$$\mathbb{D}(\psi) = \sum_{X_i = \text{orth. basis } \mathcal{L}} \langle \psi | X_i^2 | \psi \rangle - \langle \psi | X_i | \psi \rangle^2 \quad (23)$$

which is *independent of the basis*  $X_i$  and measures overall quantum fluctuations of the system in state  $\psi$ .  $\sum_i X_i^2$  is known as *Casimir operator*.

### Example

For state  $\psi$  of  $N$  qubit

$$N \leq \mathbb{D}(\psi) \leq N \left( \frac{3}{2} \right).$$

The minimum corresponds to *separable states*, and the maximum to *completely entangled* ones.

## Synopsis of math approach to entanglement.

- In *completely entangled state*  $\psi$  the system is at the center of its quantum fluctuations

$$\langle \psi | X | \psi \rangle = 0, \forall X \in \mathcal{L}$$

Entanglement  
equation

(24)

This ensure maximality of the total variance (23).

- Eqn (24) identifies  $\psi$  with *vector of minimal length* in its complex orbit  $\{g\psi | g \in G_{\mathbb{C}}\}$ . The minimal vector is unique up to action of  $G$ .
- $G_{\mathbb{C}}$  is group of invertible SLOCC operations, cf Ex.0.1.

## Example

Entanglement equation (24) implies that  $\psi \in \mathcal{H}_{ABC} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$  is completely entangled iff its marginals  $\rho_A, \rho_B, \rho_C$  are scalar operators, cf. ??.

From operational point of view state  $\psi \in \mathcal{H}$  is *entangled* iff one can filter out from  $\psi$  a completely entangled state  $\psi_0$  using SLOCC operations, i.e.  $\psi_0 = g\psi$  for some  $g \in G_{\mathbb{C}}$ . In GIT such states are called *stable* (or *semistable* if  $\psi_0$  can be reached only asymptotically).

## Dictionary

Quantum Information	Invariant Theory
Entangled state	Semitable vector
SLOCC operations	Complexified group
Completely entangled state $\psi_0$ prepared from $\psi$ by SLOCC	Minimal vector $\psi_0$ in complex orbit of $\psi$



Characterization of entangled states, i.e. criteria for (semi)stability, is one of the central problems in GIT.

**Classical Criterion:**  $\psi$  is *semistable* iff it can be separated from zero by an invariant polynomial

$$f(\psi) \neq f(0), \quad f(gx) = f(x), \forall g \in G.$$

### Example

For two component system the basic invariant is  $\det[\psi_{ij}]$ , related to concurrence by equation  $C = 2 |\det[\psi_{ij}]|$ . Unique basic invariant for 3-qubit is *Cayley hyperdeterminant*  $\text{Det}[\psi_{ijk}]$ . There are 4 basic invariants for 4-qubits, and starting from 5-qubits the invariants are still unknown.

In a broader context [Bryce S. DeWitt](#) described the situation as follows:

*“Why should we not go directly to invariants? The whole of physics is contained in them. The answer is that it would be fine if we could do it. But it is not easy.”*

*Geometric Invariant Theory* was created by Hilbert at the end of 19th century just to overcome this difficulty.

**Hilbert-Mumford Criterion:** State  $\psi \in \mathcal{H}$  is *semistable* iff every observable  $X \in \mathcal{L} = \text{Lie}(G)$  of the system in state  $\psi$  assumes both nonnegative  $\geq 0$  and nonpositive  $\leq 0$  values.

### Example

Let  $X = X_A \otimes 1 + 1 \otimes X_B$  be observable of two qubit system  $\mathcal{H}_A \otimes \mathcal{H}_B$  with

$$\text{Spec } X_A = \pm\alpha, \quad \text{Spec } X_B = \pm\beta.$$

Then  $X$  assumes those values  $\pm\alpha \pm \beta$  for which  $\langle \psi | \pm\alpha \pm \beta \rangle \neq 0$ . If all the values are strictly positive then  $\psi$  is separable, i.e. Hilbert-Mumford criterion characterizes entangled qubits.

The general form of H-M criterion may shed some light on the nature of entanglement. However, the criterion was originally designed for application to *geometric objects*, like linear subspaces or hypersurfaces of higher degree, and its effectiveness entirely depends on our ability to spell it out in terms of *geometric properties* of the underlying objects.

### Example

H-M criterion for forms  $F(x_1, x_2, \dots, x_n)$  of degree  $d$  w.r. to  $G = \mathrm{SU}(n)$  can be expressed in terms of *singularities* of hypersurface  $S : F(x_1, x_2, \dots, x_n) = 0$ , e.g. nonsingular hypersurfaces are always stable.

Let's apply this philosophy to a system of observables  $X_\alpha : \mathcal{H} \rightarrow \mathcal{H}$ . We associate with operator  $X_\alpha$  its *spectral filtration*, i.e. one parametric family of subspaces

$$\mathcal{H}^\alpha(t) = \left\{ \begin{array}{l} \text{subspace spanned by eigenspaces of } X_\alpha \\ \text{with eigenvalues } \geq t \end{array} \right\}, \quad t \in \mathbb{R}.$$

*Spectral decomposition*

$$X_\alpha = \int_{-\infty}^{\infty} P^\alpha(t) dt, \quad P^\alpha(t) = \text{projector onto } \mathcal{H}^\alpha(t)^\perp.$$

recovers operator  $X_\alpha$  from its spectral filtration.

The spectral filtration, being a collection of labeled subspaces, is a geometrical substitution for Hermitean operator.

To put filtrations in framework of GIT we have first to coordinatize them by vectors in a Hilbert space.

### Example

Following Grassmann  $d$ -subspace  $V = \langle \psi_1, \psi_2, \dots, \psi_d \rangle \subset \mathcal{H}$  can be described by decomposable skew symmetric tensor

$$V \mapsto \psi_1 \wedge \psi_2 \wedge \dots \wedge \psi_d \in \wedge^d \mathcal{H}$$

known to physicists as *Slater determinant*.

In a similar way filtrations ( = operators  $X_\alpha$ ) with fixed integral spectrum  $\lambda_\alpha = \text{Spec}(X_\alpha)$  can be coordinatized by *highest vectors*  $\psi_\alpha \in \mathcal{H}(\lambda_\alpha)$  in irreducible representation of  $\text{GL}(\mathcal{H})$  with *highest weight*  $\lambda_\alpha$ .

Finally the whole system of observables  $X_\alpha$  can be described by tensor  $\bigotimes_\alpha \psi_\alpha \in \bigotimes_\alpha \mathcal{H}(\lambda_\alpha)$ , and we can ask about stability of this tensor w.r. to say full group  $SU(\mathcal{H})$ .

### Theorem

*Family of observables  $X_\alpha : \mathcal{H} \rightarrow \mathcal{H}$  is semistable w.r. to  $G = SU(\mathcal{H})$  iff the following inequality*

$$\sum_\alpha \iint \dim[\mathcal{H}^\alpha(s) \cap \mathcal{H}^0(t)] ds dt \leq \frac{1}{\dim \mathcal{H}} \sum_\alpha \iint \dim \mathcal{H}^\alpha(s) \dim \mathcal{H}^0(t) ds dt.$$

*holds for all “test” operators  $X_0 : \mathcal{H} \rightarrow \mathcal{H}$ .*

Entanglement eqn (24) for the system  $X_\alpha$  gives

$$\sum_\alpha X_\alpha = \text{scalar operator.} \quad (25)$$

*Remark.* For fixed  $\alpha$  the test filtrations with given dimensions  $\dim(\mathcal{H}^\alpha(s) \cap \mathcal{H}^0(t))$  form *Schubert cell*  $c_{w_\alpha}$  corresponding to some permutation  $w_\alpha \in S_n$ ,  $n = \dim \mathcal{H}$ . In terms of these permutations Theorem 0.1 amounts to inequalities

$$\sum_{\alpha} \lambda_{w_\alpha(i)}^0 \lambda_i^\alpha \leq 0$$

each time  $\bigcap_{\alpha} c_{w_\alpha} \neq \emptyset$ . These inequalities are equivalent to solvability entanglement equation (25). In simplest case this gives all constraints on spectra of Hermitean operators  $A$ ,  $B$ , and  $A + B$ , see

A. Klyachko, *Selecta Math.* **4**(1998), 419–445.



Actually Theorem 0.1 holds for arbitrary subgroup  $G \subset \text{SU}(\mathcal{H})$  with test operator  $X_0$  taken from the corresponding Lie algebra  $\mathcal{L} = \text{Lie}(G)$ . Entanglement equation in this case takes form (cf. Eqn 25)

$$\sum_{\alpha} X_{\alpha} \in \mathcal{L}^{\perp} = \{Y | \text{Tr}(XY) = 0, \quad \forall X \in \mathcal{L}\}.$$

### Example

Taking  $\mathcal{H} = \mathcal{H}_A \oplus \mathcal{H}_B$ ,  $G = \text{SU}(\mathcal{H}_A) \times \text{SU}(\mathcal{H}_B)$  we get a solution of the *quasiclassical MP* (22).

### Example

Another choice  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ ,  $G = \text{SU}(\mathcal{H}_A) \times \text{SU}(\mathcal{H}_B)$  solves the mixed QMP (28).

## Example

Exterior  $\mathcal{H} = \bigwedge^n \mathcal{H}_1$  and symmetric  $\mathcal{H} = S^n \mathcal{H}_1$  powers lead to so called *N-representability problem* discussed in the next section.

# $N$ -representability problem

QMP may be complicated by additional constraints on state  $\psi$ . For example, Pauli principle implies

$$(\text{State space of } N \text{ identical particles}) = \begin{cases} S^N \mathcal{H}, & \text{for bosons,} \\ \bigwedge^N \mathcal{H}, & \text{for fermions.} \end{cases}$$

For such systems reduced matrices appear in the second quantization formalism in the form

$$\begin{aligned} \rho^{(1)} &= \langle \psi | a_i^\dagger a_j | \psi \rangle = \text{1 particle RDM,} \\ \rho^{(2)} &= \langle \psi | a_i^\dagger a_j^\dagger a_k a_l | \psi \rangle = \text{2 particle RDM, etc.} \end{aligned}$$

Their physical importance stems from the observation that, say for *fermionic system*, like multi electron atom or molecule, with pairwise interaction

$$H = \sum_i^N H_i + \sum_{i < j} H_{ij}$$

the energy of state  $\psi$  depends only on 2-point RDM

$$E = \binom{N}{2} \text{Tr} (H^{(2)} \rho^{(2)}),$$

where  $H^{(2)} = \frac{1}{N-1} [H_1 + H_2] + H_{12}$  is reduced two particle Hamiltonian.

This allows, for example, to express the energy of ground state  $E_0$  via 2-point RDM

$$E_0 = \binom{N}{2} \min_{\rho^{(2)}=\text{RDM}} \text{Tr}(H^{(2)}\rho^{(2)}).$$

The problem however is that it is not obvious what conditions the RDM itself should satisfy. This is what the QMP is about. In this settings it is known from late 50-th as  *$N$ -representability problem*.

*"Until these conditions have been elucidated it is going to be difficult to make much progress along this line."* C.A. Coulson, *Rev. Mod. Phys.*, 32(1960),175.

Later in mid 90-th the  $N$ -representability problem was regarded as one of ten most prominent research challenges in quantum chemistry.

F.H. Stillinger et al. National Research Council, National Academy Press, 1995.

Its solution allows to calculate nearly all properties of matter which are of interest to chemists and physicists. This notwithstanding little or no progress has been made in this area in the last decade.

# One point $N$ -representability

Following chemists we interpret one point reduced matrix  $\rho^{(1)}$  as electron density and use normalization  $\text{Tr } \rho^{(1)} = \mathbf{N}$ . There are few cases where complete rigorous solution was known prior 2005.

(i) Pauli principle:  $0 \leq \lambda_i \leq 1$ ,  $\lambda = \text{Spec } \rho^{(1)}$ .

This condition provides a criterion for *mixed  $N$ -representability*.

(ii) Criterion for two particles  $\bigwedge^2 \mathcal{H}_r$  or two holes  $\bigwedge^{r-2} \mathcal{H}_r$  is given by even degeneration of all eigenvalues, except 0 (resp. 1) for odd  $r = \dim \mathcal{H}_r$ .

A.J. Coleman, Rev. Mod. Phys., 35(1963), 668.

(iii) Criterion for system  $\bigwedge^3 \mathcal{H}_6$ :

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

where  $\text{Spec} \rho^{(1)} : \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq \lambda_5 \geq \lambda_6$ .

P.E. Borland and K. Dennis, J. Phys B, 5(1972),7.

*"We have no apology for consideration of such a special case. The general  $N$ -representability problem is so difficult and yet so fundamental for many branches of science that each concrete result is useful in shedding light on the nature of general solution."*

For more than 30 years no other solution of  $N$ -representability problem has been found.



Borland and Dennis derived their criterion from an extensive computer experiment, and later proved it with help provided by M.B. Ruskai and R.L. Kingsly. They also conjectured criteria for systems  $\bigwedge^3 \mathcal{H}_7, \bigwedge^4 \mathcal{H}_7, \bigwedge^4 \mathcal{H}_8$ , e.g. for  $\bigwedge^3 \mathcal{H}_7$  the one point representability is given by 4 inequalities

$$\begin{aligned}\lambda_1 + \lambda_6 + \lambda_7 &\geq 1, & \lambda_2 + \lambda_5 + \lambda_7 &\geq 1, \\ \lambda_3 + \lambda_4 + \lambda_7 &\geq 1, & \lambda_3 + \lambda_5 + \lambda_6 &\geq 1,\end{aligned}$$

but they were unable to prove them. The conjectures turn out to be true and covered by the following general result.

## Theorem

For system  $\bigwedge^n \mathcal{H}_r$  all constraints on spectra  $\lambda = \text{Spec } \rho$  and  $\mu = \text{Spec } \rho^{(1)}$  are given by inequalities

$$\sum_i a_i \mu_{v(i)} \leq \sum_j (\wedge^n a)_j \lambda_{w(j)}$$

for all “test spectra”  $a : a_1 \geq a_2 \geq \dots \geq a_r, \sum a_i = 0$ . Here  $\wedge^n a = \{a_{i_1} + a_{i_2} + \dots + a_{i_n}\} \downarrow$  and  $v \in S_r, w \in S_{\binom{n}{r}}$  are permutations subject to **geometric condition**  $c_w^v(a) \neq 0$  to be explained below.

**Explanation.** For the test spectra  $a$  define *flag variety*  $\mathcal{F}_a(\mathcal{H}) := \{A | \mathrm{Spec}(A) = a\}$  and morphism

$$\begin{aligned}\varphi_a : \mathcal{F}_a(\mathcal{H}) &\rightarrow \mathcal{F}_{\wedge^n a}(\wedge^n \mathcal{H}), \\ A &\mapsto A^{(n)}, \\ A^{(n)} : x \wedge y \wedge \cdots &\mapsto Ax \wedge y \wedge \cdots + x \wedge Ay \wedge \cdots\end{aligned}$$

The induced morphism of cohomology

$$\varphi_a^* : H^*(\mathcal{F}_{\wedge^n a}(\wedge^n \mathcal{H})) \rightarrow H^*(\mathcal{F}_a(\mathcal{H}))$$

in the basis of *Schubert cocycles*  $\sigma_w$  is given by

$\varphi_a^* : \sigma_w \mapsto \sum_v c_w^v(a) \sigma_v$ . Calculation of the coefficients  $c_w^v(a)$  is a pretty tricky problem, but it can be solved and implemented into a computer program.

## Example

For system  $\wedge^2 \mathcal{H}_4$  the marginal constraints on  $\lambda = \text{Spec}(\rho)$  and  $\mu = \text{Spec}(\rho^{(1)})$  are given by inequalities

$$2\mu_1 \leq \lambda_1 + \lambda_2 + \lambda_3, \quad 2\mu_4 \leq \lambda_4 + \lambda_5 + \lambda_6$$

$$2(\mu_1 + \mu_4) \leq \lambda_1 + \lambda_2 - \lambda_5 - \lambda_6,$$

$$\mu_1 + \mu_2 - \mu_3 - \mu_4 \leq \lambda_1 - \lambda_6,$$

$$\mu_1 - \mu_2 + \mu_3 - \mu_4 \leq \min(\lambda_1 - \lambda_5, \lambda_2 - \lambda_6),$$

$$|\mu_1 - \mu_2 - \mu_3 + \mu_4| \leq \min(\lambda_1 - \lambda_4, \lambda_2 - \lambda_5, \lambda_3 - \lambda_6),$$

$$2 \max(\mu_1 - \mu_3, \mu_2 - \mu_4) \leq \min(\lambda_1 + \lambda_3 - \lambda_5 - \lambda_6, \lambda_1 + \lambda_2 - \lambda_4 - \lambda_6),$$

$$2 \max(\mu_1 - \mu_2, \mu_3 - \mu_4) \leq \min(\lambda_1 + \lambda_3 - \lambda_4 - \lambda_6, \lambda_2 + \lambda_3 - \lambda_5 - \lambda_6),$$

$$\lambda_1 + \lambda_2 - \lambda_4 - \lambda_5,$$

## Example

Compatibility conditions for  $\wedge^2 \mathcal{H}_5$  contain **460** independent inequalities.

# Representation theory

Let  $S^\lambda$  be irreducible representation of the *symmetric group*  $S_n$  corresponding to *Young diagram*

$\lambda : \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k > 0, |\lambda| := \sum_i \lambda_i = n.$

$$\lambda = (5, 4, 2, 1) = \begin{array}{|c|c|c|c|c|} \hline \square & \square & \square & \square & \square \\ \hline \square & \square & \square & \square & \\ \hline \square & \square & & & \\ \hline \square & & & & \\ \hline \end{array}, \quad \tilde{\lambda} := \frac{1}{n}\lambda.$$

$S^\lambda \otimes S^\mu$  splits into irreducible components

$$S^\lambda \otimes S^\mu = \sum_{\nu} g(\lambda, \mu, \nu) S^\nu, \quad |\lambda| = |\mu| = |\nu|,$$

with multiplicities  $g(\lambda, \mu, \nu)$  known as *Kronecker coefficients*.

Calculation of the Kronecker coefficients is a tricky problem, arguably considered as “... *the last major problem in ordinary representation theory of  $S_n$* ”, Y. Dvir, *J. of Algebra* **154** (1993), 125–140.

### Theorem

*If  $g(\lambda, \mu, \nu) \neq 0$  then  $(\tilde{\lambda}, \tilde{\mu}, \tilde{\nu})$  are marginal spectra of a pure state  $\psi \in \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$  and such spectra are dense in the space of all marginal spectra (for pure QMP).*

A beautiful proof of this theorem based on quantum information technic was found recently by M. Christandl & G. Mitchison, [quant-ph/0409016](#).

$\text{QMP} \Leftrightarrow \text{Asymptotic support of } g(\lambda, \mu, \nu).$

## Example

It is known (134) that maximal length of the first row of Young diagrams  $\nu$  s.t.  $S^\nu \subset S^\lambda \otimes S^\mu$  is equal to  $|\lambda \cap \mu| = \sum_i \min(\lambda_i, \mu_i)$ . Thm. 0.3 recasts this into information about *maximal eigenvalue* of state  $\rho_{AB}$  with given margins

$$\max_{\rho_{AB}} \lambda_1^{AB} = \sum_i \min(\lambda_i^A, \lambda_i^B) \geq \min(\lambda_1^A, \lambda_1^B).$$

For *separable state*  $\rho_{AB}$ , Nielsen-Kempe majorization inequality  $\lambda^A \succ \lambda^{AB}$  implies just the opposite:  $\lambda_1^A \geq \lambda_1^{AB}$ . Hence  $\rho_{AB}$  with maximal possible  $\lambda_1^{AB}$  is entangled, provided neither  $\rho_A$  nor  $\rho_B$  is a pure state. *Separability can't be detected by reduces states.*

## Example

Pure QMP for 3 qutrits  $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$  was solved independently by [M. Franz, J. Lie Theory, 12, 539–549 \(2002\)](#) and [A. Higuchi, quant-ph/0309186 \(2003\)](#):

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

where  $a, b, c$  is a permutation of  $A, B, C$ .