

Quantum marginal problem

Alexander Klyachko

Department of Mathematics
Bilkent University

August 3, 2009

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 ρ_A, ρ_B, ρ_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 ρ_{AB} of two component system $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ and its reduced states ρ_A, ρ_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 λ_i of the marginal states ρ_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 λ_A, λ_B are minimal eigenvalues of ρ_A, ρ_B ;
 $\lambda_1^{AB} \geq \lambda_2^{AB} \geq \lambda_3^{AB} \geq \lambda_4^{AB}$ is spectrum of ρ_{AB} .

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

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 $\Phi \in \bigotimes_{\alpha} \wedge^{d_{\alpha}} \mathcal{H}$.

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 $\Phi \in \bigotimes_{\alpha} \wedge^{d_{\alpha}} \mathcal{H}$.

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 Φ and the configuration are said to be **stable**. Vectors Φ 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**.

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**.

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.

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.

Kempf-Ness unitary trick (1978)

The following conditions are equivalent

- Vector Φ 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 Φ_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 Φ defines unique up to proportionality metric in which Φ 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.

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.

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_{α} = orthogonal projector onto F_{α} 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_α 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 $\sum_\alpha \tilde{\ell}_\alpha = 0$.

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_α 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 $\sum_\alpha \tilde{\ell}_\alpha = 0$.

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 ℓ_α , 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_ℓ 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_{α} =orthogonal projector onto F_{α} . **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**.

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**.

To this end we first of all need a **holomorphic** metric independent substitution for Hermitean operator X_α , which would play the same role as subspace $F_\alpha = \text{Im}(P_\alpha)$ used for projector P_α . 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_α .

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 λ_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_α depends only on the **labels** of the flag (4), but not the flag itself, i.e. it is essentially a **free parameter**.

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_α depends only on the **labels** of the flag (4), but not the flag itself, i.e. it is essentially a **free parameter**.

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**.

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**.

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 $F_\alpha(s)$.

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**.

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 $F_\alpha(s)$.

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

A closer look at the integrals

Suppose the operators X_α 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: $\prod_\alpha \sigma_{I_\alpha} \neq 0$.

A closer look at the integrals

Suppose the operators X_α 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: $\prod_\alpha \sigma_{I_\alpha} \neq 0$.

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_α 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 λ, μ, ν ;
- 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 σ_K enters into decomposition of $\sigma_I \cdot \sigma_J$ with a nonzero coefficient.

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 λ, μ, ν ;
- 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 σ_K enters into decomposition of $\sigma_I \cdot \sigma_J$ with a nonzero coefficient.

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.

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.

$G \subset SU(\mathcal{H})$ – 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.

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.

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 ≤ 1 . Then

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

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 **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.

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^{φ} 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^{φ} 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 ν, w s.t. Schubert cocycle σ_{ν} 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 ρ_A, ρ_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 ρ^{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** σ_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 ρ_{AB} of $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ with margins ρ_A, ρ_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 ≤ 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 φ_{ab}^* directly in terms of σ_w .

Back to Schubert cocycles

An explicit formula for Schubert cocycle σ_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 $\ell = \ell(w)$.

Back to Schubert cocycles

An explicit formula for Schubert cocycle σ_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 $\ell = \ell(w)$.

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
2×2	2	7[4]
$2 \times 2 \times 2$	3	40[38]
2×3	3	41
2×4	4	234
3×3	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,??].

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 ρ 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

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

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

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

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

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

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

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

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

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

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

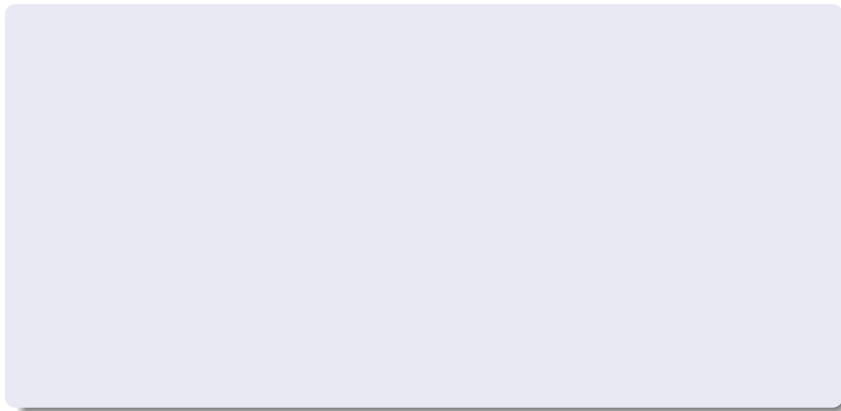
where $\Delta_i = \lambda_1^{(i)} - \lambda_2^{(i)}$, $\Delta_1 \leq \Delta_2 \leq \Delta_3$. The transposed eigenvalues and added signs are shown in color.

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

Original version(s) of Pauli principle



Original version(s) of Pauli principle

- Initial form (1925): No quantum state can be occupied by more than one electron (no wavefunctions at that time!).

Original version(s) of Pauli principle

- Initial form (1925): No quantum state can be occupied by more than one electron (no wavefunctions at that time!).
- Restatement in terms of density matrix:

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

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

Original version(s) of Pauli principle

- Initial form (1925): No quantum state can be occupied by more than one electron (no wavefunctions at that time!).
- Restatement in terms of density matrix:

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

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

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

Heisenberg refinement

Heisenberg refinement

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

$$\Psi \in \wedge^N \mathcal{H} \subset \mathcal{H}^{\otimes N}, \quad \mathcal{H} = \text{one-electron space.}$$

Heisenberg refinement

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

$$\Psi \in \wedge^N \mathcal{H} \subset \mathcal{H}^{\otimes N}, \quad \mathcal{H} = \text{one-electron space.}$$

- The impact of this replacement on the density matrix ρ 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 ρ^N be a mixed state of a system $\wedge^N \mathcal{H}_r$ and ρ 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 $c_w^v(\alpha)$ 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* σ_w

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

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} .

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} .
- It determines the characteristic classes and shapes the topology of the manifold \mathcal{M} .

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} .
- 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 .

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} .
- 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 .
- The above theorem (avw) in this case imposes constraints on spectra $\mu = \text{Spec } R$ and $\lambda = \text{Spec } Ric$ of Riemann and Ricci operators,

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} .
- 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 .
- The above theorem (avw) in this case imposes constraints on spectra $\mu = \text{Spec } R$ and $\lambda = \text{Spec } Ric$ of Riemann and Ricci operators,
- and sets a limit on the influence of matter on geometry and topology of space \mathcal{M} .

A sample of results

A sample of results

- In 4-space \mathcal{M}^4 the constraints on spectra $\mu = \text{Spec } R$ and $\lambda = \text{Spec Ric}$ are given by the inequalities

$$2\lambda_1 \leq \mu_1 + \mu_2 + \mu_3, \quad 2\lambda_4 \leq \mu_4 + \mu_5 + \mu_6$$

$$2(\lambda_1 + \lambda_4) \leq \mu_1 + \mu_2 - \mu_5 - \mu_6,$$

$$\lambda_1 + \lambda_2 - \lambda_3 - \lambda_4 \leq \mu_1 - \mu_6,$$

$$\lambda_1 - \lambda_2 + \lambda_3 - \lambda_4 \leq \min(\mu_1 - \mu_5, \mu_2 - \mu_6),$$

$$|\lambda_1 - \lambda_2 - \lambda_3 + \lambda_4| \leq \min(\mu_1 - \mu_4, \mu_2 - \mu_5, \mu_3 - \mu_6),$$

$$2 \max(\lambda_1 - \lambda_3, \lambda_2 - \lambda_4) \leq \min(\mu_1 + \mu_3 - \mu_5 - \mu_6, \mu_1 + \mu_2 - \mu_4 - \mu_6),$$

$$2 \max(\lambda_1 - \lambda_2, \lambda_3 - \lambda_4) \leq \min(\mu_1 + \mu_3 - \mu_4 - \mu_6, \mu_2 + \mu_3 - \mu_5 - \mu_6, \mu_1 + \mu_2 - \mu_4 - \mu_5).$$

A sample of results

- In 4-space \mathcal{M}^4 the constraints on spectra $\mu = \text{Spec } R$ and $\lambda = \text{Spec Ric}$ are given by the inequalities

$$2\lambda_1 \leq \mu_1 + \mu_2 + \mu_3, \quad 2\lambda_4 \leq \mu_4 + \mu_5 + \mu_6$$

$$2(\lambda_1 + \lambda_4) \leq \mu_1 + \mu_2 - \mu_5 - \mu_6,$$

$$\lambda_1 + \lambda_2 - \lambda_3 - \lambda_4 \leq \mu_1 - \mu_6,$$

$$\lambda_1 - \lambda_2 + \lambda_3 - \lambda_4 \leq \min(\mu_1 - \mu_5, \mu_2 - \mu_6),$$

$$|\lambda_1 - \lambda_2 - \lambda_3 + \lambda_4| \leq \min(\mu_1 - \mu_4, \mu_2 - \mu_5, \mu_3 - \mu_6),$$

$$2 \max(\lambda_1 - \lambda_3, \lambda_2 - \lambda_4) \leq \min(\mu_1 + \mu_3 - \mu_5 - \mu_6, \mu_1 + \mu_2 - \mu_4 - \mu_6),$$

$$2 \max(\lambda_1 - \lambda_2, \lambda_3 - \lambda_4) \leq \min(\mu_1 + \mu_3 - \mu_4 - \mu_6, \mu_2 + \mu_3 - \mu_5 - \mu_6, \mu_1 + \mu_2 - \mu_4 - \mu_5).$$

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

A sample of results for pure N-representability

Three electron system $\wedge^3 \mathcal{H}_r$ of even rank $r = \dim \mathcal{H}_r$

A sample of results for pure N-representability

Three electron system $\wedge^3 \mathcal{H}_r$ of even rank $r = \dim \mathcal{H}_r$

- $\lambda_{k+1} + \lambda_{r-k} \leq 1$, $0 \leq k < r$. For $r = 6$ turn into B-D equations due to the normalization $\text{Tr } \rho = 3$.

A sample of results for pure N-representability

Three electron system $\wedge^3 \mathcal{H}_r$ of even rank $r = \dim \mathcal{H}_r$

- $\lambda_{k+1} + \lambda_{r-k} \leq 1$, $0 \leq k < r$. For $r = 6$ turn into B-D equations due to the normalization $\text{Tr } \rho = 3$.
- $$\begin{array}{ll} \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \leq 2, & \lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \leq 2, \\ \lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2, & \lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2; \end{array}$$

A sample of results for pure N-representability

Three electron system $\wedge^3 \mathcal{H}_r$ of even rank $r = \dim \mathcal{H}_r$

- $\lambda_{k+1} + \lambda_{r-k} \leq 1, \quad 0 \leq k < r$. For $r = 6$ turn into B-D equations due to the normalization $\text{Tr } \rho = 3$.
- $\lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \leq 2, \quad \lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \leq 2,$
 $\lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2, \quad \lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2;$
- $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 + \lambda_{11} + \lambda_{16} + \lambda_{22} + \lambda_{29} + \cdots \leq 2.$

A sample of results for pure N-representability

Three electron system $\wedge^3 \mathcal{H}_r$ of even rank $r = \dim \mathcal{H}_r$

- $\lambda_{k+1} + \lambda_{r-k} \leq 1, \quad 0 \leq k < r$. For $r = 6$ turn into B-D equations due to the normalization $\text{Tr } \rho = 3$.
- $\lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \leq 2, \quad \lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \leq 2,$
 $\lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2, \quad \lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2;$
- $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 + \lambda_{11} + \lambda_{16} + \lambda_{22} + \lambda_{29} + \cdots \leq 2.$

Complete set of constraints

To give an idea of complexity of the problem note that

A sample of results for pure N-representability

Three electron system $\wedge^3 \mathcal{H}_r$ of even rank $r = \dim \mathcal{H}_r$

- $\lambda_{k+1} + \lambda_{r-k} \leq 1$, $0 \leq k < r$. For $r = 6$ turn into B-D equations due to the normalization $\text{Tr } \rho = 3$.
- $\lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \leq 2$, $\lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \leq 2$,
 $\lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2$, $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2$;
- $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 + \lambda_{11} + \lambda_{16} + \lambda_{22} + \lambda_{29} + \cdots \leq 2$.

Complete set of constraints

To give an idea of complexity of the problem note that

- $\wedge^3 \mathcal{H}_{10}$ is bounded by 93 inequalities;

A sample of results for pure N-representability

Three electron system $\wedge^3 \mathcal{H}_r$ of even rank $r = \dim \mathcal{H}_r$

- $\lambda_{k+1} + \lambda_{r-k} \leq 1, \quad 0 \leq k < r$. For $r = 6$ turn into B-D equations due to the normalization $\text{Tr } \rho = 3$.
- $\lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \leq 2, \quad \lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \leq 2,$
 $\lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2, \quad \lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2;$
- $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 + \lambda_{11} + \lambda_{16} + \lambda_{22} + \lambda_{29} + \cdots \leq 2.$

Complete set of constraints

To give an idea of complexity of the problem note that

- $\wedge^3 \mathcal{H}_{10}$ is bounded by 93 inequalities;
- $\wedge^4 \mathcal{H}_{10}$ is bounded by 125 inequalities;

A sample of results for pure N-representability

Three electron system $\wedge^3 \mathcal{H}_r$ of even rank $r = \dim \mathcal{H}_r$

- $\lambda_{k+1} + \lambda_{r-k} \leq 1$, $0 \leq k < r$. For $r = 6$ turn into B-D equations due to the normalization $\text{Tr } \rho = 3$.
- $\lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \leq 2$, $\lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \leq 2$,
 $\lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2$, $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2$;
- $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 + \lambda_{11} + \lambda_{16} + \lambda_{22} + \lambda_{29} + \cdots \leq 2$.

Complete set of constraints

To give an idea of complexity of the problem note that

- $\wedge^3 \mathcal{H}_{10}$ is bounded by 93 inequalities;
- $\wedge^4 \mathcal{H}_{10}$ is bounded by 125 inequalities;
- $\wedge^5 \mathcal{H}_{10}$ is bounded by 161 inequalities;

A sample of results for pure N-representability

Three electron system $\wedge^3 \mathcal{H}_r$ of even rank $r = \dim \mathcal{H}_r$

- $\lambda_{k+1} + \lambda_{r-k} \leq 1$, $0 \leq k < r$. For $r = 6$ turn into B-D equations due to the normalization $\text{Tr } \rho = 3$.
- $\lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \leq 2$, $\lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \leq 2$,
 $\lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2$, $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2$;
- $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 + \lambda_{11} + \lambda_{16} + \lambda_{22} + \lambda_{29} + \cdots \leq 2$.

Complete set of constraints

To give an idea of complexity of the problem note that

- $\wedge^3 \mathcal{H}_{10}$ is bounded by 93 inequalities;
- $\wedge^4 \mathcal{H}_{10}$ is bounded by 125 inequalities;
- $\wedge^5 \mathcal{H}_{10}$ is bounded by 161 inequalities;
- $\wedge^3 \mathcal{H}_{11}$ is bounded by 121 inequalities.

Taking into account spin

Taking into account spin

- In the above setting we can't address specific spin effects buried in joint spin-orbital space $\mathcal{H}_r = \mathcal{H}_\ell \otimes \mathcal{H}_s$.

Taking into account spin

- In the above setting we can't address specific spin effects buried in joint spin-orbital space $\mathcal{H}_r = \mathcal{H}_\ell \otimes \mathcal{H}_s$.
- The orbital \mathcal{H}_ℓ degrees of freedom, via Coulomb interaction, are primary responsible for dynamics,

Taking into account spin

- In the above setting we can't address specific spin effects buried in joint spin-orbital space $\mathcal{H}_r = \mathcal{H}_\ell \otimes \mathcal{H}_s$.
- The orbital \mathcal{H}_ℓ degrees of freedom, via Coulomb interaction, are primary responsible for dynamics,
- whereas the spin ones \mathcal{H}_s , disregarding a small relativistic correction, are purely kinematic.

Taking into account spin

- In the above setting we can't address specific spin effects buried in joint spin-orbital space $\mathcal{H}_r = \mathcal{H}_\ell \otimes \mathcal{H}_s$.
- The orbital \mathcal{H}_ℓ degrees of freedom, via Coulomb interaction, are primary responsible for dynamics,
- whereas the spin ones \mathcal{H}_s , disregarding a small relativistic correction, are purely kinematic.
- The total N -fermion system decomposes into spin-orbital components parameterized by Young diagrams ν

$$\wedge^N (\mathcal{H}_\ell \otimes \mathcal{H}_s) = \sum_{|\nu|=N} \mathcal{H}_\ell^\nu \otimes \mathcal{H}_s^{\nu^t}, \quad (21)$$

Taking into account spin

- In the above setting we can't address specific spin effects buried in joint spin-orbital space $\mathcal{H}_r = \mathcal{H}_\ell \otimes \mathcal{H}_s$.
- The orbital \mathcal{H}_ℓ degrees of freedom, via Coulomb interaction, are primary responsible for dynamics,
- whereas the spin ones \mathcal{H}_s , disregarding a small relativistic correction, are purely kinematic.
- The total N -fermion system decomposes into spin-orbital components parameterized by Young diagrams ν

$$\wedge^N (\mathcal{H}_\ell \otimes \mathcal{H}_s) = \sum_{|\nu|=N} \mathcal{H}_\ell^\nu \otimes \mathcal{H}_s^{\nu^t}, \quad (21)$$

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 ν, ν^t .

Spin resolved states

Spin resolved states

- For spin resolved state $\Psi \in \mathcal{H}_\ell^\nu \otimes \mathcal{H}_s^{\nu^t}$ the Pauli constraints amount to linear inequalities between orbital λ_i and spin μ_j natural occupation numbers.

Spin resolved states

- For spin resolved state $\Psi \in \mathcal{H}_\ell^\nu \otimes \mathcal{H}_s^{\nu^t}$ the Pauli constraints amount to linear inequalities between orbital λ_i and spin μ_j natural occupation numbers.
- 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.

Spin resolved states

- For spin resolved state $\Psi \in \mathcal{H}_\ell^\nu \otimes \mathcal{H}_s^{\nu^t}$ the Pauli constraints amount to linear inequalities between orbital λ_i and spin μ_j natural occupation numbers.
- 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 μ_B .

Who cares about extended Pauli constraints?

Who cares about extended Pauli constraints?

- The Pauli principle is a purely *kinematic* constraint on available states of a multi-electron system. Not even a minuscule its violation has been detected so far.

Who cares about extended Pauli constraints?

- The Pauli principle is a purely *kinematic* constraint on available states of a multi-electron system. Not even a minuscule its violation has been detected so far.
- Therefore whenever a dynamical trend is in conflict with Pauli constraints, the latter would prevail and the system eventually will be trapped in the boundary of the manifold of allowed states.

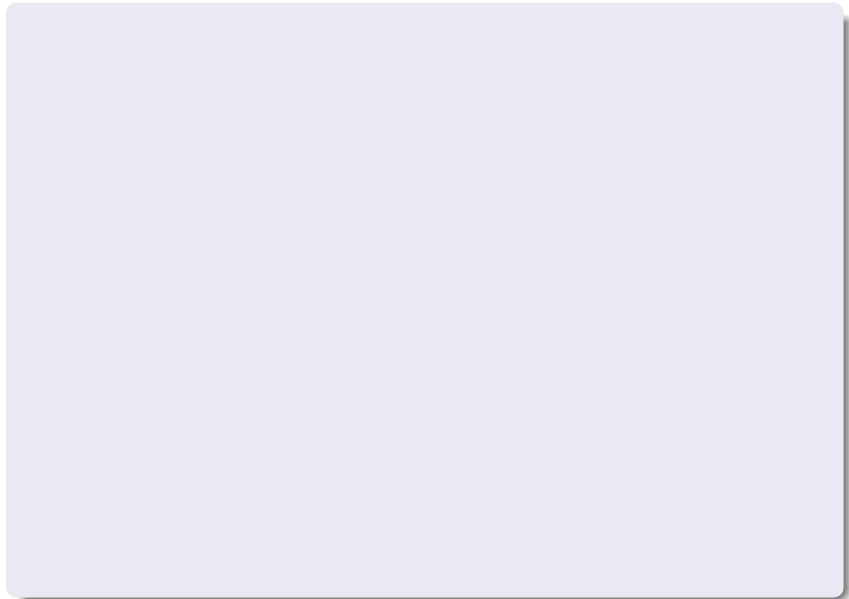
Who cares about extended Pauli constraints?

- The Pauli principle is a purely *kinematic* constraint on available states of a multi-electron system. Not even a minuscule its violation has been detected so far.
- Therefore whenever a dynamical trend is in conflict with Pauli constraints, the latter would prevail and the system eventually will be trapped in the boundary of the manifold of allowed states.
- This can manifest itself in degeneration some of the extended Pauli inequalities into equations. In this case the system and its state vector will be called *pinned* to the degenerate Pauli inequalities.

Who cares about extended Pauli constraints?

- The Pauli principle is a purely *kinematic* constraint on available states of a multi-electron system. Not even a minuscule its violation has been detected so far.
- Therefore whenever a dynamical trend is in conflict with Pauli constraints, the latter would prevail and the system eventually will be trapped in the boundary of the manifold of allowed states.
- This can manifest itself in degeneration some of the extended Pauli inequalities into equations. In this case the system and its state vector will be called *pinned* to the degenerate Pauli inequalities.
- A pinned system is essentially a new physical entity with its own dynamics and kinematics.

Physical example: Iron magnetic moment



Physical example: Iron magnetic moment

- **An old puzzle:** reduction of magnetic moment of iron atom in cubic (bcc) crystal relative to its value in free space.

Physical example: Iron magnetic moment

- **An old puzzle:** reduction of magnetic moment of iron atom in cubic (bcc) crystal relative to its value in free space.
- The magnetic moment comes from d -shell which contains 7 electrons and can have magnetic moment up to $3 \mu_B$, whereas the observed moment is $2.22 \mu_B$.

Physical example: Iron magnetic moment

- **An old puzzle:** reduction of magnetic moment of iron atom in cubic (bcc) crystal relative to its value in free space.
- The magnetic moment comes from d -shell which contains 7 electrons and can have magnetic moment up to $3 \mu_B$, whereas the observed moment is $2.22 \mu_B$.
- In cubic crystal field d -shell splits into two irreps of dimension 3 and 2 called t_{2g} and e_g subshells.

Physical example: Iron magnetic moment

- **An old puzzle:** reduction of magnetic moment of iron atom in cubic (bcc) crystal relative to its value in free space.
- The magnetic moment comes from d -shell which contains 7 electrons and can have magnetic moment up to $3 \mu_B$, whereas the observed moment is $2.22 \mu_B$.
- In cubic crystal field d -shell splits into two irreps of dimension 3 and 2 called t_{2g} and e_g subshells.
- The orbital density matrix retains the crystal symmetry, and reduces to scalars n_t and n_e on the above subshells.

Physical example: Iron magnetic moment

- **An old puzzle:** reduction of magnetic moment of iron atom in cubic (bcc) crystal relative to its value in free space.
- The magnetic moment comes from d -shell which contains 7 electrons and can have magnetic moment up to $3\mu_B$, whereas the observed moment is $2.22\mu_B$.
- In cubic crystal field d -shell splits into two irreps of dimension 3 and 2 called t_{2g} and e_g subshells.
- The orbital density matrix retains the crystal symmetry, and reduces to scalars n_t and n_e on the above subshells.
- 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 .

Physical example: Iron magnetic moment

- **An old puzzle:** reduction of magnetic moment of iron atom in cubic (bcc) crystal relative to its value in free space.
- The magnetic moment comes from d -shell which contains 7 electrons and can have magnetic moment up to $3\mu_B$, whereas the observed moment is $2.22\mu_B$.
- In cubic crystal field d -shell splits into two irreps of dimension 3 and 2 called t_{2g} and e_g subshells.
- The orbital density matrix retains the crystal symmetry, and reduces to scalars n_t and n_e on the above subshells.
- 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 .
- The occupation number for iron $n_t = 1.46$ was found by W.Jauch&M.Reehuis, Phys. Rev. B, **76**, 235121 (2007).

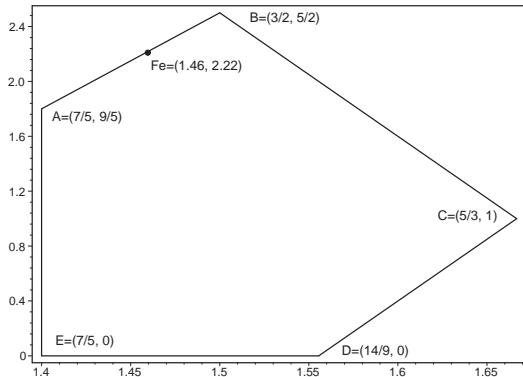


Figure: Pauli constraints on spin magnetic moment (μ_B) for 7 electrons in d -shell in cubic crystal field versus the occupation number n_t of a t_{2g} orbital. All points within the pentagon $ABCDE$ are admissible. A black dot represents experimental data for iron.