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# School on New Trends in Quantum Dynamics and Quantum Entanglement

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## ESSENTIAL ENTANGLEMENT

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## I. Introduction

Entanglement is considered to be the key feature that distinguishes quantum from classical behaviour.

Inasmuch as quantum theory is intrinsically a statistical theory, and makes (statistical) predictions on measurement results, entanglement manifests in correlations of measurement results on different system components, that ~~are "stronger" than classical ones~~ are incompatible with classical probability theory as formulated by Kolmogorov.

Historically, entanglement was brought up by Schrödinger (1935), debated by Einstein, Podolsky and Rosen (1935), quantified by Bell (1964), and since demonstrated in a plenty of experiments (Aspect et al., Zeilinger et al. ...), in particular after the "invention" of the concept of a quantum computer (Shor, ...).

Recently, communities distinct from quantum engineering got interested in entanglement – e.g. strong field fragmentation of helium (U. Becker et al., R. Dörner et al., ...), and quantum chemists who study coherence effects in excitation and charge transport e.g. in biological tissues. While "engineered" by nature, these systems are very different from strongly screened systems that so far exist in human labs. In particular, they are widely open, noisy, and large, and thus define new challenges for theory.

This lecture will provide the elementary tools to ~~understand~~ describe entanglement in such systems.

"complete set of observables $A, B, C, \ldots$"

a) $A, B, C \ldots$ are pairwise commuting

$$AB = BA, \quad AC = CA, \quad BC = CB, \ldots$$

$$[A, B] = 0 \quad \ldots$$

i.e. simultaneously diagonalizable

b) The eigenvalues $\{a_j, b_j, c_j, \ldots\}$ of $A, B, C, \ldots$ allow for an unambiguous identification of each eigenvector $|j\rangle$. $\{a_j, b_j, c_j, \ldots\}$ are the "quantum numbers" characterizing $|j\rangle$.

# II. Pure state entanglement

## II.1. Tensor structure of ~~composite or multidimensional~~ quantum systems with multiple degrees of freedom

Given a complete set of observables $A, B, C, \ldots$ for the description of a quantum system, we can associate each observable with its Hilbert space, eigenvalues and eigenvectors:

$$\begin{aligned} A|a\rangle &= a|a\rangle \quad \text{on } \mathcal{H}_A \\ B|b\rangle &= b|b\rangle \quad \text{on } \mathcal{H}_B \\ C|c\rangle &= c|c\rangle \quad \text{on } \mathcal{H}_C \\ &\vdots \end{aligned} \qquad (\text{II}.1)$$

We then define the "tensor product" or "product space" of $\mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_C, \ldots$

$$\mathcal{H} := \mathcal{H}_A \underset{\uparrow \atop \text{"tensor"}}{\otimes} \mathcal{H}_B \otimes \mathcal{H}_C \,, \qquad (\text{II}.2)$$

as the vector space spanned by linear combinations of tensor products

$$|a\rangle \otimes |b\rangle \otimes |c\rangle := |a\rangle|b\rangle|c\rangle := |a,b,c\rangle . \qquad (\text{II}.3)$$

Example:

Polarization states $|0\rangle$ (horizontal) and $|1\rangle$ (vertical) of two photons live in a space spanned by

$|0\rangle \otimes |0\rangle, \quad |0\rangle \otimes |1\rangle, \quad |1\rangle \otimes |0\rangle, \quad |1\rangle \otimes |1\rangle,$

generated by linear ~~pr~~ superpositions like

$$\frac{1}{\sqrt{2}}\,|0,0\rangle + \frac{1}{\sqrt{2}}\,|1,1\rangle .$$

For our following discussion we consider ourselves with two factor spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. The generalization for more than two factors is straightforward (as much as the construction of the product state is concerned).

Nomenclature:

two factors $\mathcal{H}_A, \mathcal{H}_B$ $:\Longleftrightarrow$ "bipartite system"

more than two factors $:\Longleftrightarrow$ "multipartite system"

$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ is again a vector space, by virtue of

$$\begin{aligned}\lambda\left(|a\rangle \otimes |b\rangle\right) &= \left(\lambda\,|a\rangle\right) \otimes |b\rangle \\ &= |a\rangle \otimes \left(\lambda\,|b\rangle\right)\end{aligned} \qquad (\text{II}.4)$$

and

$$\begin{aligned}\left(|a_1\rangle + |a_2\rangle\right) \otimes |b\rangle &= |a_1\rangle \otimes |b\rangle + |a_2\rangle \otimes |b\rangle \\ |a\rangle \otimes \left(|b_1\rangle + |b_2\rangle\right) &= |a\rangle \otimes |b_1\rangle + |a\rangle \otimes |b_2\rangle\end{aligned} \qquad (\text{II}.5)$$

Given dimensions $d_{\mathcal{H}_A}$ and $d_{\mathcal{H}_B}$ of the factor spaces, $\mathcal{H}$ has dimension

$$d_{\mathcal{H}} = d_{\mathcal{H}_A} \cdot d_{\mathcal{H}_B} , \qquad (\text{II}.6)$$

and is spanned by products of the basis vectors of $\mathcal{H}_A$ and $\mathcal{H}_B$,

$$\left\{ |a_j\rangle \otimes |b_k\rangle \right\}_{\substack{j=1,\dots,d_{\mathcal{H}_A} \\ k=1,\dots,d_{\mathcal{H}_B}}} \qquad (\text{II}.7)$$

Accordingly, each vector given as a product of two arbitrary vectors

$|\varphi\rangle \in \mathcal{H}_A$ and $|\chi\rangle \in \mathcal{H}_B$ has the decomposition

$$|\psi\rangle = |\varphi\rangle \otimes |\chi\rangle = \Big(\sum_j c_j |a_j\rangle\Big) \otimes \Big(\sum_k r_k |b_k\rangle\Big)$$

$$= \sum_{jk} c_j r_k \, |a_j\rangle \otimes |b_k\rangle \qquad (\text{II}.8)$$

The scalar product on $\mathcal{H}$ is induced by those on $\mathcal{H}_A$ and $\mathcal{H}_B$: for $|\psi\rangle, |\xi\rangle \in \mathcal{H}$ with $|\psi\rangle = |\varphi\rangle \otimes |\chi\rangle$ and $|\xi\rangle = |\eta\rangle \otimes |\zeta\rangle$ one defines

scalar multiplication

$$\langle \xi | \psi \rangle := \underbrace{\langle \eta | \varphi \rangle}_{\text{scalar product on } \mathcal{H}_A} \cdot \underbrace{\langle \zeta | \chi \rangle}_{\text{on } \mathcal{H}_B} \qquad (\text{II}.9)$$

Tensor products of operators $A$ and $B$ on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, act on $\mathcal{H}$ as

$$(A \otimes B)\, |\varphi\rangle \otimes |\chi\rangle = A|\varphi\rangle \otimes B|\chi\rangle, \qquad (\text{II}.10)$$

where

$$A \otimes B = (A \otimes \mathbb{1}_B)(\mathbb{1}_A \otimes B) = A \cdot \mathbb{1}_A \otimes \mathbb{1}_B \cdot B \qquad (\text{II}.11)$$

The most general operator on $\mathcal{H}$ is of the form

$$R = \sum_j S_{jA} \otimes T_{jB}, \qquad (\text{II}.12)$$

and the most general vector in $\mathcal{H}$ is written

$$|\psi\rangle = \sum_{jk} c_{jk} |\varphi_j\rangle \otimes |\chi_k\rangle, \qquad (\text{II}.13)$$

where $|\varphi_j\rangle$ and $|\chi_k\rangle$ <u>need not</u> be basis vectors of $\mathcal{H}_A$ or $\mathcal{H}_B$, respectively.

Not each operator on $\mathcal{H}$ can be written as a simple tensor product of operators on $\mathcal{H}_A$ and $\mathcal{H}_B$, and the analogous statement holds for vectors in $\mathcal{H}$.

In particular, states $|\psi\rangle \in \mathcal{H}$ with

$$|\psi\rangle \neq |\varphi\rangle \otimes |\chi\rangle \qquad (\text{II } 14)$$
$$\forall\, |\varphi\rangle \in \mathcal{H}_A,\ |\chi\rangle \in \mathcal{H}_B$$

are called "<u>entangled</u>". States of the form $|\psi\rangle = |\varphi\rangle \otimes |\chi\rangle$ are called "<u>separable</u>".

## II 2 Schmidt decomposition of states of bipartite quantum systems

The representation (II 8) of an arbitrary state vector $|\psi\rangle \in \mathcal{H}$ runs over two summation indices $j$ and $k$. Given a specific state $|\psi\rangle$, we can rewrite that as follows:

$$|\psi\rangle \underset{(\text{II } 8)}{=} \sum_{jk} c_j r_k\, |a_j\rangle \otimes |b_k\rangle = \qquad (\text{II } 15)$$

$$= \sum_{jk} d_{jk}\, |a_j\rangle \otimes |b_k\rangle ,$$

$d_{jk} = c_j r_k$

Hence $d_{jk} = \langle a_j | \otimes \langle b_k | \psi\rangle$. Arbitrary unitary transformations $U$ and $V$ on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, induce the transformations

$$|\tilde{a}_j\rangle = U|a_j\rangle \qquad |\tilde{b}_k\rangle = V|b_k\rangle \qquad (\text{II } \cancel{16}\ 12)$$

$$\tilde{d}_{jk} = \langle \tilde{a}_j | \otimes \langle \tilde{b}_k | \psi\rangle =$$

$$\underset{(\text{II } 16)}{=} \langle a_j | U^\dagger \otimes \langle b_k | V^\dagger | \psi\rangle =$$

Singular value decomposition: For any $A \in \mathbb{C}^{m\times n}$ $\exists$ $U \in \mathbb{C}^{m\times m}$ and $V \in \mathbb{C}^{n\times n}$ : $U^+ A V = \mathrm{diag}(\sigma_1, \ldots, \sigma_p) \in \mathbb{R}^{m\times n}$,

$p = \min\{m, n\}$, where $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_p \geq 0$.

[s. G. H. Golub, C. F. van Loan, Matrix Computations, John Hopkins Univ. Press 1996]

$\{|a_j^s\rangle\}_j$, $\{|b_j^s\rangle\}$ local ONB's !

$$= \sum_{pq} \underbrace{\langle a_j | u^+ | a_p \rangle}_{=: u_{jp}} \underbrace{\langle b_k | V^+ | b_q \rangle}_{=: v_{qk}} \underbrace{\langle a_p | \otimes \langle b_q | \psi \rangle}_{\underset{(II.15)}{=} d_{pq}}$$

$\{a_p\}, \{b_q\}$ ONB on $\mathcal{H}_1, \mathcal{H}_2$

(sic!)

$$= \left[ u\, d\, v \right]_{jk}$$

Therefore,

$$|\psi\rangle \underset{(II.15,16)}{=} \sum \left[ u d v \right]_{jk} |a_j\rangle |b_k\rangle \qquad (II.\cancel{17}\ 13)$$

Since any complex matrix $d$ can be diagonalized by unitary transformations $u$ and $v$, to yield its <u>singular value decomposition</u> with real, non-negative diagonal entries – "singular values" – $\sqrt{\lambda_j}$, we can always find local bases $\{|a_j^s\rangle\}_j$ and $\{|b_j^s\rangle\}_j$ such that

$$|\psi\rangle = \sum_j \sqrt{\lambda_j}\, |a_j^s\rangle \otimes |b_j^s\rangle \qquad (II.\cancel{18}\ 14)$$

with the summation over one index alone. (II.18) is the <u>Schmidt decomposition of $|\psi\rangle$</u>, with the <u>Schmidt coefficients $\lambda_j$</u>.

1

## II.3 (Reduced) density matrices

With (II.4,5,8,9) we have embedded all states of $\mathcal{H}_A$ and $\mathcal{H}_B$ into $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Since in the sense of (II.12,13), $\mathcal{H}$ is "larger" than the set of products of states of $\mathcal{H}_A$ and $\mathcal{H}_B$, we can ask to which extent it is possible to associate any state ~~of $\mathcal{H}$~~ in $\mathcal{H}$ with a state in $\mathcal{H}_A$ and $\mathcal{H}_B$.

To follow up this question, we now represent a state $|\psi\rangle$ in $\mathcal{H}$ by the associated projector on $\mathcal{H}$:

$$|\psi\rangle\langle\psi| \underset{(\text{II}.18)}{=} \sum_{j,j'} \mu_j \mu_{j'} \, |a_j^S\rangle\langle a_{j'}^S| \otimes |b_j^S\rangle\langle b_{j'}^S| \qquad (\text{II}.19)$$

where we set $\mu_j := \sqrt{\lambda_j}$

Let us first assume that the right hand side (RHS) of (II.19) contains only one non-vanishing term, i.e. $\mu_j = \delta_{j0}$, then

$$|\psi\rangle\langle\psi| = |a_0^S\rangle\langle a_0^S| \otimes |b_0^S\rangle\langle b_0^S| \qquad (\text{II}.20)$$

A partial trace of $|\psi\rangle\langle\psi|$ over a complete basis of $\mathcal{H}_B$ gives

$$\operatorname{tr}_B |\psi\rangle\langle\psi| = \sum_m \underbrace{{}_B\langle m|}_{\text{ONB on } \mathcal{H}_B}\psi\rangle\langle\psi\underbrace{|m\rangle_B}_{\text{ONB on } \mathcal{H}_B} =$$

$$\underset{(\text{II}.20)}{=} \sum_m |a_0^S\rangle\langle a_0^S| \; {}_B\langle m|b_0^S\rangle\langle b_0^S|m\rangle_B =$$

$$= |a_0^S\rangle\langle a_0^S| \, \langle b_0^S|b_0^S\rangle \underset{(\text{II}.18)}{=} |a_0^S\rangle\langle a_0^S| ,$$

$$\operatorname{tr}_B |\psi\rangle\langle\psi| = |a_0^S\rangle\langle a_0^S| , \qquad (\text{II}.21)$$

and thus a unique mapping between $|\psi\rangle$ and $|a_0^S\rangle \in \mathcal{H}_A$.
Strictly analogously, the ~~trace~~ partial trace over $\mathcal{H}_A$ maps $|\psi\rangle$ on $|b_0^S\rangle \in \mathcal{H}_B$.

The qualitative content of (II.21) is that the deliberate ignorance of the state of subsystem B does not affect the identification of $|\psi\rangle$ with a state of subsystem A.

The situation changes, though, if the right hand side of (II.19) contains more than one term; partial trace over B leads to

$$\mathrm{tr}_B |\Psi\rangle\langle\Psi| = \sum_m \sum_{jj'} \mu_j \mu_{j'} |a_j^S\rangle\langle a_{j'}^S| \, \underbrace{{}_B\langle m|b_j^S\rangle}_{\delta_{mj}} \underbrace{\langle b_{j'}^S|m\rangle}_{\delta_{mj'}}$$

$$= \sum_m \mu_m^2 |a_m^S\rangle\langle a_m^S| \,, \qquad \text{(II.22)}$$

which is a diagonal operator with eigenvalues $\mu_m^2 < 1$, on $\mathcal{H}_A$. Since any projector $|\varphi\rangle\langle\varphi|$ on ~~[illegible]~~ $|\varphi\rangle$ in $\mathcal{H}_A$ has eigenvalues 0 and 1, $\mathrm{tr}_B |\Psi\rangle\langle\Psi|$ <u>cannot</u> be identified with a state vector on $\mathcal{H}_A$!

Partial trace ~~[illegible]~~ of states on $\mathcal{H}$ over $\mathcal{H}_A$ or $\mathcal{H}_B$ in general generates operator-valued objects of the form (II.22), which can be identified with state vectors $|\varphi\rangle$ or $|\chi\rangle$ on $\mathcal{H}_A$ or $\mathcal{H}_B$ <u>only if</u> $|\Psi\rangle$ is separable.

$$\rho_A := \mathrm{tr}_B |\Psi\rangle\langle\Psi| \,, \quad \rho_B := \mathrm{tr}_A |\Psi\rangle\langle\Psi| \qquad \text{(II.23)}$$

are the <u>reduced density matrices of $|\Psi\rangle$</u> on $\mathcal{H}_A$ and $\mathcal{H}_B$, ~~respectively~~, and operate on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively.

Comparison of (II.18, 19, 22) furthermore shows that the Schmidt coefficients of $|\Psi\rangle$ can be obtained as the (non-vanishing) eigenvalues of the reduced density matrices $\rho_A$ or $\rho_B$ of $|\Psi\rangle$.

The number of non-vanishing Schmidt coefficients of a state $|\Psi\rangle$ is called the <u>Schmidt rank</u> of $|\Psi\rangle$.
The vector ~~[illegible]~~ $\vec{\lambda}$ with dimension $d = \min\{\dim(\mathcal{H}_A), \dim(\mathcal{H}_B)\}$

and the Schmidt coefficients as entries in non-increasing order is called the ___Schmidt vector___.

According to (II 14, 20, 21), separable states have only one non-vanishing ~~eigen~~ Schmidt ~~value~~ coefficient $\lambda_0 = 1$.

Correspondingly, a ___maximally entangled state___ has Schmidt vector
$$\vec{\lambda} = \underbrace{\left( \frac{1}{d}, \ldots, \frac{1}{d} \right)}_{d \text{ entries!}}$$

While the reduced density matrix of a separable state is pure, since
$$\operatorname{tr}_A \rho^2_{A,sep} = \operatorname{tr} \begin{pmatrix} 1 & & \\ & 0 & \\ & & 0 \end{pmatrix}^2 = 1 ,$$
the reduced state of the maximally entangled state is maximally mixed, i.e.
$$\operatorname{tr}_A \rho^2_{A,max.ent.} = \operatorname{tr} \begin{pmatrix} 1/d & & 0 \\ & \ddots & \\ 0 & & 1/d \end{pmatrix}^2 = d \cdot \frac{1}{d^2} = \frac{1}{d} ,$$

and the purity $\operatorname{tr} \rho^2_{A|B}$ of the reduced density matrix of a state $|\psi\rangle$ thus ~~defines a~~ can be used as an entanglement indicator for pure states.

## II.4 Local operations and classical communication (LOCC)

LOCC's provide some framework for the classification of entangled states (in the sense of being more or less entangled).

They ~~include~~ comprise all manipulations that are allowed by the laws of quantum mechanics, including measurements, coherent driving, interactions with auxiliary degrees of freedom, under the condition that

that they are restricted to either one of the individual subsystems.

Operations that require an interaction between the subsystems do not fall into this category, and quantum correlations that cannot be generated by local operations. Only classical communication is here admissible to create correlations. E.g. the result of a measurement can be communicated to a receiver ready to execute a local operation on the other subsystem, and this subsequent measurement can be conditioned on the classically communicated measurement result. This will only create classical correlations between both subsystems, and no entanglement can be generated when starting from a separable state.

Consequently, one considers a state $\rho_2$ less or equally entangled than a state $\rho_1$, if $\rho_2$ can be obtained from $\rho_1$ by LOCC. Maximally entangled states are then such states which allow to reach any other state by LOCC. In two-qubit systems, the Bell states

$$|\psi^\pm\rangle = \frac{1}{\sqrt{2}}\left(|0,1\rangle \pm |1,0\rangle\right)$$
$$|\phi^\pm\rangle = \frac{1}{\sqrt{2}}\left(|0,0\rangle \pm |1,1\rangle\right) \qquad (\text{II}.24)$$

are maximally entangled, and maximally entangled states of bipartite systems with sub-dimension $d$ are of the form

$$|\psi\rangle = \frac{1}{\sqrt{d}} \sum_{j=1}^{d} |j\rangle \otimes |j\rangle \qquad (\text{II}.25)$$

The situation gets considerably more complicated in multi-partite states with more than two subsystems, since there inequivalent entanglement classes do exist. A well known example is provided by

GHZ - and W-states, on $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$, $\mathcal{H}_j \equiv \mathbb{C}^2$,

$$|GHZ\rangle = \frac{1}{\sqrt{2}}\left[|000\rangle + |111\rangle\right],$$

$$|W\rangle = \frac{1}{\sqrt{3}}\left[|001\rangle + |010\rangle + |100\rangle\right] \qquad (\overline{\text{II}}\ 26)$$

Neither

While $|GHZ\rangle$ as well as $|W\rangle$ are strongly entangled in some sense, neither $|GHZ\rangle$ is reachable from $|W\rangle$ through LOCC, nor the inverse.

## II.5 Pure state entanglement quantifiers

As a consequence of the above, two states that can be transformed into each other by invertible LOCC's are ascribed equivalent entanglement properties. Invertible LOCC's are (precisely) local unitary transformations induced by single-particle Hamiltonians

$$U = U_1 \otimes U_2 = e^{-i\left(H_A \otimes 1_B + 1_A \otimes H_B\right)t/\hbar} \qquad (\overline{\text{II}}\ 27)$$

Any entanglement quantifier therefore has to be invariant under such transformations. For bipartite systems, the Schmidt coefficients $\lambda_j$ are precisely the invariants under transformations of type $(\overline{\text{II}}\ 27)$. Consequently, the $\lambda_j$ fully describe the entanglement properties of ~~an~~ a pure bipartite state.

Non-increasing functions (E) of the $\lambda_j$ under LOCC's are called 'entanglement monotones'.

Entanglement monotones that satisfy some additional axioms are called '<u>entanglement measures</u>', though there is no uniquely accepted list of axioms. Some found in the literature are

- $E(|\psi\rangle)$ vanishes for separable states (unless ...!)
- $E(|\psi\rangle^{\otimes n}) = n \cdot E(|\psi\rangle)$ 'additivity'
- $E(|\psi\rangle \otimes |\phi\rangle) \leq E(|\psi\rangle) + E(|\phi\rangle)$ 'subadditivity'
- $E(\lambda|\psi\rangle + (1-\lambda)|\phi\rangle) \leq \lambda E(|\psi\rangle) + (1-\lambda) E(|\phi\rangle)$, for $0 \leq \lambda \leq 1$ 'convexity'

[in general formulated for density matrices on $\mathcal{H}$, $|\psi\rangle \to \rho$, $|\phi\rangle \to \rho'$ see below chap. IV]

Some popular entanglement monotones are:

- <u>Schmidt rank $s$</u>: the number of non-vanishing coefficients in (II.18)

- <u>Schmidt number $K$</u>: $K = \left[\sum_{j=1}^{s} \lambda_j^2\right]^{-1} = \left[\operatorname{tr} \rho_A^2\right]^{-1}$

$K \in [1; d]$ ~ <u>inverse participation number</u> (II.28)

- <u>the ~~von~~ entanglement entropy</u>: $S_E(|\psi\rangle) = -\sum_{j=1}^{s} \lambda_j \ln \lambda_j$

- <u>the concurrence</u>:

$$C(|\psi\rangle) = \cancel{\sqrt{\frac{s}{s-1}\left(1-\sum_{j=1}^{s}\lambda_j^2\right)}} \sqrt{2\left(1-\sum_{j=1}^{s}\lambda_j^2\right)}$$

## II.6 Quantum and classical correlations

To relate our above (rather formal) definitions to our opening remarks concerning correlations of measurement results, consider the maximally entangled state (II.25) and the state

$$\text{(II.29)}\qquad \rho = \frac{1}{d}\sum_{j=1}^{d} |\psi_j\rangle\langle\psi_j| \ , \quad |\psi_j\rangle = |j\rangle\otimes|j\rangle$$

(an experimentalist prepares both subsystems always in the same random state $|j\rangle$, with balanced probabilities $\frac{1}{d}=p_j$). A projective measurement in the (orthonormal) basis $\{|j\rangle\}$ on the first subsystem of (II.25) has completely random outcome, with probability $\frac{1}{d}$ for each of the possible results, though a subsequent measurement on the second subsystem has a certain result (the first measurement projects the two-particle state on a random result $|j_0\rangle\otimes|j_0\rangle$, and the outcome of a measurement on the second subsystem is then certain). However, precisely the same is true for a measurement in the $\{|j\rangle\}$ basis is performed on $\rho$ in (II.29).

Only when the measurement is performed in another, distinct basis $\{|\alpha_p\rangle\}$ does the difference between (II.25) and (II.29) emerge:

Given the measurement outcome $\alpha_p$ on the first subsystem of (II.25), the two-body state $|\Psi\rangle$ is projected on

$$|\alpha_p\rangle\otimes\frac{1}{\sqrt{d}}\sum_j \langle\alpha_p|j\rangle\,|j\rangle = |\alpha_p\rangle\otimes|\tilde{\alpha}_p\rangle$$

with $|\tilde{\alpha}_p\rangle = \frac{1}{\sqrt{d}}\sum\langle\alpha_p|j\rangle|j\rangle$. The $|\tilde{\alpha}_p\rangle$ $(p=1,\dots,d)$ are mutually orthogonal, since $\langle\tilde{\alpha}_q|\tilde{\alpha}_p\rangle = \frac{1}{d}\sum_{k,j}\langle k|\alpha_q\rangle\langle\alpha_p|j\rangle\langle k|j\rangle = \frac{1}{d}\langle\alpha_p|\alpha_q\rangle = \delta_{pq}$ modulo renormalization. The ~~only~~ result of a subsequent measurement on the second subsystem in the basis $\{|\tilde{\alpha}_p\rangle\}$ is therefore deterministic. In contrast, a measurement on (II.29) in the basis $\{|\alpha_p\rangle\}$ projects onto $|\alpha_p\rangle\langle\alpha_p|\rho|\alpha_p\rangle\langle\alpha_p| = |\alpha_p\rangle\langle\alpha_p|\otimes\frac{1}{d}\sum|\langle\alpha_p|j\rangle|^2|j\rangle\langle j|$, ~~and attached~~ with the second subsystem in a mixed state. A subsequent measurement on the second subsystem will thus in general provide an uncertain result!

# III. Mixed state entanglement

While the Schmidt decomposition (II.18) provides a versatile tool to analyze the entanglement properties of pure bipartite states of arbitrary (finite) subdimension, and the difficulties of pure state entanglement characterization fully emerge only for multipartite states, it is much more demanding to characterize the entanglement content of mixed states of systems larger than $2\times 2$ — though this is precisely the challenge when one wants to assess the role of entanglement e.g. in photochemical reactions / transport processes in complex systems.

## III.1 Mixed state entanglement measures

A mixed state $\rho$ acting on $\mathcal{H}$ (that can be understood to be generated in a way very analogous to our above construction of the reduced density matrices $\rho_A$ and $\rho_B$) is called a "product state" if it can be written as

$$\rho = \rho_A \otimes \rho_B \qquad (III.1)$$

with $\rho_A$ and $\rho_B$ acting on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. Such state bears no correlations between local measurements at all.

A mixed state of the form

$$\rho = \sum p_j \, \rho_A^{(j)} \otimes \rho_B^{(j)} \qquad (III.2)$$

with $\rho_A^{(j)}$ and $\rho_B^{(j)}$ acting on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, and $p_j \geq 0$, $\sum p_j = 1$ is called "separable", since it bears only classical correlations (fully explained in terms of probabilities $p_j$). Mixed states that cannot be written

Indeed, ($\overleftarrow{\mathrm{III}}$.4) generates all quasi Jack decompositions of $g$!

in the form (III.2) are called 'entangled'.

Since, upon diagonalization, each mixed state can be written ~~as~~ in its eigenstates ~~$|\phi_j\rangle\langle\phi_j|$~~ $|\phi_j\rangle$ with eigenvalues $\mu_j$ (distinct from those in (III.18)!),

$$\rho = \sum \mu_j \, |\phi_j\rangle\langle\phi_j| \,, \qquad (\text{III}.3)$$

it ~~may~~ is suggestive to define the entanglement of $\rho$ as the weighted average of the entanglement of the $|\phi_j\rangle$, by

$$\text{"} E(\rho) \text{"} = \sum \mu_j \, E(|\phi_j\rangle) \,. \qquad (\text{III}.3a)$$

~~However, as already~~

However, any linear combination

$$\sum_j V_{ij} \sqrt{\mu_j} \, |\phi_j\rangle =: \sqrt{p_i} \, |\psi_i\rangle \qquad (\text{III}.4)$$

defines another valid decomposition of $\rho$, provided $V$ is left-unitary, i.e.

$$\sum_k V^\dagger_{ik} V_{kj} = \delta_{jk} \,, \qquad (\text{III}.5)$$

since

$$\sum_i p_i \, |\psi_i\rangle\langle\psi_i| \underset{(\text{III}.4)}{=} \sum_{ijk} V_{ij} \sqrt{\mu_j} \, |\phi_j\rangle\langle\phi_k| \sqrt{\mu_k} \, V^*_{ik}$$

$$= \sum_{ijk} V^\dagger_{ki} V_{ij} \sqrt{\mu_j \mu_k} \, |\phi_j\rangle\langle\phi_k| =$$

$$\underset{(\text{III}.5)}{=} \sum_{jk} \delta_{kj} \sqrt{\mu_j \mu_k} \, |\phi_j\rangle\langle\phi_k| = \sum_j \mu_j \, |\phi_j\rangle\langle\phi_j|$$

"convex roof construction"

$\rho_{PT}$ does depend on the basis used, but the eigenvalues of $\rho_{P}^{PT}$ do not!

Consequently, the pure state decomposition of $\rho$ is not unique, and neither is a weighted average à la (III.5a).

A valid mixed state generalization of entanglement that is ~~invariant under~~ LOCC non-increasing under LOCC is provided by taking the infimum over all pure state decompositions,

$$E(\rho) = \inf_{\{|\psi_j\rangle, p_j\}} \sum p_j \, E(|\psi_j\rangle) \qquad (\text{III}.6)$$

In systems larger than $2\times 2$ no ~~explicit~~ general, explicit algebraic solution does exist for the optimization problem implicit in (III.6), and one generally needs to optimize over all left unitaries $V$ in (III.4), which need to be chosen ~~of dimension~~ $V \in \mathbb{C}^{n^2\times n}$, where $n$ is the rank of $\rho$. Thus, one deals with an optimization space of dimension $\sim n^3$, which rapidly grows with the subsystem Hilbert space dimensions.

The exact solution to (III.6) for $2\times 2$ systems has been given by Wootters in 1998.

## III.2 Mixed state negativity

Due to the computationally demanding evaluation of (III.6) another entanglement monotone has been introduced which can be evaluated algebraically, the "negativity $N(\rho)$". $N(\rho)$ is given in terms of the eigenvalues of the partial transpose of the state of a bipartite quantum system.

For an arbitrary bipartite state

$$\rho = \sum_{ij,kl} \rho_{ij,kl} \, |\varphi_i\rangle\langle\varphi_j| \otimes |\chi_k\rangle\langle\chi_l| \qquad (\text{III}.7)$$

its partial transpose is defined as

$$\rho^{T_2} = \sum_{ij,kl} \rho_{ij,lk} \, |\varphi_i\rangle\langle\varphi_j| \otimes |\chi_k\rangle\langle\chi_l| \qquad (\text{III}.8)$$

If ~~the~~ $\rho^{PT}$ has eigenvalues $\lambda_j$, then the negativity of $\rho$ is defined as

$$N(\rho) = \frac{\sum_j |\lambda_j| - 1}{2} \qquad (\overline{\text{III}}.9)$$

$N(\rho)$ takes positive values if $\rho^{PT}$ has at least one negative eigenvalue, though vanishes whenever $\rho^{PT}$ is positive semi-definite.

Since in systems larger than $2\times 2$ there exist entangled states with positive partial transpose, $N(\rho)$ is not strictly larger than zero for all entangled states and thus cannot detect all mixed state entanglement. However, it is especially the monotone which is easiest to evaluate for higher dimensional bipartite systems.

## III.3 Trace distance

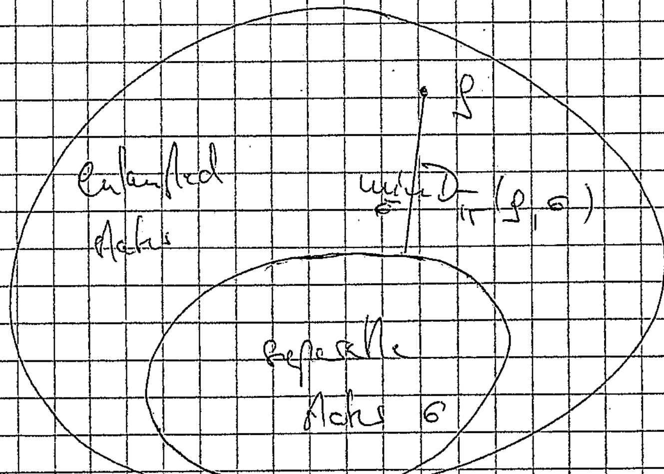
Since no straightforward generalization of the Schmidt decomposition or of negativity is available for multipartite systems with more than two factor spaces, other entanglement measures have been designed through measures of the distance between a given state and the set of ~~and~~ separable states in state space. We ~~will~~ here briefly introduce the trace norm between two states, which quantifies their distance through

$$D_{Tr}(\rho, \omega) = Tr|\rho - \omega| = \|\rho - \omega\|_{Tr} \qquad (\text{III}.10)$$

The minimal distance of a given state $\rho$ from the separables,

$$E_{Tr}(\rho) = \min_{\sigma \text{ separable}} D_{Tr}(\rho, \sigma) \qquad (\overline{\text{III}}.11)$$

then defines an entanglement measure, which is ~~unique~~ well-defined due to the convexity of the set of separable states (every straight line between two separable states contains only separable states).




Remark: Note that (III.9) actually can be rewritten as

$$N(\rho) = \frac{\|\rho^{PT}\|_{tr} - 1}{2} . \qquad (\text{III}.12)$$

## IV. ~~[illegible]~~ Benchmarking entanglement evolution

So far, we inferred the open system entanglement evolution directly from the time evolution of the system density matrix.

$$\begin{tikzcd}
C(t_0) \arrow[r, dashed, "?"] & C(t) \\
\rho(t_0) \arrow[u] \arrow[r, "\text{Breuer}"', "\text{Vecchini}"] & \rho(t) \arrow[u]
\end{tikzcd}$$

As the system size increases, it gets ever more demanding to ~~[illegible]~~ transport the entire density matrix.

$\longrightarrow$ IS THERE SOME SORT OF UNIVERSAL BEHAVIOUR?

Whenever

- approach large system sizes
- ignore system details $\longrightarrow$ STATISTICAL approach!
- need to live with uncontrolled errors

~~→ seek robust features, universal~~

## VI.1 Pure states of d-level systems

$$|\psi\rangle \in \mathbb{C}^d \simeq \mathbb{R}^{2d} \qquad (\text{IV}.1) \qquad \cancel{(\text{IV}.A)}$$

global phase irrelevant $\longrightarrow \mathbb{R}^{2d-1}$

normalization $\longrightarrow$ hypersphere $S^{2d-2} \simeq \{|\psi\rangle \in \mathbb{R}, \||\psi\|=1\}$

(two level atom $\rightarrow$ Bloch sphere $S^2$)

## VI.2 Dynamics of quantum states

open system dynamics ($\rightarrow$ Breuer, Vacchini)

$$\begin{cases} \rho(0) \longmapsto \rho(t) = \mathrm{tr}_{env}\left[U_{tot}(t)\, \rho_{tot}(0)\, U^{+}_{tot}(t)\right] \\ \qquad =: \Lambda_t\left[\rho(0)\right] = \Lambda_t\, \rho(0) \qquad (\text{IV}.2) \\ \text{with } \rho_{tot}(0) = \rho(0) \otimes \rho_{env}(0) \end{cases}$$

$\Lambda_t$ CPT (completely positive trace-preserving)

We are interested to characterize the global behavior of generic initial states under $\Lambda_t$, hence need to compare the dynamics of different initial states.

$\longrightarrow$ use trace distance of two states $\rho, \sigma$:

$$D_{tr}(\rho, \sigma) = \|\rho - \sigma\|_{tr} = tr|\rho - \sigma| = tr\sqrt{(\rho-\sigma)^\dagger(\rho-\sigma)} \quad (\boxed{IV}3)$$

Ruskai 1994 (+ intuition):

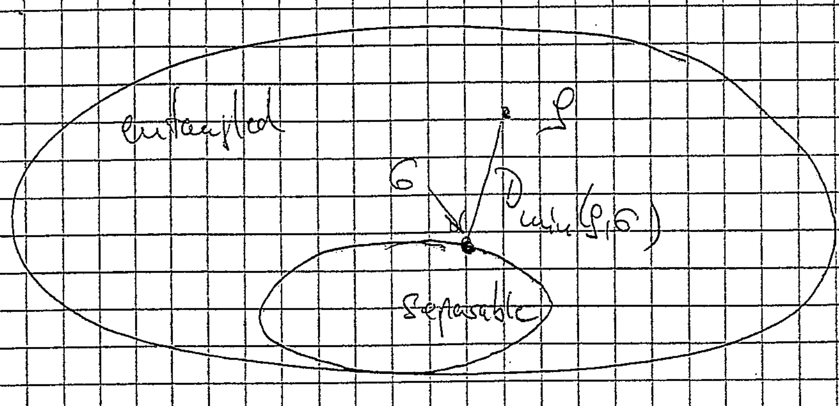
$$D_{tr}\left[\Lambda_t(\rho), \Lambda_t(\sigma)\right] \leq D_{tr}(\rho, \sigma) \quad (\boxed{IV}\,\cancel{4})$$

$$\forall \text{ CPT-maps } \Lambda_t$$

|| i.e. open system dynamics induces some sort of contraction on state space ||

## VI.3 A distance based entanglement measure

Rather than first introducing entanglement of ~~ ~~ pure states and ~~therefore deriving mixed~~ subsequently generalizing for mixed states (comp. chap III.1, (III.6)) it is in some sense more direct to start directly from the structure of state space:



→ entanglement ≡ minimal distance from separables

$$E(\rho) = \min_{\substack{\sigma \in S \\ \uparrow \text{ separables}}} D_{tr}(\rho, \sigma) \qquad (\text{IV}.5)$$

→ Further down we will need that $E(\rho)$ is <u>Lipschitz-continuous</u> on such space.

<u>Lipschitz</u>

→ A function $f: U \to V$ is <u>Lipschitz continuous</u>

$$:\Longleftrightarrow \quad \|f(x) - f(y)\|_V \le \eta \, \|x - y\|_U \quad \forall x, y \in U, \qquad (\text{IV}.6)$$

with <u>Lipschitz constant</u> $\eta$

→ Indeed,

$$\left| E(\rho_1) - E(\rho_2) \right| \underset{(\text{IV}.5)}{=} \left| D_{tr}(\rho_1, \sigma_1) - D_{tr}(\rho_2, \sigma_2) \right|$$

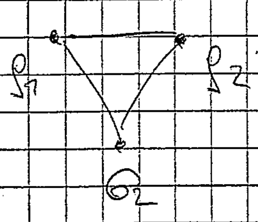
and $\sigma_1, \sigma_2$ respectively closest separables

$$\le \left| D_{tr}(\rho_1, \sigma_2) - D_{tr}(\rho_2, \sigma_2) \right|$$

$$\le D_{tr}(\rho_1, \rho_2)$$

triangle inequality

$$\rightsquigarrow \quad |E(\rho_1) - E(\rho_2)| \le D_{tr}(\rho_1, \rho_2) \qquad (\text{IV}.7)$$




$E$ Lipschitz with $\eta_E = 1$

$$D(\rho_1, \sigma_2) \le D(\rho_1, \rho_2) + D(\rho_2, \sigma_2)$$

## IV.4 Entanglement evolution

We start out from pure initial states, which we propagate with $\Lambda_t$

$$\rho = \Lambda_t(|\chi\rangle\langle\chi|) \qquad \omega = \Lambda_t(|\psi\rangle\langle\psi|) \qquad (\text{IV}.8)$$

Due to (IV.3,7) (E Lipschitz):

$$|E(\rho) - E(\omega)| \leq \eta_E \|\rho - \omega\|_{tr} =$$

$$\underset{(\text{IV}.8)}{=} \eta_E \|\Lambda_t(|\chi\rangle\langle\chi|) - \Lambda_t(|\psi\rangle\langle\psi|)\|_{tr}$$

$$\underset{(\text{IV}.4)}{\leq} \eta_E \eta_{\Lambda_t} \| |\chi\rangle\langle\chi| - |\psi\rangle\langle\psi| \|_{tr} \leq$$

~~$\eta_{\Lambda_t} = 1$ for unitary $\Lambda_t$~~

$$\leq 2\, \eta_E \eta_{\Lambda_t} \| |\chi\rangle - |\psi\rangle \|$$

$\| |\psi\rangle \| := \sqrt{\langle\psi|\psi\rangle}$ euclidean norm

$$\| |\chi\rangle\langle\chi| - |\psi\rangle\langle\psi| \|_{tr} \leq 2 \| |\chi\rangle - |\psi\rangle \|$$

$$\curvearrowright \quad |E(\Lambda_t(|\chi\rangle\langle\chi|)) - E(\Lambda_t(|\psi\rangle\langle\psi|))| \leq 2\, \eta_E \eta_{\Lambda_t} \| |\chi\rangle - |\psi\rangle \| \qquad (\text{IV}.9)$$

Hence, $E$ is Lipschitz continuous function from $\mathbb{R}^{2d^2}$ to $\mathbb{R}$, with Lipschitz constant $2\eta_E \eta_{\Lambda_t}$

## IV.5 Concentration of measure – Levy's Lemma

[→ See e.g. M. Ledoux: The Concentration of Measure Phenomenon, Mathematical Surveys and Monographs, AMS 2001]

Levy's Lemma: For $f: S^n \to \mathbb{R}$ Lipschitz continuous with Lipschitz constant $\eta$:

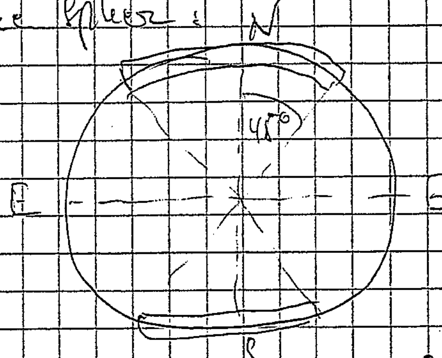
$$\Pr\left( \left| f(x) - \langle f \rangle \right| > \varepsilon \right) \leq 4 \exp\left( -C \frac{(n+1)\, \varepsilon^2}{\eta^2} \right) \quad (\text{IV}.10)$$

Idea: $|f(x) - f(y)| \leq \eta\, |x-y|$ by construction.

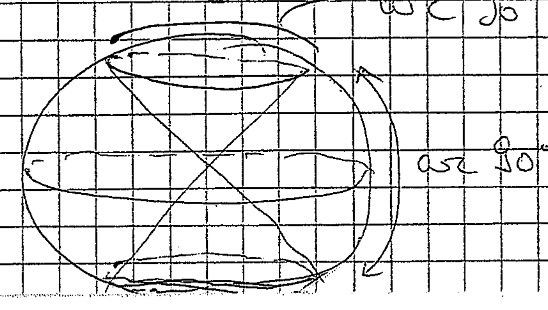
If large subvolume of the domain of $f$ concentrates in a narrow region around $y$, then the variation of $f$ on this large subvolume ~~is bounded~~ is bounded in a narrow interval.

Uniform sampling of the values of $f$ on its entire domain will thus give a strongly suppressed probability for large variations.

→ on the sphere:




polar regions same area as equatorial regions




equatorial arc $360° = 4 \cdot 90°$

⤳ equatorial area $\geq 2 \times$ polar area

$S^n \rightarrow$ concentration of surface volume around equator !

$n \to \infty \rightarrow$ volume concentrates exponentially around equator

## IV.6 Entanglement concentration of open system dynamics

(IV.9) $\Rightarrow$ $E$ is Lipschitz with constant $\eta_E \eta_{\Lambda_t}$ on $S^{2d-2}$

$\overrightarrow{(IV.10)}$

$$\Pr\left[ E(\rho(t)) - \langle E\rangle(t) \right] \leq 4\exp\left[-C \frac{(2d-1)\,\varepsilon^2}{4\eta_E^2\,\eta_{\Lambda_t}^2}\right] \quad (IV.11)$$

$$\langle E\rangle(t) = \int E\left[\Lambda_t(|\psi\rangle\langle\psi|)\right] d|\psi\rangle$$

$\eta_{\Lambda_t}$ time dependent through $\Lambda_t$

(IV.11) $\Rightarrow$ In high dimensions, can predict entanglement evolution of all states with high precision, if know fate of only one (generic, benchmark) state !

## IV.7 Example for N qubits under phase decoherence

$\rightarrow$ Private bath decoherence, single-qubit map

$$\Lambda_t(\rho_0) = (1-p)\rho_0 + p\left[|\uparrow\rangle\langle\uparrow|\rho_0|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\rho_0|\downarrow\rangle\langle\downarrow|\right]$$

with $p = 1-\exp(-\Gamma t)$

→ N-qubit map:

$$\rho_t = \underbrace{\Lambda_t \otimes \ldots \otimes \Lambda_t}_{N \text{ times}} |\chi\rangle\langle\chi|$$

→ bipartite entanglement of one qubit with respect to N-1 remaining qubits, measured by negativity, (cal 9),

$$N(\rho) = \frac{\|\rho^{PT}\|_{tr} - 1}{2} = \sum_{\lambda_i < 0} |\lambda_i|$$

eigenvalues of $\rho^{PT}$