## universität innsbruck

Bachelor's thesis

# Geometric aspects of the set of quantum states 

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July 28, 2022

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## Contents

1 Introduction ..... 3
2 Quantum states ..... 5
2.1 Density matrices ..... 5
2.2 Pure and mixed states ..... 6
3 The set of quantum states ..... 7
3.1 The shape and center of $\mathrm{D}(\mathcal{H})$ ..... 7
3.2 Eigenvalue picture ..... 9
3.3 Size estimates ..... 11
4 Bipartite quantum systems ..... 13
4.1 Separability and entanglement ..... 13
4.2 The partial transpose ..... 15
4.3 Size estimates ..... 15
5 Multipartite quantum systems ..... 19
6 Conclusion ..... 20
Bibliography ..... 22

## 1 Introduction

The truth is, quantum mechanics is hard. It is not a rarity to find yourself confused while doing a long calculation, forgetting about the physical meaning behind the mathematical rigor necessary in order to obtain a quantitative result. A good intuition about these abstract concepts is therefore a necessary skill for theoretical physicists. This thesis analyses the set of all possible states, denoted by $\mathrm{D}(\mathcal{H})$, a quantum mechanical system can be in - a very abstract set of complex matrices. Using the fact that this set is convex, some interesting visualisations are created via the mathematics of convex geometry. The two main goals of this thesis are to

1. create appropriate, geometric pictures useful to gain an intuition for the set of quantum states $\mathrm{D}(\mathcal{H})$.
2. give quantitative size estimations for $\mathrm{D}(\mathcal{H})$ and some of its subsets dependent on Hilbert space of the system.

These estimates will be done by calculating the radii $r_{\text {in }}$ and $r_{\text {out }}$ of the biggest hypersphere completely inside the set and the smallest one outside. These are the higher dimensional generalizations of the in- and outward circle in classical euclidian geometry, as seen in Figure 1.1.

The main source for this work was the book Alice and Bob meet Banach - The Interface of Asymptotic Geometric Analysis and Quantum Information Theory by Guillaume Aubrun and Stanslaw J. Szarek. It explains, how the mathematics of convexity and cone geometry can be used in order to gain insights into quantum information theory. While many arguments presented in this thesis can also be found there (as well as many others), most calculations are presented here more detailed and in a


Figure 1.1: A visualization of the inward and outward circle of a pentagon. Their higher dimensional generalization will be used to estimate the size of the set of quantum states $\mathrm{D}(\mathcal{H})$. more beginner-friendly way, avoiding advanced mathematical concepts whenever it is possible.

This thesis is structured as follows: Chapter 2 talks about quantum states in general, introducing the concept of density matrices and the differences between pure and mixed states - a important distinction used in quantum information theory. Chapter 3 is about the set of all possible quantum states $\mathrm{D}(\mathcal{H})$, characterising its center and shape. Furthermore the eigenvalue picture, being a geometric visualization for $\mathrm{D}(\mathcal{H})$, will be defined and used in order to measure the values for $r_{i n}$ and $r_{\text {out }}$. Chapter 4 looks at bipartite systems, consisting of two distinct subsystems. Here,
the concept of separability and entanglement will emerge, after which in- and outward radii for the $\mathrm{D}(\mathcal{H})$ 's subsets $\operatorname{SEP}(\mathcal{H})$ and $\operatorname{PPT}(\mathcal{H})$ will be calculated. Chapter 5 tries to generalize these results to a Hilbert space consisting of more than two parties, while Chapter 6 summarizes the results presented throughout the thesis and motivates some interesting further question in this field of study.
One should note that the hyperspheres with a radius $r_{i n} / r_{\text {out }}$ will always be denoted as the set's in- and outward circle, even though they will typically be of much higher dimension.

## 2 Quantum states

This chapter answers the question, what a quantum state of a given system is and how we are able to describe it. Afterwards, the distinction between pure and mixed states is introduced. This will be done using the concept of density matrices, which give a more natural way of describing mixed states in comparison to the typical Hilbert space vector formulation of quantum mechanics.

### 2.1 Density matrices

When talking about quantum mechanics, one always also talks about probabilities. It is very important though to distinguish, if a system's uncertainty arises from its quantum nature (=quantum uncertainty) or if one simply does not have enough information to describe it in more detail (=classical uncertainty). The typical formulation of quantum mechanics, which describes a system via normed vectors $|\Psi\rangle$ in a Hilbert space $\mathcal{H}$, can describe the quantum uncertainty of a system very well. However, when trying to introduce classical certainty, one will realize that this is very unintuitive in this formulation.
A more natural way of describing classical probability is via so called density matrices. One can, when having a Hilbert space vector $|\Psi\rangle$, form the corresponding density matrix $\rho=|\Psi\rangle\langle\Psi|$. The advantage of density matrices can be seen, when wanting to describe a system, that has (classical) probability $1 / 2$ of being in the state $|\Psi\rangle$ and $1 / 2$ for state $|\Phi\rangle$. This can be described by the density matrix

$$
\rho=\frac{1}{2}(|\Psi\rangle\langle\Psi|+|\Phi\rangle\langle\Phi|)
$$

which would not be possible in a simillar way using Hilbert space vectors. A density matrix is therefore any quadratic matrix of the form

$$
\begin{equation*}
\rho=\sum_{k} p_{k}\left|\Psi_{k}\right\rangle\left\langle\Psi_{k}\right| \tag{2.1}
\end{equation*}
$$

with $\left|\Psi_{k}\right\rangle \in \mathcal{H}$ and some coefficients $p_{k}$, which state the probability to measure $\rho$ as $\left|\Psi_{k}\right\rangle\left\langle\Psi_{k}\right|{ }^{1}$ It follows, that all the coefficients have to be non-negative and sum to 1 .
In order for a matrix to describe a physical state and be of the form 2.1, it must obey three conditions:

## 1. Hermiticity

A matrix A is said to be hermitian, if its adjoint $A^{\dagger}$ is itself. This can be checked, as

$$
\rho^{\dagger}=\left(\sum_{k} p_{k}\left|\Psi_{k}\right\rangle\left\langle\Psi_{k}\right|\right)^{\dagger}=\sum_{k} p_{k}\left(\left|\Psi_{k}\right\rangle\left\langle\Psi_{k}\right|\right)^{\dagger}=\sum_{k} p_{k}\left|\Psi_{k}\right\rangle\left\langle\Psi_{k}\right|=\rho
$$

[^0]2. Normalization

A matrix is normalised, if its norm $\|A\|$ is equal to one. The corresponding norm is the matrix trace (the sum over its diagonal elements). It follows from

$$
\begin{aligned}
\operatorname{Tr}(\rho) & =\operatorname{Tr}\left(\sum_{k} p_{k}\left|\Psi_{k}\right\rangle\left\langle\Psi_{k}\right|\right)=\sum_{k} p_{k} \operatorname{Tr}\left(\left|\Psi_{k}\right\rangle\left\langle\Psi_{k}\right|\right)=\sum_{k} p_{k} \operatorname{Tr}\left(\left\langle\Psi_{k}\right|\left|\Psi_{k}\right\rangle\right)= \\
& =\sum_{k} p_{k}\left\langle\Psi_{k}\right|\left|\Psi_{k}\right\rangle=\sum_{k} p_{k}=1
\end{aligned}
$$

where the linearity and the invariance under cyclic permutations of the trace are used.
3. Positive semidefinitness

A matrix is positive semidefinite, if the product $x^{\top} A x$ is non-negative for any vector $x$ of appropriate size. This is equivalent with saying all eigenvalues of the matrix have to be non-negative. In braket notation this can be seen for density matrices via

$$
\langle x| \rho|x\rangle=\sum_{k} p_{k}\left\langle x \mid \Psi_{k}\right\rangle\left\langle\Psi_{k} \mid x\right\rangle=\sum_{k} p_{k}\left|\left\langle\Psi_{k} \mid x\right\rangle\right|^{2} \geq 0
$$

where the semipositivity of the absolute value is used.
Now that the defining properties of density matrices and their ability to describe quantum states are understood, lets introduce a very important distinction in quantum information theory, which is the difference between pure and mixed states.

### 2.2 Pure and mixed states

The destinction into pure and mixed states is deeply connected to the difference between classical and quantum uncertainty. A pure state is defined as a density matrix for which a normed Hilbert space element $|\Psi\rangle$ exists, such that

$$
\begin{equation*}
\rho_{\text {pure }}=|\Psi\rangle\langle\Psi| \tag{2.2}
\end{equation*}
$$

They are therefore all the density matrices to which a single Hilbert space vector corresponds. Their classical uncertainty is therefore zero. Mixed states, however, do carry classical uncertainty about what quantum state the system actually is in. Such a density matrix is of the form

$$
\begin{equation*}
\rho_{\text {mixed }}=\sum_{k} p_{k}\left|\Psi_{k}\right\rangle\left\langle\Psi_{k}\right| \tag{2.3}
\end{equation*}
$$

where all the $p_{k}$ have to be non-negative and sum up to 1 . In the language of convexity, one can say that the mixed states are convex combinations of pure ones - which is equivalent to saying mixed states are of the form 2.3. This makes the set of all states a convex set with the pure states as its extreme points, studyable via the tools of convex geometry.
A very special state, whose importance will arise in the next chapter, is the so called maximally mixed state denoted by $\rho_{*}$. It's density matrix is

$$
\begin{equation*}
\rho_{*}:=\frac{1}{d} I_{d} \tag{2.4}
\end{equation*}
$$

where $d$ gives the (complex) dimension of the Hilbert space and $I_{d}$ is the identity matrix of size $d \times d$.

## 3 The set of quantum states

This chapter analyses the set of all possible quantum states, denoted by $\mathrm{D}(\mathcal{H})$. Using it's convexity, we will be able to deduce some facts about the size of this set. By doing that, one can derive interesting geometrical pictures describing $\mathrm{D}(\mathcal{H})$. The main result of this chapter will be a derivation of it's in- and outward radii $r_{i n}$ and $r_{\text {out }}$ dependent on the dimension of the Hilbert space. The norm used for this will be the Hilbert-Schmidt norm $\|A\|=\sqrt{\langle A, A\rangle}=\sqrt{\operatorname{Tr}\left(A^{2}\right)}$.

### 3.1 The shape and center of $\mathbf{D}(\mathcal{H})$

The set of quantum states includes all the matrices of $\operatorname{size} \operatorname{dim}(\mathcal{H}) \times \operatorname{dim}(\mathcal{H})$, being hermitian, normed and positive semidefinite. However, as positive semidefiniteness implies hermiticity, there really are two conditions necessary to be fulfilled by a quadratic matrix in order to describe a quantum state. A sketch, how one might visualize the set of quantum states, can be seen in Figure 3.1.


Figure 3.1: A visualisation of the set of quantum states on a finite dimensional Hilbert space $\mathcal{H}=\mathbb{C}^{d}$. One can see the hyperplane of trace one matrices embedded in the space of all hermitian matrices of size $\mathrm{d} \times \mathrm{d}$. Also the cone of semidefinite matrices is visible. The set of states corresponds to the intersection of hyperplane and cone. There is also a point drawn in its center, corresponding to the maximally mixed state $\rho_{*}$. Taken from Geometrical aspects of entanglement, Leinaas et al., Figure 1. [2]

When talking about the center of a convex set, one needs to clarify what being the center actually means. There are more possibilities in defining this. One choice, for example, would be the set's center of mass ${ }^{1}$. However, the definition used in this thesis will be, that the center of a body must be the focus point of its in- and outward circle.
For most „typical" shapes, like circles, cubes or pyramids for example, these definitions will yield

[^1]the same point as a center. Nevertheless, as even rectangles have different possible choices for the focus point of their inward circle, as shown in Figure 3.2, while there is always just one center of mass, the choosen center is in general dependent on the used definition.


Figure 3.2: A visualisation of the ambiguity of the inward circle of a rectangle. All points along the ocher colored line are possible choices for the center of the inward circle. This picture should raise awareness, that one has to be mindful when talking about the centers of convex bodies.

Theorem 1. The maximally mixed state $\rho_{*}=\frac{1}{d} I_{d}$ is the center for the set of states $D(\mathcal{H})$. If this selection is ambiguous, one can always use $\rho_{*}$ as a chanonical choice.

As $\mathrm{D}(\mathcal{H})$ is a convex set, one knows that an inward circle (=cirlce with maximal radius, whose points are all inside or on the border of $\mathrm{D}(\mathcal{H})$ ) as well as an outward circle (=circle with minimal radius, whose points are all outside or on the border of $\mathrm{D}(\mathcal{H})$ ) must exist. The proof will show, that the center - though in general ambiguous - can always be chosen to be $\rho_{*}$.

Proof. The proof will be done in two parts, the first showing that $\rho_{*}$ is a chanonical choice for the inward circle's focus and the second doing the same for the outward radius. As they both yield $\rho_{*}$ as a result, it can be chosen as the general center.

## 1. inwards circle:

Let M be a possible focus for the inward circle of $\mathrm{D}(\mathcal{H})$ and let A be a state with distance $r_{i n}$ from M. As the norm is invariant under unitary transformations

$$
\|A-M\|=\left\|U^{\dagger} A U-U^{\dagger} M U\right\|=r_{i n}
$$

and unitary transformations do not change the spectrum (=set of eigenvalues) of a matrix

$$
\operatorname{Spect}(A)=\operatorname{Spect}\left(U^{\dagger} A U\right)
$$

one concludes, that $U^{\dagger} A U$ will again be a quantum state with distance $r_{i n}$ to $U^{\dagger} M U$. As this is true for any state on the incirlce around $\mathrm{M}, U^{\dagger} M U$ must also be a possible focus point (which is true for any unitary matrix U ), showing that $\left\{U^{\dagger} M U \mid \mathrm{U}\right.$ unitary $\}$ must be a subset of all choosable focii. As the set of all possible centers of a convex set must also be convex, one can be sure that also all convex combinations of elements in $\left\{U^{\dagger} M U \mid \mathrm{U}\right.$ unitary $\}$ will yield choosable focus points. By calculating its center of mass one will get $\tilde{M}$ as

$$
\tilde{M}=\int_{U(d)} U^{\dagger} M U d U
$$

where $\mathrm{U}(\mathrm{d})$ is the unitary group of size d . By definition, $\tilde{M}$ has to be invariant under all unitary transformations, as for any unitary matrix V

$$
\begin{aligned}
V^{\dagger} \tilde{M} V & =V^{\dagger}\left(\int_{U(d)} U^{\dagger} M U d U\right) V=\int_{U(d)} V^{\dagger} U^{\dagger} M U V d U=\int_{U(d)}(U V)^{\dagger} M(U V) d U= \\
& =\int_{U(d)}\left(U^{\prime}\right)^{\dagger} M U^{\prime} d U^{\prime}=\tilde{M}
\end{aligned}
$$

The only matrices invariant under all unitary transforamtions are matrices of the form $\tilde{M}=\alpha \cdot I_{d}$ for $\alpha \in \mathbb{C}$. From the normalisation constraint $\operatorname{Tr}(\tilde{M})=1$ follows $\alpha=1 / d$.
2. outwards circle:

Again, one picks a possible choice N for the focus of the outwards circle and an point B with the maximal distance $r_{\text {out }}$ from it. Using the same argumentation as before, one sees that also $\left\|U^{\dagger} B U-U^{\dagger} N U\right\|=r_{\text {out }}$ for any unitary U. Again, as this argument is true for any B with maximal distance, $U^{\dagger} B U$ will yield another outcircle focus for every unitary U . By averaging over the unitary group of corresponding size $\mathrm{U}(\mathrm{d})$,

$$
\tilde{N}=\int_{U(d)} U^{\dagger} N U d U
$$

arises, which again is invariant under all unitary transformations (the calculation is the same as in the first part of the proof), yielding $\tilde{N}=\alpha I_{d}$ with $\alpha \in \mathbb{C}$. The normalization gives $\alpha=1 / d$.

This says that no point in $\mathrm{D}(\mathcal{H})$, when choosen as the midpoint of the in- and outward cirlces, yields a bigger value for $r_{i n}$ and smaller one for $r_{\text {out }}$. Therefore, all derivations of these values will correspond the calculations of the form

$$
\begin{align*}
& r_{i n}=\left\|\rho_{\text {in }}-\rho_{*}\right\|=\sqrt{\operatorname{Tr}\left(\left(\rho_{\text {in }}-\rho_{*}\right)^{2}\right)} \\
& r_{\text {out }}=\left\|\rho_{\text {out }}-\rho_{*}\right\|=\sqrt{\operatorname{Tr}\left(\left(\rho_{\text {out }}-\rho_{*}\right)^{2}\right)} \tag{3.1}
\end{align*}
$$

for some $\rho_{\text {in }} / \rho_{\text {out }}$ fullfilling the condition to be on either the in- or outward circle's line. The goal of the next section is to characterise states fullfilling these conditions. This will yield a very interesting geometric interpretation of $\mathrm{D}(\mathcal{H})$, by thinking about the set of all possible eigenvalues, density matrices can have.

### 3.2 Eigenvalue picture

Using equations 3.1, the following theorem shows that the distance of any state $\rho \in \mathrm{D}(\mathcal{H})$ towards the maximally mixed state $\rho_{*}$ specifically does only depend on its eigenvalues.

Theorem 2. The metric defined in 3.1 is only dependent on the eigenvalues $\lambda_{k}$ of a density matrix $\rho$.

$$
r=\left\|\rho-\rho_{*}\right\|=\left\|\left(\begin{array}{c}
\lambda_{1} \\
\ldots \\
\lambda_{d}
\end{array}\right)-\frac{1}{d}\left(\begin{array}{c}
1 \\
\ldots \\
1
\end{array}\right)\right\|
$$

Distances from the set's center can therefore be measured in $\mathbb{R}^{d}$ instead of $\operatorname{Herm}\left(\mathbb{C}_{d \times d}\right)$.

Proof. As norms are invariant under unitary transformations,

$$
r=\left\|\rho-\rho_{*}\right\|=\left\|U^{\dagger} \rho U-U^{\dagger} \rho_{*} U\right\|
$$

follows for every unitary matrix $U$. Therefore, one can always do the transformation with a unitary $U_{\rho}$, which diagonalises $\rho$ into $D_{\rho}$. As $\rho_{*}$ is just a scalar times the identity matrix, it will commute with $U_{\rho}$ and stay invariant, making sure that $D_{\rho}-\rho_{*}$ is diagonal.
$r=\left\|U_{\rho}^{\dagger} \rho U_{\rho}-U_{\rho}^{\dagger} \rho_{*} U_{\rho}\right\|=\left\|D_{\rho}-\rho_{*}\right\|=\sqrt{\operatorname{Tr}\left(\left(D_{\rho}-\rho_{*}\right)^{2}\right)}=\sqrt{\sum_{k}\left(D_{\rho, k}-\rho_{* k}\right)^{2}}=\sqrt{\sum_{k}\left(\lambda_{k}-\frac{1}{d}\right)^{2}}$
Here $\lambda_{k}$ denotes the k -th eigenvalue of $\rho$. As every density matrix $\rho$ has to be hermitian, its eigenvalues - which are the diagonal entries in $D_{\rho}$ - are real. The distance a density matrix has from $\rho_{*}$ is therefore only dependent on the entries of its diagonalized form, which in fact are the eigenvalues of $\rho$.

When measuring distances on $\mathrm{D}(\mathcal{H})$ towards the maximally mixed state $\rho_{*}$ specifically, one can therefore simplify the problem by looking at the eigenvalue picture. The set can be visualised as a convex subset of $\mathbb{R}^{d}$, corresponding to all points, whose coordinates yield a density matrix when used as its eigenvalues. As these have to sum up to 1 (normalisation) and all be non-negative (positive semidefinitness), the set of states can be visualised as seen in Figures 3.3 and 3.4.


Figure 3.3: The set of states for Hilbert space $\mathcal{H}=\mathbb{C}^{3}$ in the eigenvalue picture. The convex set is the intersection of points, whose coordinates sum up to 1 and the first octant with the coordinate axes(for an arbitrary dimension this is called the positive cone of $\mathbb{R}^{d}$ ). This follows from the fact, that density matrices have to be positive semidefinite and of trace one.

Such a convex body in $\mathbb{R}^{d}$ having $d+1$ extreme points is called d-simplex. It is the generalization of the equilateral triangle ( $=2$-simplex) and tetrahedron ( $=3$-simplex). By analysing these higher dimensional geometric bodies, interesting facts about $\mathrm{D}(\mathcal{H})$ can be deduced.


Figure 3.4: The set of states for the $\mathcal{H}=\mathbb{C}^{4}$ in the eigenvalue picture. The tetrahedron is the intersection of the hyperplane of points in $\mathbb{R}^{4}$, whose coordinates sum up to 1 with the cone of points, whose coordinates are all positive.

### 3.3 Size estimates

The goal of this section is to caluculate the values of $r_{\text {in }}$ and $r_{\text {out }}$ for $\mathrm{D}(\mathcal{H})$ on a finite dimensional Hilbert space $\mathcal{H}=\mathbb{C}^{d}$. As Theorem 2 states, distances from the set's center $\rho_{*}$ can be calculated in the eigenvalue picture. This way of thinking about $\mathrm{D}(\mathcal{H})$ makes it much easier to characterise states fullfilling the condition to lie on the in- or outward cirlce's line. As the set corresponds to a d-simplex in $\mathbb{R}^{d}$, geometric arguments can be used in order to find such special states.
A visualisation of this is shown in Figure 3.5


Figure 3.5: A visualization of the set of states for $\mathcal{H}=\mathbb{C}^{3}$. The dot in the center of the triangle corresponds to the maximally mixed state $\rho_{*}$, also its inward and outward circles are drawn.

Theorem 3. For a Hilbert space $\mathcal{H}=\mathbb{C}^{d}$, the radius of $D(\mathcal{H})$ 's outward circle equals

$$
r_{\text {out }}=\sqrt{\frac{d-1}{d}}
$$

while its inward circle's radius is

$$
r_{i n}=\sqrt{\frac{1}{d(d-1)}}
$$

Proof. The calculations will be shown using the eigenvalue picture.
In order to calculate $r_{\text {out }}$, one has to find a vector $\vec{v}$ maximising $\left\|\vec{v}-\overrightarrow{\rho_{\rho_{*}}}\right\|=\sqrt{\sum_{k}\left(v_{k}-1 / d\right)^{2}}$
for $\overrightarrow{v_{\rho_{*}}}=\frac{1}{d}(1, \ldots, 1)^{\top}$ under the constraints $\sum_{k} v_{k}=1$ and $\forall k: v_{k} \geq 0$. This can be done via the use of lagrange parameters, for example. Otherwise, one can also look at Figure 3.5, see that the extreme points have a 1 in one coordinate and 0 for every other and generalize this to higher dimensions. Both ways yield as a possible choice for such a vector $\vec{v}=(1,0, \ldots, 0)^{\top}$ (or every vector with permutated coordinates). Such a state's distance from $\rho_{*}$ can be calculated via

$$
\begin{aligned}
r_{\text {out }} & =\left\|\vec{v}-\overrightarrow{v_{\rho_{*}}}\right\|=\left\|\left(\begin{array}{c}
1 \\
0 \\
\ldots \\
0
\end{array}\right)-\frac{1}{d}\left(\begin{array}{c}
1 \\
1 \\
\ldots \\
1
\end{array}\right)\right\|=\sqrt{\left(1-\frac{1}{d}\right)^{2}+(d-1) \frac{1}{d^{2}}}= \\
& =\sqrt{\frac{1}{d^{2}}-\frac{2}{d}+1+\frac{d-1}{d^{2}}}=\sqrt{1-\frac{1}{d}}=\sqrt{\frac{d-1}{d}}
\end{aligned}
$$

In order to find vectors $\vec{w}$ which lie on the incirlce, some geometric argumentation is needed. The inward radius can be characterised as the minimal distance, a point on the surface of a body has to its center. For tetrahedra it is quite obvious, that these points must be the centers of the bodies faces, which are equilateral triangles. For a general dimension, the faces of $d$ simplex will be a (d-1)-simplex. The orientation of these ( $\mathrm{d}-1$ )-simplices in $\mathbb{R}^{d}$ is such, that the simplex is orthogonal to the one extreme point not touching it. This means, that the vector, which connects the center of the ( $\mathrm{d}-1$ )-simplex to the opposite extreme point, is orthogonal to every vector connecting two points inside the ( $\mathrm{d}-1$ )-simplex. This can be visualized nicely by the 3 -simplex (=tetrahedron), whose surface is made up by 42 -simplices (=equilateral triangles), which are in fact by themselves constructed from 3 2-simplices ( $=$ lines) each.
The eigenvalue picture shows that the center of a $\tilde{d}$-simplex is $\overrightarrow{v_{\rho_{*}}}=1 / \tilde{d}(1, \ldots, 1)^{\top}$. Embedding this point in a space 1 dimension higher, in the orthogonal plane to a extreme point $\vec{v}=(1,0, \ldots, 0)^{\top}$, will give the center of the face opposite to $\vec{v}$. The centers of the different ( $\mathrm{d}-1$ )-simplices are therefore all vectors $\vec{w}=\frac{1}{d-1}(0,1, \ldots 1)^{\top}$ (as well as all vectors with permutated coordinates). Using this, the inwards radius can be calculated via

$$
\begin{aligned}
r_{i n} & =\left\|\vec{w}-\overrightarrow{v_{\rho_{*}}}\right\|=\left\|\frac{1}{d-1}\left(\begin{array}{c}
0 \\
1 \\
\ldots \\
1
\end{array}\right)-\frac{1}{d}\left(\begin{array}{c}
1 \\
1 \\
\ldots \\
1
\end{array}\right)\right\|=\sqrt{\frac{1}{d^{2}}+(d-1)\left(\frac{1}{d-1}-\frac{1}{d}\right)^{2}}= \\
& =\sqrt{\frac{1}{d^{2}}+(d-1)\left(\frac{1}{d(d-1)}\right)^{2}}=\sqrt{\frac{d-1}{d^{2}(d-1)}+\frac{1}{d^{2}(d-1)}}=\sqrt{\frac{1}{d(d-1)}}
\end{aligned}
$$

Theorem 3 says, that for large Hilbert spaces $r_{i n}$ goes towards 0 , while $r_{\text {out }}$ slowly approaches 1 . Therefore, one might visualize the set of all quantum states of a system as an ellipsoid, as shown in Figure 3.1, with highly differing major- and minor-semi axes.

## 4 Bipartite quantum systems

This chapter focuses on bipartite systems, which consist of two distinct subsystems able to interact. As both of these parties are quantum systems, one is able to describe them each with Hilbert space $\mathcal{H}_{A / B}$ respectivley. The structure of this situation (having two distinct subsystems) can mathematically be expressed by a tensor product, yielding the system's Hilbert space $\mathcal{H}=$ $\mathcal{H}_{A} \otimes \mathcal{H}_{B}$. While all results of the last chapter remain true for this global system, the tensor decomposition of $\mathcal{H}$ gives rise to some physically important subsets of $\mathrm{D}(\mathcal{H})$ with an interesting geometry.
After an introduction of entanglement and separability, the set of positive partial transpose $\operatorname{PPT}(\mathcal{H})$ will be defined. This is a subset of $\mathrm{D}(\mathcal{H})$ used for approximating the set of separable states $\operatorname{SEP}(\mathcal{H})$. Afterwards, the in- and outwards radii of those two sets will be calculated and compared to the results from Theorem 3.

### 4.1 Separability and entanglement

Bipartite quantum systems are all systems described by a Hilbert space of the form

$$
\begin{equation*}
\mathcal{H}=\mathcal{H}_{A} \otimes \mathcal{H}_{B} \tag{4.1}
\end{equation*}
$$

where $\mathcal{H}_{A}$ and $\mathcal{H}_{B}$ are the Hilbert spaces of the two parties on their own. In order to describe states on this global Hilbert space, the definition of a pure product state

$$
\rho=|\phi\rangle\langle\phi| \otimes|\psi\rangle\langle\psi|
$$

with $|\phi\rangle \in \mathcal{H}_{A}$ and $|\psi\rangle \in \mathcal{H}_{B}$, is needed. These are all the states corresponding to one pure state on both subsystems. If a system is described by a pure product state, its subsystems do not interfere with eachother and do not carry classical uncertainty. This can be seen, as the partial trace over one of the Hilbert spaces $\operatorname{Tr}_{A}(\rho)=|\psi\rangle\langle\psi|$ stays invariant under measuring subsystem B in an arbitrary state $|\alpha\rangle$. This will be discussed in more detail once entanglement is introduced. In order to also describe systems with classical uncertainty, one has to allow convex combinations

$$
\begin{equation*}
\rho=\sum_{k} c_{k}\left|\phi_{k}\right\rangle\left\langle\phi_{k}\right| \otimes\left|\psi_{k}\right\rangle\left\langle\psi_{k}\right| \tag{4.2}
\end{equation*}
$$

States writable in this form are called separable. The set of separable states, consisting of all density matrices of the form 4.2 , therefore is a convex subset of $\mathrm{D}(\mathcal{H})$ with the pure product states as its extreme points. This is also the set of all solely classical correlated states. ${ }^{1}$

However, not all states on $\mathcal{H}$ are writable in this form. The ones that are not are called entangled. Some typical examples for entangled states are the four Bell states on $\mathcal{H}=\mathbb{C}^{2} \otimes \mathbb{C}^{2}$ shown below. [3] The two pure basis states of $\mathbb{C}^{2}$ are denoted by $|0\rangle$ and $|1\rangle$. Also the tensor product $|0\rangle\langle 0| \otimes|0\rangle\langle 0|$ gets surpressed into $|00\rangle\langle 00|$ to simplify the notations.

[^2]\[

$$
\begin{align*}
\left|\Phi^{+}\right\rangle\left\langle\Phi^{+}\right| & =\frac{1}{2}(|00\rangle\langle 00|+|00\rangle\langle 11|+|11\rangle\langle 00|+|11\rangle\langle 11|) \\
\left|\Phi^{-}\right\rangle\left\langle\Phi^{-}\right| & =\frac{1}{2}(|00\rangle\langle 00|-|00\rangle\langle 11|-|11\rangle\langle 00|+|11\rangle\langle 11|) \\
\left|\Psi^{+}\right\rangle\left\langle\Psi^{+}\right| & =\frac{1}{2}(|01\rangle\langle 01|+|01\rangle\langle 10|+|10\rangle\langle 01|+|10\rangle\langle 10|)  \tag{4.3}\\
\left|\Psi^{-}\right\rangle\left\langle\Psi^{-}\right| & =\frac{1}{2}(|01\rangle\langle 01|-|01\rangle\langle 10|-|10\rangle\langle 01|+|10\rangle\langle 10|)
\end{align*}
$$
\]

The Bell states are not of the form 4.2 , as not all terms in 4.3 are density matrices, as for example

$$
|00\rangle\langle 11|=|0\rangle\langle 1| \otimes|0\rangle\langle 1| \doteq\left(\begin{array}{ll}
0 & 1 \\
0 & 0
\end{array}\right) \otimes\left(\begin{array}{ll}
0 & 1 \\
0 & 0
\end{array}\right)
$$

which is neither positive semidefinite nor normed.
The key distinction between these Bell states (or any other entangled state) and separable ones is, that measurements on one subsystem of the states in 4.3 do affect the other party's state. When looking at a system described by $\left|\Phi^{+}\right\rangle\left\langle\Phi^{+}\right|$for example, both of the subsystems are in a superposition of $|0\rangle$ and $|1\rangle$. The state on subsystem $B$ would be

$$
\rho_{B}=\operatorname{Tr}_{A}\left(\left|\Phi^{+}\right\rangle\left\langle\Phi^{+}\right|\right)=\left\langle\left. 0\right|_{A} \mid \Phi^{+}\right\rangle\left\langle\Phi^{+} \mid 0\right\rangle_{A}+\left\langle\left. 1\right|_{A} \mid \Phi^{+}\right\rangle\left\langle\Phi^{+} \mid 1\right\rangle_{A}=\frac{1}{2}\left(|0\rangle\left\langle\left. 0\right|_{B}+\mid 1\right\rangle\left\langle\left. 1\right|_{B}\right)\right.
$$

where the index denotes state's system. However, when taking a measurement on A before measuring $B$ this result is no longer true, as measuring system $A$ in the $|1\rangle_{A}$ state for example

$$
\left\langle\left. 1\right|_{A} \mid \Phi^{+}\right\rangle\left\langle\Phi^{+} \mid 1\right\rangle_{A}=|1\rangle\left\langle\left. 1\right|_{B}\right.
$$

The measurement done on A therefore changed the state on B, which corresponds to Einstein's "spooky action at a distance", as this is true no matter how far the subsystems are apart.
The Bell state $\left|\Phi^{+}\right\rangle\left\langle\Phi^{+}\right|$(as well as $\left|\Phi^{-}\right\rangle\left\langle\Phi^{-}\right|$) therefore yields perfectly correlated measurements, while the results for $\left|\Psi^{ \pm}\right\rangle\left\langle\Psi^{ \pm}\right|$would be perfectly anticorrelated. In general, the defining property of entanglement is, that measurements on one subsystem affect the state of the other one, which does not happen with a separable state as in 4.2. The subsystems are therefore non-classically correlated.

Even though separable and entangled states behave differently under measurements, it is not clear on first sight what conditions a density matrix has to fullfill in order to be writable as in 4.2. In order to be able to answer the question, if a given state is separable or not, the concept of the partial transpose will get introduced in the next section. From this a necessary condition for separabilty arises.

### 4.2 The partial transpose

The partial transpose operator is defined as

$$
\begin{equation*}
\Gamma_{B}:=I_{d} \otimes T \tag{4.4}
\end{equation*}
$$

It acts as the identity on the first subsystem and does a matrix transpose on the second one. As the matrix transpose is a positive, though not completely positive, $\operatorname{map}^{2}[6]$, the transpose of a density matrix will always yield another density matrix. As the eigenvalues can change under a partial transposition, this is not true for partially transposed states. Therefore one is able to define the set of positive partially transposed states, which consits of all density matrices remaining states after getting partially transposed

$$
\begin{equation*}
\operatorname{PPT}:=\left\{\rho \in \mathrm{D}(\mathcal{H}): \Gamma_{B} \rho \in \mathrm{D}(\mathcal{H})\right\} \tag{4.5}
\end{equation*}
$$

$\rho$ being an element of PPT therefore is equivalent to saying that $\Gamma_{B} \rho$ only has non-negative eigenvalues, as the trace of a matrix is not affected by such a transformation. This definition of PPT is independent of the choice, which of the two subsystems is transposed, as the partial transpose on system B just gives the global transpose of the partial transpose on A.

$$
\Gamma_{B} \rho=\left(I_{d} \otimes T\right) \rho=T \otimes T\left(T \otimes I_{d}\right) \rho=T_{\text {global }}\left(\Gamma_{A} \rho\right)
$$

When taking the partial transpose of a separable state
$\Gamma_{B} \rho=\left(I_{d} \otimes T\right) \sum_{k} c_{k}\left|\phi_{k}\right\rangle\left\langle\phi_{k}\right| \otimes\left|\psi_{k}\right\rangle\left\langle\psi_{k}\right|=\sum_{k} c_{k}\left|\phi_{k}\right\rangle\left\langle\phi_{k}\right| \otimes T\left|\psi_{k}\right\rangle\left\langle\psi_{k}\right|=\sum_{k} c_{k}\left|\phi_{k}\right\rangle\left\langle\phi_{k}\right| \otimes\left|\tilde{\psi}_{k}\right\rangle\left\langle\tilde{\psi}_{k}\right|$
it remains separable. This follows from the fact that the density matrices $\left|\psi_{k}\right\rangle\left\langle\psi_{k}\right|$ all get transposed globally and must therefore not change their eigenvalues. This is stated in the PeresHorodecki criterion, yielding a necessary condition for separability.[4]

$$
\begin{equation*}
\mathrm{SEP} \subset \mathrm{PPT} \tag{4.6}
\end{equation*}
$$

Interestingly, for the low dimensional Hilbert spaces $\mathcal{H}=\mathbb{C}^{2} \otimes \mathbb{C}^{2}$ and $\mathcal{H}=\mathbb{C}^{2} \otimes \mathbb{C}^{3}$, this condition is not only necessary, but also sufficient.[4]

### 4.3 Size estimates

Similar to Theorem 3, this section will be dedicated to calculate the values for $r_{i n}$ and $r_{\text {out }}$ for the two sets $\operatorname{SEP}(\mathcal{H})$ and $\operatorname{PPT}(\mathcal{H})$, consisting of all separable/positive partially transposable states on a general bipartite Hilbert space.

Theorem 4. The outward radii $r_{\text {out }}$ of $\operatorname{SEP}(\mathcal{H})$ and $\operatorname{PPT}(\mathcal{H})$ match for an arbitrary bipartite Hilbert space $\mathcal{H}=\mathbb{C}^{d_{1}} \otimes \mathbb{C}^{d_{2}}$. Its value is

$$
r_{\text {out }}=\sqrt{\frac{d-1}{d}}
$$

with $d$ being the global Hilbert space dimension $d=d_{1} \cdot d_{2}$.

[^3]Proof. At first the statement will be shown for the separable states. As $\mathrm{SEP}(\mathcal{H})$ is a convex set, it follows that the maximal distance from the center $\left\|\rho-\rho_{*}\right\|$ will get realised for a extreme point of the set, which corresponds to a product state $\rho=\Lambda \otimes \Phi$ with $\Lambda \in \operatorname{Herm}_{\mathrm{d}_{1} \times \mathrm{d}_{1}}$ and $\Phi \in \operatorname{Herm}_{\mathrm{d}_{2} \times \mathrm{d}_{2}}$. The distance such a state has towards $\rho_{*}$ is therefore

$$
\begin{aligned}
\left\|\rho-\rho_{*}\right\| & =\sqrt{\operatorname{Tr}\left(\left(\Lambda \otimes \Phi-\frac{1}{d} I_{d}\right)^{2}\right)}=\sqrt{\operatorname{Tr}\left(\Lambda^{2} \otimes \Phi^{2}-\frac{2}{d} \Lambda \otimes \Phi+\frac{1}{d^{2}} I_{d}\right)}= \\
& =\sqrt{\operatorname{Tr}\left(\Lambda^{2}\right) \operatorname{Tr}\left(\Phi^{2}\right)-\frac{2}{d} \operatorname{Tr}(\Lambda) \operatorname{Tr}(\Phi)+\frac{1}{d^{2}} \operatorname{Tr}\left(I_{d}\right)}=\sqrt{\operatorname{Tr}\left(\Lambda^{2}\right) \operatorname{Tr}\left(\Phi^{2}\right)-\frac{2}{d}+\frac{1}{d}}= \\
& =\sqrt{\operatorname{Tr}\left(\Lambda^{2}\right) \operatorname{Tr}\left(\Phi^{2}\right)-\frac{1}{d}}
\end{aligned}
$$

where $\operatorname{Tr}(\Lambda)=\operatorname{Tr}(\Phi)=1$ was used. As the outward radius corresponds to the maximal distance a state can have from the center, $r_{\text {out }}$ can be calculated via

$$
r_{o u t}=\max \left(\left\|\rho-\rho_{*}\right\|\right)=\max \left(\sqrt{\operatorname{Tr}\left(\Lambda^{2}\right) \operatorname{Tr}\left(\Phi^{2}\right)-\frac{1}{d}}\right)=\sqrt{1-\frac{1}{d}}=\sqrt{\frac{d-1}{d}}
$$

which coincides with the outward radius of $\mathrm{D}(\mathcal{H})$. As $\mathrm{SEP} \subset \mathrm{PPT} \subset \mathrm{D}$ implies that $r_{\text {out }}(\mathrm{SEP}) \leq$ $r_{\text {out }}(\mathrm{PPT}) \leq r_{\text {out }}(\mathrm{D})$ holds, the same follows for $\operatorname{PPT}(\mathcal{H})$.

Theorem 5. The inward radii $r_{i n}$ of $S E P(\mathcal{H})$ and $P P T(\mathcal{H})$ match for an arbitrary bipartite Hilbert space $\mathcal{H}=\mathbb{C}^{d_{1}} \otimes \mathbb{C}^{d_{2}}$. Its value is

$$
r_{i n}=\sqrt{\frac{1}{d(d-1)}}
$$

with $d$ being the global Hilbert space dimension $d=d_{1} \cdot d_{2}$.
Proof. At first, one may choose an orthogonal basis of the set of Hermitian matrices Herm ${ }_{d \times d}$, such that $e_{0}=\rho_{*}$ aswell as $\operatorname{Tr}\left(e_{i}\right)=0$ and $\left\|e_{i}\right\|=1$ for $i=1, \ldots, N$. Using this basis, an arbitrary density matrix can be expressed as $\rho=\rho_{*}+\sum_{k} r_{k} e_{k}$ for some coordinate vector $\vec{r} \in \mathbb{R}^{N}$. The set $\mathrm{D}(\mathcal{H})$, as well as all of its subsets can therefore be associated with subsets of $\mathbb{R}^{N}$. Furthermore, let K be defined as the set of all states, lying inside the hypersphere of radius $\sqrt{\frac{1}{d(d-1)}}$ around $\rho_{*}$, so $\left\|\rho-\rho_{*}\right\|^{2} \leq \frac{1}{d(d-1)}$ for every $\rho \in \mathrm{K}$. This can be simplified to the condition $\|\vec{r}\|^{2} \leq \frac{1}{d(d-1)}$, as

$$
\left\|\rho-\rho_{*}\right\|^{2}=\operatorname{Tr}\left(\left(\rho-\rho_{*}\right)^{2}\right)=\operatorname{Tr}\left(\left(\sum_{k} r_{k} e_{k}\right)^{2}\right)=\operatorname{Tr}\left(\left(\sum_{k} r_{k}^{2} e_{k}^{2}\right)=\sum_{k} r_{k}^{2} \operatorname{Tr}\left(e_{k}^{2}\right)=\sum_{k} r_{k}^{2}=\|\vec{r}\|^{2}\right.
$$

Instead of showing the inclusion $\mathrm{K} \subset$ SEP implied by the theorem, one can make use of the bipolar theorem in $\mathbb{R}^{N}$ and change to the polar of these sets, denoted by a ${ }^{*}$, and show $\mathrm{SEP}^{*} \subset \mathrm{~K}^{*} .3$ As K just corresponds to a hypersphere with radius $\mathrm{r}=\sqrt{\frac{1}{d(d-1)}}$ around the origin in $\mathbb{R}^{N}$, one deduces that its polar is a hypersphere of inverted radius. This can be seen as $\langle\vec{r}, \vec{x}\rangle \geq-1$ implies that a $\vec{x}$ being anti-parallel to a vector $\vec{r}$ can maximally be of lenght $\frac{1}{r}$ in order to be in the polar.

We will now characterise elements of SEP*. It is known, that the dual of the separable cone which corresponds to all separable matrices ignoring the normalization constraint - is the cone of

[^4]all block-positive matrices[1]. This means, that saying a matrix M is block positive is equivalent to $\langle M, S\rangle \geq 0 \forall S \in$ SEP. By restricting us to elements in the hyperplane of unit trace, this scalar product equals
$$
\langle M, S\rangle=\operatorname{Tr}\left(\rho_{*}^{2}\right)+\langle\vec{m}, \vec{s}\rangle=\frac{1}{d}+\langle\vec{m}, \vec{s}\rangle
$$
where $\vec{m}$ and $\vec{s}$ are the coordinate vectors of the block-positive/separable matrix in the chosen basis. For a matrix M to be block-positive can therfore be expressed as a criterion for its coordinate vector $\vec{m}$
$$
d\langle\vec{m}, \vec{s}\rangle=\langle d \vec{m}, \vec{s}\rangle \geq-1
$$

Comparing this result to the definition of the polar, we see that a matrix $\mathrm{M}=\rho_{*}+\sum_{k} m_{k} e_{k}$ is block-positive, if and only if its scaled coordinate vector $d \vec{m}$ is inside the polar. We can therefore describe the polar of the separable set SEP* as the set of all vectors $\vec{a}$, for which $\rho_{*}+\sum_{k} \frac{a_{k}}{d} e_{k}$ yields a block-positve density matrix.
The inclusion $\mathrm{SEP}^{*} \subset \mathrm{~K}^{*}$ is therefore equivalent to showing that such a vector $\vec{a}$ is an element of the hypersphere of radius $\sqrt{d(d-1)}$ in $\mathbb{R}^{N}$ or prooving, that all block-positive density matrices ly inside the hypersphere of radius $\sqrt{\frac{d-1}{d}}$ around $\rho_{*}$.
By calculating $\left\|\rho-\rho_{*}\right\|^{2}$

$$
\left\|\rho-\rho_{*}\right\|^{2}=\operatorname{Tr}\left(\left(\rho-\rho_{*}\right)^{2}\right)=\operatorname{Tr}\left(\rho^{2}\right)-2 \operatorname{Tr}\left(\rho \rho_{*}\right)+\operatorname{Tr}\left(\rho_{*}^{2}\right)=\operatorname{Tr}\left(\rho^{2}\right)-\frac{2}{d}+\frac{1}{d}=\|\rho\|^{2}-\frac{1}{d}
$$

one gets a general condition to prove

$$
\|\rho\|^{2} \leq \frac{d-1}{d}+\frac{1}{d}=1
$$

for a general bipartite block-positive density matrix. By using the tensor decomposition, any matrix $\rho$ can be expressed as $\rho=\sum_{i, j} E_{i j} \otimes \rho_{i j}$, where $E_{i j}$ is an matrix unit of size $d_{1} \times d_{1}$, meaning its only nonzero entry is a 1 at the $(\mathrm{i}, \mathrm{j})$-spot, $\rho_{i, j}$ is the matrix block of size $d_{2} \times d_{2}$ at the $(\mathrm{i}, \mathrm{j})$-spot. By using the identity $E_{i j} \cdot E_{k l}=\delta_{j k} E_{i l}$, one gets

$$
\rho^{2}=\left(\sum_{i, k} E_{i k} \otimes \rho_{i k}\right) \cdot\left(\sum_{l, j} E_{l j} \otimes \rho_{l j}\right)=\sum_{i, j} E_{i j} \otimes \sum_{k} \rho_{i k} \rho_{k j}
$$

Taking the trace, this simplifies to

$$
\operatorname{Tr}\left(\rho^{2}\right)=\sum_{i, j, k} \operatorname{Tr}\left(E_{i j}\right) \cdot \operatorname{Tr}\left(\rho_{i k} \rho_{k j}\right)=\sum_{i, k} \operatorname{Tr}\left(\rho_{i k} \rho_{k i}\right)=\sum_{i, k} \operatorname{Tr}\left(\rho_{i k} \rho_{i k}^{\dagger}\right)=\sum_{i, k}\left\|\rho_{i k}\right\|^{2}
$$

where the hermiticity of the matrix and its blocks was used.
Finally, one must apply Lemma 9.16 in [1], which states for a self adjoint, block-positive matrix in the Hilbert space $\mathcal{H}=\mathbb{C}^{n} \otimes \mathbb{C}^{2}$, representable as

$$
\left(\begin{array}{rr}
A & B \\
B^{\dagger} & C
\end{array}\right)
$$

the inequallity $\|B\|^{2} \leq \operatorname{Tr}(A) \operatorname{Tr}(C)$ must hold. From this

$$
\operatorname{Tr}\left(\rho^{2}\right)=\sum_{i, k}\left\|\rho_{i k}\right\|^{2} \leq \sum_{i, k} \operatorname{Tr}\left(\rho_{i i}\right) \operatorname{Tr}\left(\rho_{k k}\right)=\operatorname{Tr}(\rho)^{2}=1
$$

follows, completing the proof for $\operatorname{SEP}(\mathcal{H})$. Simillar to the proof of Theorem 4 , from $\mathrm{SEP} \subset \mathrm{PPT} \subset \mathrm{D}$ follows that $r_{i n}(\mathrm{SEP}) \leq r_{\text {in }}(\mathrm{PPT}) \leq r_{i n}(\mathrm{D})$ holds. As the inward radii of $\mathrm{SEP}(\mathcal{H})$ and $\mathrm{D}(\mathcal{H})$ match, the same must be true for $\operatorname{PPT}(\mathcal{H})$.

It should be stated here, that the radii calculated in Theorem 4 and 5 are always measured in regard to $\rho_{*}$. While Theorem 1 proved that this state is the center of $\mathrm{D}(\mathcal{H})$, this was not shown for $\operatorname{SEP}(\mathcal{H})$ and $\operatorname{PPT}(\mathcal{H})$. In other words, it must also be shown that there is no state in both these sets, that yields bigger values for $r_{i n}$ or $r_{\text {out }}$ when used as their center. However, as their in- and outward circle match the ones of $\mathrm{D}(\mathcal{H})$, one can conclude that such points can not exist as they would have to violate the condition $r_{\text {in/out }}(\mathrm{SEP}) \leq r_{\text {in/out }}(\mathrm{PPT}) \leq r_{\text {in/out }}(\mathrm{D})$ implied by $\mathrm{SEP} \subset \mathrm{PPT} \subset \mathrm{D}$.
Interestingly, the in- and outward radii for the set $\operatorname{SEP}(\mathcal{H})$ and $\operatorname{PPT}(\mathcal{H})$ do not depend on the tensor decomposition of the Hilbert space in 4.1 , but only on the dimension of the global Hilbert space. Theorems 4 and 5 yield the same values for $r_{\text {in }}$ and $r_{\text {out }}$ for the sets $\operatorname{PPT}(\mathcal{H})$ and $\operatorname{SEP}(\mathcal{H})$ as Theorem 3 for the set of all states $\mathrm{D}(\mathcal{H})$. This seems surprising, as it is a well-known fact in quantum information theory, that in the limit of large hilbert spaces, the probability for a randomly choosen state to be entangled is $1 .[5]$ However, it should be noted that there are other size estimates (for example the mean-width as shown in Chapter 9 in [1]) for which the sets $\operatorname{SEP}(\mathcal{H}), \operatorname{PPT}(\mathcal{H})$ and $\mathrm{D}(\mathcal{H})$ yield different values.

## 5 Multipartite quantum systems

Multipartite systems are systems with two or more parties. As the bipartite case was discussed in detail in the last chapter, the focus will lie on Hilbert spaces with at least 3 subsystems. This has a big effect on the definition of $\operatorname{PPT}(\mathcal{H})$, which was independent of the choice which subsystem was transposed for the bipartite case. As this is no longer the case for Hilbert spaces with three or more parties, this chapter only discusses the set of separable states.
A general multipartite Hilbert space is of the form

$$
\begin{equation*}
\mathcal{H}=\bigotimes_{k=1}^{N} \mathcal{H}_{k} \tag{5.1}
\end{equation*}
$$

Interestingly, the in- and outward circle of the set $\operatorname{SEP}(\mathcal{H})$ behave highly different for a Hilbert space of the form 5.1.

Theorem 6. The radius of the outward circle $r_{\text {out }}$ of the set of separable states $S E P(\mathcal{H})$ yields

$$
r_{o u t}=\sqrt{\frac{d-1}{d}}
$$

for an arbitrary Hilbert space of the form 5.1.
Proof. Smilliar to the proof of Theorem 4 one can argue, that from $\operatorname{SEP}(\mathcal{H})$ being convex follows that $r_{\text {out }}$ - being the maximal distance from the body's center - must be realised toward its extreme points. These, being product states, are of the form $\rho=\bigotimes_{k=1}^{N} \Lambda_{k}$ for some $\Lambda_{k} \in \mathrm{D}\left(\mathcal{H}_{k}\right)$. The metric can then be calculated via

$$
\begin{aligned}
\left\|\rho-\rho_{*}\right\| & =\sqrt{\operatorname{Tr}\left(\left(\rho-\rho_{*}\right)^{2}\right)}=\sqrt{\operatorname{Tr}\left(\bigotimes_{k=1}^{N} \Lambda_{k}^{2}-\frac{2}{d} \bigotimes_{k=1}^{N} \Lambda_{k}-\frac{1}{d^{2}} I_{d}\right)}= \\
& =\sqrt{\operatorname{Tr}\left(\bigotimes_{k=1}^{N} \Lambda_{k}^{2}\right)-\frac{2}{d} \operatorname{Tr}\left(\bigotimes_{k=1}^{N} \Lambda_{k}\right)+\frac{1}{d^{2}} \operatorname{Tr}\left(I_{d}\right)}=\sqrt{\prod_{k=1}^{N} \operatorname{Tr}\left(\Lambda_{k}^{2}\right)-\frac{1}{d}}
\end{aligned}
$$

As $\operatorname{Tr}\left(\Lambda_{k}^{2}\right)$ is maximal, if $\Lambda_{k}^{2}=\Lambda_{k}, r_{\text {out }}$ can be calculated via

$$
r_{\text {out }}=\max \left(\left\|\rho-\rho_{*}\right\|\right)=\max \left(\sqrt{\prod_{k=1}^{N} \operatorname{Tr}\left(\Lambda_{k}^{2}\right)-\frac{1}{d}}\right)=\sqrt{\prod_{k=1}^{N} \operatorname{Tr}\left(\Lambda_{k}\right)-\frac{1}{d}}=\sqrt{1-\frac{1}{d}}=\sqrt{\frac{d-1}{d}}
$$

However, while the outward radius of $\operatorname{SEP}(\mathcal{H})$ and $\mathrm{D}(\mathcal{H})$ match for an arbitrary Hilbert space $\mathcal{H}$, the inward radius of $\operatorname{SEP}(\mathcal{H})$ is highly dependent on the form of the tensor decomposition of the Hilbert space in 5.1 and very hard to calculate even for specific cases. To give an example, in Chapter 9 in Alice and Bob meet Banach the authors are able to calculate that the inward radius for a N -qubit system is proportional to $6^{-\frac{N}{2}} .[\mathbf{1}]$

## 6 Conclusion

Now that we discussed the set of states on its own, looked at bipartite systems and how the sets $\operatorname{PPT}(\mathcal{H})$ and $\operatorname{SEP}(\mathcal{H})$ behave for a two party Hilbert space and also shortly discussed the multipartite case, lets summarize. Though the set of all quantum states of a system is an abstract set of complex matrices, fullfilling some conditions enabling us to interpret them in a physical way, we have been able to conclude some interesting facts about its structure. Being centered about the maximally mixed states $\rho_{*}=\frac{1}{d} I_{d}$, its rich geometry yields the eigenvalue picture, associating $\mathrm{D}\left(\mathbb{C}^{d}\right)$ with a (d-1)-dimensional simplex. This reduction enabled us not only to gain a visual interpretation of the set of states, unraveling some of its hidden beauty and symmetry, but also to calculate the in- and outward radii in a real vectorspace picture. This made the derivation less abstract and more intuitive, which is of course more than welcome.
Afterwards, we focussed on bipartite systems with a Hilbert space of the form $\mathcal{H}=\mathbb{C}^{d_{1}} \otimes \mathbb{C}^{d_{2}}$. In this context, the distinction into separable and entangled states was introduced, which brought us to the analysation of the set of positive partial transposed states $\operatorname{PPT}(\mathcal{H})$. The partial transpose - being a positive, though not completely positve map [6] - brought us the Peres-Horodeckicriterion; a necessary condition for separability. Furthermore, the radii of the in- and outward circle have been derived for these sets as well. Theorems 4 and 5 proved, that their size is only dependent on the global Hilbert space dimension and not on the specific form of the tensor decomposition. What is more, $r_{\text {in }}$ and $r_{\text {out }}$ have the same value for all three sets $\mathrm{D}(\mathcal{H}), \operatorname{PPT}(\mathcal{H})$ and $\operatorname{SEP}(\mathcal{H})$ ), as long as the Hilbert space is bipartite. This result was surprising, as the sets differ highly in volume and have to be convex. A picture, on how one might interpret this result and therefore visualize the different sets can be seen in Figure 6.1.


Figure 6.1: An illustration showing how different convex sets can share their in- and outward circle while differing in volume. The figure shows $\operatorname{SEP}\left(\mathcal{H}_{1} \otimes \mathcal{H}_{2}\right)$ (green), $\operatorname{PPT}\left(\mathcal{H}_{1} \otimes \mathcal{H}_{2}\right)$ (union of green and orange) and $\mathrm{D}\left(\mathcal{H}_{1} \otimes \mathcal{H}_{2}\right)$ (union of green, orange and blue) for the bipartite case. It should be noted that the shape of the different sets was chosen to illustrate this fact and has no other physical justification.

Even for a general multipartite system we have been able to prove that $\operatorname{SEP}(\mathcal{H})$ 's outward radius always matches with the one of all states. This says, that for every Hilbert space, there are some separable states near the border of the set $\mathrm{D}(\mathcal{H})$. Using the eigenvalue picture, one concludes that every Hilbert space has to have separable states with some of its eigenvalues being arbitrary small. However, the inward radius of the set of separable states depends highly non-trivially on the tensor decomposition of the Hilbert space, which makes it very difficult to calculate it. To obtain deeper insights into the reasons why this is the case and how one might overcome this hurdles, seems like an interesting topic for futher research. Some other very interesting questions would be to try to find other cases than the bipartite one, where the inward radii of $\operatorname{SEP}(\mathcal{H})$ and $\mathrm{D}(\mathcal{H})$ match or use other ways of measuring sizes for these sets and find out, which one yield the same result for the different sets and which do not. I think that doing this will yield some interesting facts about entanglement and, in the long run, increase our understanding for this very counterintuitive quantum behaviour.
To conclude, the internal structure of the set of quantum states enables us to find interesting pictures in order to characterize it. Describing this theoretical abstraction as a part of reality lets us derive further facts about quantum mechanics; helping us to not only understand our theories better, but also nature itself.

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Ich erkläre mich mit der Archivierung der vorliegenden Bachelorarbeit einverstanden.

Innsbruck, am July 28, 2022



[^0]:    ${ }^{1}$ It should be stated, that in order to really measure $\left|\Psi_{k}\right\rangle\left\langle\Psi_{k}\right|$, one needs to transfer the matrix into the eigenbasis $\left\{\left|\Phi_{j}\right\rangle\left\langle\Phi_{j}\right|, j=1, \ldots, n\right\}$ of the measurement operator $\hat{A} .\left|\Psi_{k}\right\rangle\left\langle\Psi_{k}\right|=\sum_{j} c_{j k}\left|\Phi_{j}\right\rangle\left\langle\Phi_{j}\right|$. The measurement is described by $\hat{A} \rho=\sum_{k} p_{k} \sum_{j} c_{j k} \hat{A}\left|\Phi_{j}\right\rangle\left\langle\Phi_{j}\right|=\sum_{j, k} \lambda_{j} p_{k} c_{j k}\left|\Phi_{j}\right\rangle\left\langle\Phi_{j}\right|$. So, when measuring $\hat{A}$ of a system described by $\rho$, the result will give eigenvalue $\lambda_{j}$ with a probability of $\sum_{k} p_{k} c_{j k}$.

[^1]:    ${ }^{1}$ The center of mass is calculated by defining a density function which is constant over every point in the set and zero everywhere else and then taking a weighted average over all points.

[^2]:    ${ }^{1}$ For a state to be classically correlated means, that a measurement taken on one of the subsystems can not affect the state of the other subsystem.

[^3]:    ${ }^{2}$ This means, that the eigenvalues of a general matrix do not change when transposing it globally, while they do change under a partial transpose.

[^4]:    ${ }^{3}$ The polar $\mathrm{X}^{*}$ of a set $\mathrm{X} \subset R^{N}$ is defined as all $\mathrm{y} \in \mathbb{R}^{N}$ fullfilling the inequality $\langle x, y\rangle \geq-1$ for every $\mathrm{x} \in \mathrm{X}$.

