



NTNU – Trondheim
Norwegian University of
Science and Technology

Low Rank States with Bound Entanglement in a System of three qubits

Børge Irgens

Physics

Submission date: December 2013

Supervisor: Jan Myrheim, IFY

Norwegian University of Science and Technology
Department of Physics

Abstract

We have studied mixed quantum states in the system of three qubits with the property that all their partial transposes are positive; these are called PPT states. We classify a PPT state by the ranks of the state itself and its three single partial transposes. We have studied especially the rank 4444 and rank 5555 entangled PPT states.

We find two distinct classes of rank four states, identified by a real valued quadratic expression invariant under local $SL(2, \mathbb{C})$ transformations, mathematically equivalent to continuous Lorentz transformations. We call it a Lorentz invariant since it is also invariant under partial transpositions, which are discrete Lorentz transformations. This quadratic Lorentz invariant is non-zero for one class of states (type 1) and zero for the other class (type 2). We present analytical constructions of states of both types, general enough to reproduce all the rank four PPT states we have found numerically.

There are six product vectors in a generic five dimensional subspace. The product vectors in the ranges of a rank 5555 state and its partial transposes are used to define local SL invariants that are not invariant under partial transpositions. We find four distinct classes of states based on whether the SL invariants are invariant under the different partial transpositions or not.

As general result, we find that if the SL invariants of a state are invariant under a given partial transposition, then the state can be made symmetric under that partial transposition by an SL transformation on that subsystem alone. If the SL invariants are complex conjugated, then the state can be made symmetric under partial transposition and complex conjugation. These symmetrizations can be done on the same state independently on each subsystem.

The dimensions and geometry of the rank 5555 states have been examined. We find that states of different types lie on surfaces of different dimensions. States of different types exist on the same subspace. Different surfaces containing states of different types are found to touch the simplex of separable states on a given subspace in different ways.

Sammendrag

Målet for denne masteroppgaven har vært gjøre numeriske studier av ekstremale tilstander med positive deltransponerte (PPT-tilstander) i systemer bestående av tre qubits. Vi klassifiserer PPT-tilstander ved rangen av tilstanden selv og dens tre deltransponerte. Vi har sett spesielt på de sammenfiltrede tilstandene med rang 4444 og 5555.

Vi har funnet to distinkte klasser av rang fire-tilstander, som kan identifiseres av verdien av et kvadratisk uttrykk som er invariant under lokale $SL(2, \mathbb{C})$ transformasjoner. Vi kaller den en Lorentz-invariant siden den også er invariant under deltransponering, som er en diskret Lorentz-transformasjon. Denne kvadratiske Lorentz-invarianten er ikke-null for en klasse (type 1) og null for den andre (type 2). Vi presenterer analytiske konstruksjoner av begge typene, som er generell nok til å reprodusere alle rang fire PPT-tilstandene vi har funnet numerisk.

Det finnes seks produktvektorer i et generisk femdimensjonalt underrom. Produktvektorene i billedrommet til en rang 5555-tilstand og den deltransponerte brukes til å lage lokale SL -invarianter som ikke nødvendigvis er invariant under deltransponering. Vi finner fire distinkte klasser av tilstander, basert på om SL -invariantene er invariant under de forskjellige deltransponerte eller ikke.

Som et generelt resultat, finner vi at om SL -invariantene til en tilstand er invariant under en gitt deltransponering, så kan tilstanden gjøres symmetrisk under den deltransponeringen, av en SL -transformasjon på det delsystemet alene. Om SL -invariantene blir komplekskonjugerte, så kan tilstanden gjøres symmetrisk under deltransponering og komplekskonjugering. Disse symmetriseringene kan gjøres uavhengig på de forskjellige delsystemene.

Dimensjonene og geometrien til rank 5555 tilstandene har blitt studert. Vi finner at forskjellige typer tilstander ligger på flater med forskjellige dimensjoner. Tilstander av forskjellige typer eksisterer på det samme underrommet. Forskjellige flater av tilstander av forskjellige typer berører simplekset av separable tilstander i et gitt billedrom på forskjellige måter.

Contents

Abstract	i
Sammendrag	ii
Preface	vi
1 Introduction	1
2 Fundamentals	5
2.1 Linear algebra	5
2.1.1 Tensor products	5
2.2 The trace operator	6
2.3 Some basic quantum mechanics	6
2.3.1 Density operators	7
2.3.2 Entanglement	7
2.3.3 Ranks	8
2.3.4 Product vectors	8
3 Rank 4444 states	11
3.1 Invariants of rank 4444 states	11
3.2 Numerical search for rank four PPT states as biseparable states . . .	12
3.3 States with vanishing quadratic invariant	14
3.3.1 A random search method	14
3.3.2 Explicit construction	14
3.4 States with non-zero invariant	16
3.4.1 Explicit construction	16
4 Rank 5555 states and product vectors	19
4.1 Product vectors	20
4.1.1 Finding product vectors	20
4.2 Product vectors in the range of a rank 5555 state	21
4.2.1 A note on separable states	24
4.3 Symmetric forms	24
4.3.1 Types I and II	25
4.3.2 Type III	28

5	Perturbing states	33
5.1	Dimensions	34
5.2	Walking on the surface	35
6	Finding states on a specified subspace	39
6.1	Minimisation routine	40
6.2	Different rank 5555 states on the same subspace	41
6.3	E -orthogonal vectors of rank 5555 states	42
7	Conclusion and further work	43
A	Partial transpositions in $2 \otimes 2 \otimes 2$	47
B	$SL(2, \mathbb{C})$, Lorentz transformations, and Lorentz invariants	49
B.1	The Generators	52
C	Standard forms of sets of vectors	53
D	A problem of finding product vectors in a subspace	55
E	The split tensor product	59
F	Linear combinations of product vectors	61
G	MATLAB code	63
G.1	Symmetric forms	63
G.1.1	Type I	63
G.1.2	Type III	65
G.2	4th order Runge Kutta	66
G.3	Simulated annealing	68
	Bibliography	73

List of Figures

2.1	ρ and its partial transposes	9
4.1	Relation between the invariants and standard forms of a type I state	22
4.2	Relation between the invariants and standard forms of a type II state	23
4.3	Relations between the invariants and standard forms of a type III state.	24
4.4	Partial transposition as 2×2 matrix transposition	26
4.5	Rotation around an axis \vec{v} by θ radians	27
6.1	Edge of two different type I surfaces touching the simplex of separable states	41

Preface

This report is my thesis for earning the Master's Degree in Physics from the Norwegian University of Science and Technology (NTNU). I have studied bound entanglement in low rank systems under the supervision of Professor Jan Myrheim at the Department of Physics.

During my first years studying physics at the University, I found myself attracted to theoretical and numerical physics. When learning about how these two disciplines of physics can be combined to study quantum entanglement my choice of research topic quickly became apparent.

I am grateful to Jan for all his invaluable help and the inspiration he has provided during my work on this thesis. I want to thank Øystein Garberg for giving me his source code as a starting point and for having laid the groundwork for my work on rank 4444 states in this thesis. Finally I want to thank Leif Ove Hansen for moral support and constructive feedback.

Chapter 1

Introduction

Quantum entanglement was first described by Einstein, Podolsky, and Rosen (1935) and Schrödinger (1935) as a strange phenomenon of quantum mechanics, whereby strong correlations that cannot be explained by classical physics exists between systems that are spatially separated. Einstein et al. (1935) argued, based on the notions of realism and locality, that these strong correlations imply that quantum mechanics cannot be a complete theory. Realism means that a measurement has a predetermined outcome and locality only allows local interactions, which essentially means that two spatially separated states can only interact at the speed of light.

Based on the assumptions of realism and locality, it is possible to derive limits on the allowed correlations of measurement results (Bell et al., 1964), so called Bell inequalities. Violations of Bell inequalities have been observed experimentally, proving that either realism or locality must be violated. This effect is even more pronounced in a three-particle system where Greenberger et al. (2007) constructed a state that requires only a single set of measurements to disprove the notions of realism and locality (Mermin, 1990). These measurements have been carried out experimentally by Pan et al. (2000).

In the nineties, it was realised that quantum entanglement is not just a peculiarity of non-classical physics, it is a resource that can be used for technological applications. Most notably it is important in many parts of quantum information theory, for instance quantum computing, quantum cryptography, quantum teleportation and superdense coding.

A central problem in the study of quantum entanglement is how to determine if an arbitrary mixed state is entangled or not. A computationally inexpensive test is the Peres criterion, which says that any separable state remains positive definite under partial transposition (it is a PPT state). Representing the convex sets of separable states, PPT states and density operators, as \mathcal{S} , \mathcal{P} and \mathcal{D} respectively, the criterion says that $\mathcal{S} \subset \mathcal{P} \subset \mathcal{D}$, where \mathcal{P} is larger than \mathcal{S} in cases where the

product of the dimensions of the subsystems is greater than six. A convex set is completely described by its extremal points, which motivates our study of extremal PPT states.

These extremal states have been extensively studied analytically and numerically in the case of two and three subsystems. We know that any extremal PPT state of rank larger than one must be entangled, and a bipartite (Chen and Chen, 2008; Horodecki et al., 2003) or tripartite (Karnas and Lewenstein, 2001) entangled PPT state must have rank larger than four or higher.

Leinaas et al. (2006) studies the geometry of separability, and presents a method for determining whether a state is separable. It uses the fact that the set of separable states is convex to iteratively find the closest separable state to an arbitrary density matrix. This can be used to determine whether a state is separable or not.

Leinaas et al. (2007) presents a necessary and sufficient condition for a finite dimensional density matrix to be an extremal point of \mathcal{P} . The method can also be used to search for extremal PPT states.

Leinaas et al. (2010b) presents numerical algorithms for finding PPT states with specified ranks and product vectors in a specified subspace. These methods were extended to three subsystems by Garberg (2012) and is a large part of the basis for my own work in this thesis.

Bennett et al. (1999) shows how to construct an analytical low rank extremal PPT state using an unextendible product basis (UPB). We define a UPB as an unextendible set of orthogonal product vectors in its kernel and no product vectors in its image. Leinaas et al. (2010a) and Sollid et al. (2011) generalised this construction to a nonorthogonal UPB by applying a nonsingular product transformation. They present numerical evidence indicating that all rank four extremal PPT states 3×3 dimensions can be constructed this way. This construction also works in $2 \times 2 \times 2$ dimensions, though a generic four states does not have a UPB in its kernel in this case.

Hansen et al. (2012) uses perturbation theory to construct rank five entangled states close to known rank four entangled states, and to study the geometry of surfaces of PPT states. They also show how to use (a sufficient number of) product vectors in the kernel to reconstruct a PPT state of low rank.

In this thesis we examine low rank entangled extremal PPT states in a system of three qubits, i.e. states composed of three subsystems of dimension two. In particular the rank four and rank five states, which are the lowest rank PPT states that can be entangled.

My work on rank four states continues the work Øyvind Garberg did in his master thesis (Garberg, 2012) and has been published in (Garberg et al., 2013). He used two numerical algorithms to locate PPT states with specified ranks and extremal states, finding a large number of numerical examples of extremal PPT states. None of which had product vectors in their kernel.

He found limitations on the possible ranks of extremal PPT states and their partial transposes, in particular that the partial transposes of rank four entangled PPT states also have rank four. The rank four states were studied in more detail. He constructed a quadratic and four quartic quantities that are invariant under $SL \otimes SL \otimes SL$ transformations, and must therefore have the same value for all the states in an equivalence class. Calculating these invariants for the different rank four states gave one group of states with a seemingly continuous range of values of all the invariants (and therefore different equivalence classes), and one group where the quadratic invariant was zero and the rest had identical values (indicating that they may be a part of the same equivalence class).

In Chapter 3 we show that the class with one invariant identical to zero must be supported on a subspace where all vectors ψ, ϕ in the the range of the state must satisfy $\psi^T(\epsilon \otimes \epsilon \otimes \epsilon)\phi = 0$ where ϵ is the 2×2 antisymmetric matrix. We find empirically that the states of the other class can be transformed by $SL \otimes SL \otimes SL$ transformations to a real form. In both cases we show how to analytically construct the states we have found numerically.

In Chapter 4 we examine rank five states. These states are special because there are a finite number of product vectors in a generic five dimensional subspace of $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$. We find numerically that there are six product vectors in the range of a generic rank five state. There can be only one extremal state with the same range for the state and all its partial transposes, so using the six product vectors we define invariants of the state and its partial transposes.

In Section 4.2 we classify the states into four different types according to how their invariants are conserved under partial transpositions. Invariants are important because they can be used to conclude that states are *not* $SL \otimes SL \otimes SL$ equivalent. In particular, a type I state is invariant under one partial transposition up to an $SL \otimes SL \otimes SL$ transformation. A type II state is a type I state under two different partial transpositions. A type III state is invariant under any two concurrent partial transpositions up to an $SL \otimes SL \otimes SL$ transformation. A type IV state has seemingly no relation between product vectors related to different partial transposes.

In Section 4.3 we show how we have been able to transform the states we have found with invariants conserved under partial transposition to symmetric form.

In Chapter 5 we examine the geometry of surfaces of rank five states, and find that the different types defined in Section 4.2 have qualitatively different properties. We also find that the surfaces with specified range touch the separable states in an interesting pattern.

In Chapter 6 we look for rank five states on a specified subspace, and find that only specific combinations of types share the same range. Two surfaces of type I states, with different symmetries, are found on all generic subspaces examined. In the case of a type II state, the type I states have the two symmetries of the type II state separately. No type II, III or IV states are found on the same subspace. We also find a special subspace on which there is only one surface of type I, closely

related to a non-generic type of state.

Chapter 2

Fundamentals

To study computational and geometrical aspects of entanglement we need a basic foundation of linear algebra and quantum mechanics. The material in this chapter can be found in relevant introductory literature, e.g. (Nielsen and Chuang, 2004).

2.1 Linear algebra

I will be using matrix notation and Dirac notation for vectors interchangeably. I.e. a column vector can be written either as ψ or $|\psi\rangle$ and its Hermitian conjugate either as ψ^\dagger or $\langle\psi|$.

2.1.1 Tensor products

The tensor product is a way of combining different vector spaces to make larger vector spaces. It is essential for describing multi-particle quantum systems.

If V and W are vector spaces of dimension n and m then the tensor products of the two, $V \otimes W$, is a vector space of dimension nm . The elements in this new vector space are linear combinations of tensor products $|v\rangle \otimes |w\rangle$ of elements $|v\rangle \in V$ and $|w\rangle \in W$.

Let z be a complex scalar, $|v\rangle, |v_1\rangle, |v_2\rangle$ be elements in the vector space V and $|w\rangle, |w_1\rangle, |w_2\rangle$ be elements in the vector space W . Then the tensor product has the following properties:

$$z(|v\rangle \otimes |w\rangle) = (z|v\rangle) \otimes |w\rangle = |v\rangle \otimes (z|w\rangle) \quad (2.1)$$

$$(|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle \quad (2.2)$$

$$|v\rangle \otimes (|w_1\rangle + |w_2\rangle) = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle \quad (2.3)$$

A convenient way to represent the tensor product is the Kronecker product for complex matrices. Let A be a $m \times n$ matrix and B a $p \times q$ matrix. The matrix representation of the tensor product is then,

$$A \otimes B = \begin{bmatrix} A_{11}B & A_{12}B & \dots & A_{1n}B \\ A_{21}B & A_{22}B & \dots & A_{2n}B \\ \vdots & \vdots & \vdots & \vdots \\ A_{m1}B & A_{m2}B & \dots & A_{mn}B \end{bmatrix} \quad (2.4)$$

2.2 The trace operator

One operation which is prevalent throughout the study of quantum information theory is the trace operator. It is defined as

$$\text{Tr } A \equiv \sum_i A_{ii} . \quad (2.5)$$

By the definition it has the following properties:

$$\text{Tr}(AB) = \text{Tr}(BA) \quad (2.6)$$

$$\text{Tr}(A + B) = \text{Tr } A + \text{Tr } B \quad (2.7)$$

The trace of an operator is defined as the trace of its matrix representation.

One of its uses is to define the norm of a state,

$$\|\rho\| = \sqrt{\text{Tr } \rho \rho^\dagger} \quad (2.8)$$

and since an overall normalisation factor does not influence the entanglement properties of a state we always normalise the states to unit trace:

$$\rho \leftarrow \frac{\rho}{\text{Tr } \rho} \quad (2.9)$$

2.3 Some basic quantum mechanics

Every isolated system has an associated Hilbert space \mathcal{H} , known as the state space of the system. The system is described by its state vector $|\psi\rangle \in \mathcal{H}$.

The state space of a composite system is the tensor product of the state spaces of the component systems. If the composite systems are in the states $|\psi_1\rangle, \dots, |\psi_n\rangle$, then the state of the total system is $|\psi\rangle = |\psi_1\rangle \otimes \dots \otimes |\psi_n\rangle$

2.3.1 Density operators

State vectors are adequate for describing a system when we know the state with certainty, but most real world quantum systems are disturbed by external influences. Suppose a quantum system is in one of the states $|\psi_i\rangle$, $i = 1, \dots, n$ with respective probability p_i . The density operator (also known as density matrix) of this system is,

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \quad (2.10)$$

A density matrix ρ is a positive (all eigenvalues non negative) Hermitian matrix with $\text{Tr } \rho = 1$. The set of density matrices is defined as:

$$\mathcal{D} = \{\rho \in H_N | \rho \geq 0, \text{Tr } \rho = 1\} \quad (2.11)$$

where H_N is the set of all $N \times N$ Hermitian matrices. $\rho \geq 0$ is short-hand notation for all the eigenvalues of ρ being non-negative, i.e. the matrix is semi-definite. Equivalently $\psi^\dagger \rho \psi \geq 0 \quad \forall \psi \in \mathbb{C}^N$.

Let $|\psi_i\rangle \quad i = 1, \dots, n$ be the orthonormal eigenvectors, with eigenvalues greater than zero, of a state ρ . Then the orthogonal projection

$$P = \sum_i |\psi_i\rangle \langle \psi_i| \quad (2.12)$$

projects on $\text{Im } \rho$ and the complementary projection

$$Q = \mathbb{1} - P \quad (2.13)$$

projects on $\text{Ker } \rho$.

A density operator can either be an extreme point of \mathcal{D} or a convex combination

$$\rho = x\rho_1 + (1-x)\rho_2, \quad 0 < x < 1 \quad (2.14)$$

of two other states $\rho_1, \rho_2 \in \mathcal{D}$. It follows that

$$\psi^\dagger \rho \psi = x\psi^\dagger \rho_1 \psi + (1-x)\psi^\dagger \rho_2 \psi \geq 0 \quad \forall \psi \quad (2.15)$$

or equivalently $\rho \geq 0$, proving that \mathcal{D} is a convex set. The extremal points of \mathcal{D} are the pure states $\rho = \psi\psi^\dagger$, which cannot be expressed as convex combinations of other states, and they define the set \mathcal{D} .

2.3.2 Entanglement

One of the postulates of quantum mechanics is that the state space of a composite system is the tensor product of the state spaces of the component physical systems. If we have systems numbered 1 through n and system i is prepared in the state $|\psi_i\rangle$, then the state vector of the total system is $|\psi_1\rangle \otimes \dots \otimes |\psi_n\rangle$. Interestingly,

some states cannot be decomposed in this way. Take for instance the Bell state,

$$|\psi\rangle = \frac{|00\rangle + |11\rangle}{2}. \quad (2.16)$$

There are no single qubit states $|a\rangle$ and $|b\rangle$ such that $|\psi\rangle = |a\rangle \otimes |b\rangle$. We call a state with this property an *entangled* state, and any product state is *separable*.

In the density operator formalism, a state is separable if it can be written,

$$\rho = \sum_i w_i \rho_i^1 \otimes \cdots \otimes \rho_i^n \quad (2.17)$$

Peres points out that such a separable state must remain positive when it is partially transposed with respect to one of its subsystems (Peres, 1996). E.g. in the bipartite case, the state

$$\rho^P = \sum_i w_i \rho_i^{(1)} \otimes (\rho_i^{(2)})^T \quad (2.18)$$

must have only non-negative eigenvalues. Horodecki et al. (1996) show that the Peres criterion is sufficient if and only if the product of the dimensions of the composite systems is less than six.

The partial transpose operation is well defined for entangled states as well (see Appendix A for more details). The set of all PPT states, both entangled and separable, we call \mathcal{P} or the Peres set.

If we denote the set of separable states as \mathcal{S} then the Peres test states that $\mathcal{S} \subset \mathcal{P} \subset \mathcal{D}$. That means that the question of separability is reduced to the separability of PPT states.

In our notation T_i is the partial transposition of system i and $\rho^{T_0} = \rho$.

2.3.3 Ranks

We use the notation $\text{rank } nmop$ to refer to states with $r(\rho) = n, r(\rho^{T_1}) = m, r(\rho^{T_2}) = o$ and $r(\rho^{T_3}) = p$. T_1T_2, T_1T_3, T_2T_3 are other possible partial transpositions, but they can be obtained by doing a total transposition, or equivalently a complex conjugation, of ρ^{T_i} $i = 0, 1, 2, 3$. The relation between the states can be seen in Figure 2.1, where corners diagonally across the cube are complex conjugates of each other. Note that the corners of the cube are all equivalent, i.e. PPT states with the same ranks as ρ , so we arbitrarily sort ρ^{T_i} in ascending order of their ranks.

2.3.4 Product vectors

A product vector is a tensor product of two or more vectors. In particular the pure separable states are product vectors.

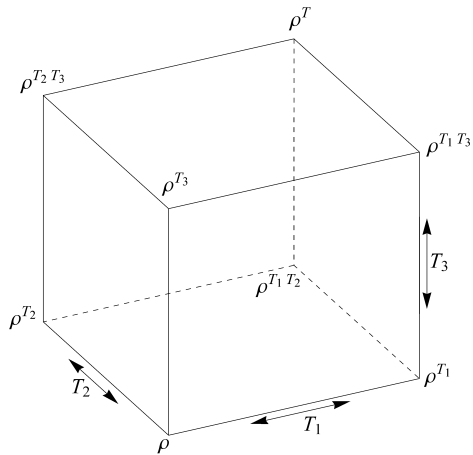


Figure 2.1: ρ and its partial transposes

Sorting states into equivalence classes

A product transformation,

$$\rho \mapsto \rho^\dagger = aV\rho V^\dagger \text{ with } V = V_A \otimes V_B \cdots \quad (2.19)$$

where a is a normalisation factor and $V_i \in \text{SL}(2, \mathbb{C})N_i$ preserves rank, positivity, separability and other interesting properties of ρ .

We want to classify the three qubit states into $\text{SL} \otimes \text{SL} \otimes \text{SL}$ equivalence classes, defining two unnormalized density matrices ρ and σ to be equivalent if

$$\sigma = (V_1 \otimes V_2 \otimes V_3) \rho (V_1 \otimes V_2 \otimes V_3)^\dagger, \quad (2.20)$$

with $V_i \in \text{SL}(2, \mathbb{C})$. This definition is useful because equivalent density matrices have the same entanglement properties, although quantitative measures of entanglement will be different. Qualitative properties will be the same, such as tensor product structure of pure states, decomposition of mixed states as convex combinations of pure states, rank and positivity of states and all their partial transposes, and so on.

The relation between the group $\text{SL}(2, \mathbb{C})$ and the group of continuous Lorentz transformations is well known, and is reviewed here in Appendix B. From a density matrix in the three qubit system we define one quadratic and four quartic real Lorentz invariants, so called because they are invariant under $\text{SL} \otimes \text{SL} \otimes \text{SL}$ transformations as in Equation 2.20. They are also invariant under partial transpositions, because a partial transposition may be interpreted as a parity transformation, which is a discrete Lorentz transformation.

This means, for example, that the ratio between one quartic Lorentz invariant and the square of the quadratic invariant will have the same value for all the states

in one equivalence class and all their partial transposes. Taking the ratio between Lorentz invariants is necessary in order to cancel out any normalization factor in the density matrix. If two density matrices are not in the same equivalence class, their non-equivalence will most likely be revealed when we calculate their invariants.

Chapter 3

Rank 4444 states

The work on rank four states continues the work Øyvind Garberg did on his master thesis (Garberg, 2012) and has been published in (Garberg et al., 2013). He used two algorithms which locate PPT states with specified ranks and extremal states respectively to find a large number of numerical examples of extremal PPT states. He found limits on the ranks of extremal PPT states and their partial transposes, in particular that the partial transposes of rank four and five entangled PPT states are also rank four and five. The rank four states were studied in more detail. He constructed quantities that are invariant under $SL \otimes SL \otimes SL$ transformations, and must therefore have the same value for all the states in an equivalence class. Calculating these invariants for the different rank four states gave one group of states with a seemingly continuous range of values of all the invariants (and therefore different equivalence classes), and one group where one invariant was zero and the rest had identical values (indicating that they may be a part of the same equivalence class).

In Section 3.1 we reintroduce the quadratic invariant that is zero for the states of the second group and use it to show that $\psi^T(\epsilon \otimes \epsilon \otimes \epsilon)\phi = 0$ for all ψ, ϕ in the range of the state and ϵ the antisymmetric matrix. In Section 3.3 we show how to analytically construct a state with invariant zero. In Section 3.4 we show how to analytically construct a state with invariant different from zero.

3.1 Invariants of rank 4444 states

We define a second order Lorentz invariant:

$$I^2(\rho) = \rho^{\mu\nu\lambda} \rho_{\mu\nu\lambda} = -\frac{1}{8} \text{Tr}(\rho E \rho^T E) \quad (3.1)$$

where

$$E = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (3.2)$$

Definition 1. If $I^2(\rho) \neq 0$ ρ is a state of type I, else it is a state of type II.

ρ is a Hermitian matrix, so it can be written as:

$$\rho = \sum_{i=1}^4 \lambda_i \psi_i \psi_i^\dagger \quad (3.3)$$

inserting into Equation 3.1 gives

$$\begin{aligned} I^2 &= \frac{1}{8} \text{Tr} \left(\sum_i \lambda_i \psi_i \psi_i^\dagger E \left(\sum_j \lambda_j \psi_j \psi_j \right)^T E \right) \\ &= \frac{1}{8} \sum_{i,j} \lambda_i \lambda_j \text{Tr} \left(\psi_i \psi_i^\dagger E \psi_j^* \psi_j^T E \right) \\ &= \frac{1}{8} \sum_{i,j} \lambda_i \lambda_j \text{Tr} \left(\psi_i^\dagger E \psi_j^* \psi_j^T E \psi_i \right) \\ &= -\frac{1}{8} \sum_{i,j} \lambda_i \lambda_j \text{Tr} \left(\psi_i^\dagger E \psi_j^* (\psi_i^\dagger E \psi_j^*)^* \right) \\ &= -\frac{1}{8} \sum_{i,j} \lambda_i \lambda_j |\psi_i^T E \psi_j|^2 \end{aligned} \quad (3.4)$$

where we have used the cyclic property of the trace and the fact that this E product is antisymmetric:

$$E^T = -E \Rightarrow \psi^T E \phi = (\psi^T E \phi)^T = -\phi^T E \psi \quad (3.6)$$

We see that $I^2 \geq 0$ when ρ is positive semidefinite, but we may have $I^2 < 0$ if ρ is not positive, since $\psi_i^T E \psi_i = 0$.

3.2 Numerical search for rank four PPT states as biseparable states

General considerations

A generic 4 dimensional subspace $\mathcal{U} \subset \mathbb{C}^8$ contains 3 sets of 4 product vectors:

$$e_i = x_i \otimes u_i \quad i = 1, \dots, 4 \quad (3.7)$$

$$f_i = y_i \otimes_s v_i \quad i = 1, \dots, 4 \quad (3.8)$$

$$g_i = w_i \otimes y_i \quad i = 1, \dots, 4 \quad (3.9)$$

where $x_i, y_i, z_i \in \mathbb{C}^2$ and $u_i, v_i, w_i \in \mathbb{C}^4$. The "split" tensor product \otimes_s is defined in Appendix E.

For a method of computing these product vectors in a given subspace \mathcal{U} see Appendix D. It was proved by Kraus et al. (2000) that a rank four state in a 2×4 system must be separable, so a density matrix with $\text{Im} \rho = \mathcal{U}$ and $\rho^{T_1} \geq 0$ must be biseparable in 2×4 dimensions, having the form:

$$\rho = \sum_{i=1}^4 \lambda_i e_i e_i^\dagger \quad (3.10)$$

Similarly, if $\rho^{T_2} \geq 0$ then ρ must be biseparable in the split tensor product and have the form

$$\rho = \sum_{i=1}^4 \mu_i f_i f_i^\dagger \quad (3.11)$$

and if $\rho^{T_3} \geq 0$ then it must be biseparable in 4×2 dimensions and have the form

$$\rho = \sum_{i=1}^4 \nu_i g_i g_i^\dagger \quad (3.12)$$

When we want a state ρ with $\rho^{T_i} \geq 0$ for $i = 0, 1, 2, 3$, we need to find a subspace \mathcal{U} where Equation 3.10, Equation 3.11 and Equation 3.12 are all compatible. This fails for a generic subspace.

We may search numerically for a subspace that fulfils the equations as follows. Equation 3.10 and Equation 3.11 are compatible when there is at least one linear dependency between the eight matrices, $e_i e_i^\dagger$ and $f_i f_i^\dagger$. We can calculate the linear dependencies between the matrices by representing each of these matrices as a real vector in \mathbb{R}^{64} and doing a singular value decomposition.

This is a minimisation problem where we can vary the subspace \mathcal{U} until the smallest singular value is zero. An output from the singular value decomposition is the two sets of coefficients μ_i and λ_i corresponding to the singular value zero. The coefficients μ_i and λ_i must be positive, but the singular value decomposition places no restriction on them. If μ_i or λ_i is all negative we simply switch all the signs. If some are positive and some are negative, we must discard the subspace and start again.

The procedure for making Equation 3.10 and Equation 3.12 compatible is the same. To make all three compatible we simply minimise the sum of the smallest singular value from each problem.

3.3 States with vanishing quadratic invariant

All four of the eigenvalues of our PPT states are positive so any product of eigenvalues must also be positive. Hence, if $I^2(\rho) = 0$, Equation 3.5 implies that

$$\psi_i^T E \psi_j = 0 \quad \forall i, j \quad (3.13)$$

Definition 2. *Two vectors ψ and ϕ are E -orthogonal if*

$$\psi^T E \phi = 0 \quad (3.14)$$

Every vector is E -orthogonal to itself,

$$\psi^T E \psi = -\psi^T E \psi \Rightarrow \psi^T E \psi = 0 \quad (3.15)$$

3.3.1 A random search method

It is easy to construct a four dimensional subspace $\mathcal{U} \in \mathbb{C}^8$ where the antisymmetric scalar product vanishes. A four dimensional subspace can be spanned by a set of four vectors $\{\psi_1, \psi_2, \psi_3, \psi_4\}$. Start with a random normalized vector ψ_1 . The conditions $\psi_1^T E \psi = 0$ and $\psi_1^\dagger \psi = 0$ restrict ψ_2 to a six dimensional subspace. The vector ψ_3 must satisfy $\psi_3^T E \psi_i = 0$ and $\psi_3^\dagger \psi_i = 0$ for $i = 1, 2$, meaning that ψ_3 is restricted to a four dimensional subspace. Finally ψ_4 is restricted to a two dimensional subspace.

This way we get four vectors with the properties:

$$\psi_i^\dagger \psi_j = \delta_{ij}, \quad \psi_i^T E \psi_j = 0 \quad (3.16)$$

Now we can use the method outlined in Section 3.2 to look for rank 4444 PPT-states with the image space spanned by $\{\psi_1, \psi_2, \psi_3, \psi_4\}$.

3.3.2 Explicit construction

Our numerical examples all have certain properties that enable us to construct them explicitly. First introduce the three sets of product vectors e_i, f_j, g_k from Equations (3.7)-(3.9) as bases for $\text{Img } \rho$. ρ is a type 2 state, so the eigenvectors in the range of ρ are all E -orthogonal. Furthermore all vectors $v \in \text{Img } \rho$ are E -orthogonal to $\text{Img } \rho$.

$$e_i^T E e_j = (x_i^T \epsilon x_j)(u_i^T (\epsilon \otimes \epsilon) u_j) = 0 \quad \text{for } i, j = 1, 2, 3, 4 \quad (3.17)$$

$x_i^T \epsilon x_j$ is zero for $i = j$, but not for $i \neq j$ so for Equation 3.17 to be satisfied we must in general have

$$(u_i^T (\epsilon \otimes \epsilon) u_j) = 0 \quad \text{for } i \neq j \quad (3.18)$$

Remarkably it turns out that in our numerical examples every u is a linear combination of two product vectors.

$$u_i = a_{ikly} y_k \otimes z_l + a_{imn} y_m \otimes z_n \quad (3.19)$$

When we transform x, y and z to the standard form defined in Appendix C we

i	$klmn$					
1	1221	1331	1441	2332	2442	3443
2	1122	1342	1432	2341	2431	3344
3	1133	1243	1423	2134	2244	3241
4	1144	1234	1324	2143	2233	3142

Table 3.1: The allowed index combinations in Equation 3.19

find that the linear dependencies listed in Table 3.1 require that $t_2 = t_3$. When that relation holds there is a unique solution for u depending on a single complex parameter $t = t_2 = t_3$:

$$u = \begin{pmatrix} 0 & t & t & t \\ 1 & 0 & 1 & -t \\ -1 & 0 & 1 & -t \\ 0 & 1 & -1 & -1 \end{pmatrix}. \quad (3.20)$$

$g_k = w_k \otimes z_k$ must be linear combinations of the vectors $e_i = x_i \otimes u_i$, implying that $t_1 = t$. The overall solution is $v = w = u$ which gives the vectors:

$$e = \begin{pmatrix} 0 & 0 & t & t^2 \\ 1 & 0 & 1 & -t^2 \\ -1 & 0 & 1 & -t^2 \\ 0 & 0 & -1 & -t \\ 0 & t & -t & t \\ 0 & 0 & -1 & -t \\ 0 & 0 & -1 & -t \\ 0 & 1 & 1 & -1 \end{pmatrix}, \quad f = \begin{pmatrix} 0 & 0 & t & t^2 \\ 1 & 0 & 1 & -t^2 \\ 0 & t & -t & t \\ 0 & 0 & -1 & -t \\ -1 & 0 & 1 & -t^2 \\ 0 & 0 & -1 & -t \\ 0 & 0 & -1 & -t \\ 0 & 1 & 1 & -1 \end{pmatrix},$$

$$g = \begin{pmatrix} 0 & 0 & t & t^2 \\ 0 & t & -t & t \\ 1 & 0 & 1 & -t^2 \\ 0 & 0 & -1 & -t \\ -1 & 0 & 1 & -t^2 \\ 0 & 0 & -1 & -t \\ 0 & 0 & -1 & -t \\ 0 & 1 & 1 & -1 \end{pmatrix} \quad (3.21)$$

Now we have found an explicit standard form for ρ , depending on a single complex parameter t :

$$\rho = a \sum_{i=1}^4 \lambda_i e_i e_i^\dagger = a \sum_{i=1}^4 \lambda_i f_i f_i^\dagger = a \sum_{i=1}^4 \lambda_i g_i g_i^\dagger \quad (3.22)$$

with

$$\lambda_1 = |t|^2|1+t|^2, \quad \lambda_2 = |1+t|^2, \quad \lambda_3 = |t|^2, \quad \lambda_4 = 1 \quad (3.23)$$

$$a = \frac{1}{5|t|^4 + 10|t|^2 + 1 + (3|t|^2 + 1)|1+t|^2} \quad (3.24)$$

3.4 States with non-zero invariant

It turns out that all the states we have found with non-zero invariant can be transformed to a standard form that is symmetric under all partial transpositions. Since a total transposition is the same as a complex conjugation the standard form of ρ is also real:

$$\rho^* = \rho^T = \rho^{T_1 T_2 T_3} = \rho \quad (3.25)$$

We compute the three sets of product vectors defined in Equations (3.7)-(3.9). Then we use a product transformation $V = V_1 \otimes V_2 \otimes V_3$ to transform x, y and z to the standard form defined in Appendix C. It turns out that $t_1 = t_2 = t_3 \in \mathbb{R}$ and that the transformation V also makes u, v and w real. The transformed matrix $V\rho V^\dagger$ is also real.

We have no proof that this must hold for *all* states with non-zero invariant, but it is very useful for constructing our states.

3.4.1 Explicit construction

We want to construct a state ρ on standard form fulfilling the following criteria:

- ρ should have the following form, up to normalisation

$$\rho = \sum_{i=1}^4 e_i e_i^\dagger = \sum_{i=1}^4 f_i f_i^\dagger = \sum_{i=1}^4 g_i g_i^\dagger \quad (3.26)$$

- ρ should be symmetric under all partial transpositions
- x should have the standard form defined in Appendix C

$$x = \begin{pmatrix} 1 & 0 & 1 & t_1 \\ 0 & 1 & -1 & 1 \end{pmatrix} \Rightarrow e = \begin{pmatrix} u_1 & 0 & u_3 & t_1 u_4 \\ 0 & u_2 & -u_3 & u_4 \end{pmatrix} \quad (3.27)$$

$$e_1 e_1^\dagger = \begin{pmatrix} u_1 u_1^T & 0 \\ 0 & 0 \end{pmatrix} \quad (3.28)$$

$$e_2 e_2^\dagger = \begin{pmatrix} 0 & 0 \\ 0 & u_2 u_2^T \end{pmatrix} \quad (3.29)$$

$$e_3 e_3^\dagger = \begin{pmatrix} u_3 u_3^T & -u_3 u_3^T \\ -u_3 u_3^T & u_3 u_3^T \end{pmatrix} \quad (3.30)$$

$$e_4 e_4^\dagger = \begin{pmatrix} t_1^2 u_4 u_4^T & t_1 u_4 u_4^T \\ t_1 u_4 u_4^T & u_4 u_4^T \end{pmatrix} \quad (3.31)$$

So ρ has the form:

$$\rho = \begin{pmatrix} A & B \\ B & C \end{pmatrix} \quad (3.32)$$

where

$$A = u_1 u_1^T + u_3 u_3^T + t_1^2 u_4 u_4^T \quad (3.33)$$

$$B = -u_3 u_3^T + t_1 u_4 u_4^T \quad (3.34)$$

$$C = u_2 u_2^T + u_3 u_3^T + u_4 u_4^T \quad (3.35)$$

As shown in Appendix A, for ρ to be symmetric under all partial transpositions A must have the general form:

$$A = \begin{pmatrix} a_1 & a_5 & a_6 & a_7 \\ a_5 & a_2 & a_7 & a_8 \\ a_6 & a_7 & a_3 & a_9 \\ a_7 & a_8 & a_9 & a_4 \end{pmatrix}, \quad a_1, \dots, a_9 \in \mathbb{R} \quad (3.36)$$

B and C must also have the same forms.

The only condition on A which is not automatically satisfied is $a_{41} = a_{32}$:

$$u_{41} u_{44} t_1^2 + u_{11} u_{14} + u_{31} u_{34} = u_{42} u_{43} t_1^2 + u_{12} u_{13} + u_{32} u_{33} \quad (3.37)$$

The condition on B which is not automatically satisfied is

$$t_1 u_{41} u_{44} - u_{31} u_{34} = t_1 u_{42} u_{43} - u_{32} u_{33} \quad (3.38)$$

$$u_{21} u_{24} + u_{31} u_{34} + u_{41} u_{44} = u_{22} u_{23} + u_{32} u_{33} + u_{42} u_{43} \quad (3.39)$$

$$u_j^T (\epsilon \otimes \epsilon) u_j = u_{i1} u_{j4} - u_{i2} u_{j3} - u_{j2} u_{i3} + u_{j1} u_{i4} \quad (3.40)$$

In particular, the formula

$$u_i^T (\epsilon \otimes \epsilon) u_i = 2(u_{i1} u_{i4} - u_{i3} u_{i2}) \quad (3.41)$$

makes it possible to rewrite Equation 3.38 as

$$t_1^2 u_4^T (\epsilon \otimes \epsilon) u_4 + u_1^T (\epsilon \otimes \epsilon) u_1 + u_3^T (\epsilon \otimes \epsilon) u_3 = 0 \quad (3.42)$$

$$-u_3^T(\epsilon \otimes \epsilon)u_3 + t_1 u_4^T(\epsilon \otimes \epsilon)u_4 = 0 \quad (3.43)$$

$$u_2^T(\epsilon \otimes \epsilon)u_2 + u_3^T(\epsilon \otimes \epsilon)u_3 + u_4^T(\epsilon \otimes \epsilon)u_4 = 0 \quad (3.44)$$

Equation 3.43 can be solved by choosing

$$t_1 = \frac{u_3^T(\epsilon \otimes \epsilon)u_3}{u_4^T(\epsilon \otimes \epsilon)u_4} \quad (3.45)$$

To solve Equation 3.42 define

$$\alpha^2 = -\frac{t_1^2 u_4^T(\epsilon \otimes \epsilon)u_4 + u_3^T(\epsilon \otimes \epsilon)u_3}{u_1^T(\epsilon \otimes \epsilon)u_1} \quad (3.46)$$

If $\alpha^2 > 0$ replace u_1 with αu_1 , else if $\alpha^2 < 0$ change the sign by interchanging $u_{11} \leftrightarrow u_{12}$ and $u_{13} \leftrightarrow u_{14}$ and then replace u_1 with αu_1 . To solve Equation 3.44 do precisely the same thing with u_2 . Finally normalize the state $\rho = \sum_{i=1}^4 e_i e_i^\dagger$ to unit trace to get a type 2 state.

Chapter 4

Rank 5555 states and product vectors

The next step is to get a better understanding of extremal rank 5555 PPT states. The quadratic and quartic Lorentz invariants defined in Appendix B give no useful information for our rank 5555 states. But as we show in Section 4.1, there are six product vectors in the range of our states that we can use to define invariants of ρ and its partial transposes. In Chapter 4 we examine rank five states. These states are special because there are a finite number of product vectors in a generic five dimensional subspace of $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$. We find numerically that there are six product vectors in the range of a generic rank five state. There can be only one extremal state with the same range for the state and all its partial transposes, so using the six product vectors we define invariants of the state and its partial transposes.

In Section 4.2 we classify the states into four different types according to how their invariants are conserved under partial transpositions. Invariants are important because they can be used to conclude that states are *not* $\text{SL} \otimes \text{SL} \otimes \text{SL}$ equivalent. In particular a type I state is invariant under one partial transposition up to an $\text{SL} \otimes \text{SL} \otimes \text{SL}$ transformation. A type II state is a type I state under two different partial transpositions. A type III state is invariant under any two concurrent partial transpositions up to an $\text{SL} \otimes \text{SL} \otimes \text{SL}$ transformation. A type IV state has seemingly no relation between product vectors related to different partial transposes.

In Section 4.3 we show how we have been able to transform the states we have found with invariants conserved under partial transposition to symmetric form. We also derive a necessary condition on the product vectors of a state for such a symmetric form to exist.

4.1 Product vectors

Rank five states have five degrees of freedom on the vectors in its range, and a $2 \otimes 2 \otimes 2$ product vector must satisfy five equations, which means there is likely a finite number of product vectors in the range. We find numerically that there are six product vectors in the range of a generic rank five state. There can only be one extremal state with the same range for the state and all its partial transposes, i.e. it is completely defined by its range and the range of its partial transposes. So we can use the six product vectors to define invariants of the state and its partial transposes.

4.1.1 Finding product vectors

We need to be able to find product vectors in the range of a given state ρ , i.e. a vector:

$$z = u \otimes v \otimes w = \begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix} \otimes \begin{pmatrix} e \\ f \end{pmatrix} = \begin{pmatrix} ace \\ acf \\ ade \\ adf \\ bce \\ bcf \\ bde \\ bdf \end{pmatrix} \quad (4.1)$$

such that $z \in \text{Img } \rho$.

If we search for a product vector in a subspace, with P the orthogonal projection on that subspace, the product vector must then satisfy the condition:

$$(I - P)(u \otimes v \otimes w) = 0 \quad (4.2)$$

The problem is to find all zeros of the non-negative function,

$$f(u, v, w) = (u^\dagger \otimes v^\dagger \otimes w^\dagger)(I - P)(u \otimes v \otimes w) \quad (4.3)$$

There are several ways available to numerically find these roots. The one I have used is based on the method used in (Leinaas et al., 2010b), extended for three subsystems by Garberg (2012).

To properly compare different sets of product vectors we need a standard form. With six product vectors $u_i \otimes v_i \otimes w_i$, $i = 1, 2, \dots, 6$ we choose to transform each factor to the form:

$$u = \begin{pmatrix} 1 & 0 & 1 & r_1 & r_2 & r_3 \\ 0 & 1 & -1 & 1 & 1 & 1 \end{pmatrix} \quad (4.4)$$

$$v = \begin{pmatrix} 1 & 0 & 1 & s_1 & s_2 & s_3 \\ 0 & 1 & -1 & 1 & 1 & 1 \end{pmatrix} \quad (4.5)$$

$$w = \begin{pmatrix} 1 & 0 & 1 & t_1 & t_2 & t_3 \\ 0 & 1 & -1 & 1 & 1 & 1 \end{pmatrix} \quad (4.6)$$

so the first product vector is $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = (1, 0, 0, 0, 0, 0, 0, 0)^T$.

For details of the transformation, see Appendix C. We call the values r_i, s_i, t_i the SL-invariants of the state. There are however $6!$ ways to permute the vectors, leading to different standard forms and invariants.

4.2 Product vectors in the range of a rank 5555 state

After generating about 100 rank 5555 states using the method outlined in (Garberg, 2012) we started examining their product vectors. There are six product vectors of the form $z = u \otimes v \otimes w$ in a generic five dimensional subspace. Let $z_j^{(i)}$ denote the product vectors of ρ^{T_i} . We have compared the product vectors and their invariants, and find that there are four distinct types of states.

About four fifths of our states are what we call type I. For these states two out of the three factors u, v and w are preserved under *one* of the partial transpositions. Assume for the sake of the argument that the relevant partial transposition is T_3 . Then T_3 conserves u and v , but not w .

When we transform all the factors of the product vectors of ρ and ρ^{T_3} to the standard form defined in Section 4.1.1, it turns out that the invariants of w are conserved under T_3 , even though w changes. Let $A = A_1 \otimes A_2 \otimes A_3$ be the matrix that transforms z^0 to standard form. The state can be written as

$$\rho = \sum_{i,j=1}^5 k_{ij} z_i^{(0)} \left(z_j^{(0)} \right)^\dagger \quad \text{with } k_{ji} = k_{ij}^* \quad (4.7)$$

Applying the transformation A to the product vectors in Equation 4.7 we define the transformed matrix

$$\tilde{\rho} = \sum_{i,j=1}^5 k_{ij} \left(Az_i^{(0)} \right) \left(Az_j^{(0)} \right)^\dagger = A\rho A^\dagger \quad (4.8)$$

which is a standard form of ρ with the product vectors in $\text{Im} \tilde{\rho}$ on standard form. Let $B = B_1 \otimes B_2 \otimes B_3$ be the matrix that transforms $z^{(3)}$ to the same standard form as $Az^{(0)}$. We find that

$$A\rho A^\dagger = B\rho^{T_3} B^\dagger \Rightarrow \rho^{T_3} = (B^{-1}A)\rho(B^{-1}A)^\dagger = Z\rho Z^\dagger. \quad (4.9)$$

u and v are conserved under T_3 so $Z = I \otimes I \otimes Z_3$ and the partial transposition is an SL-transformation on the third subsystem. Partially transposing the equation

$$\rho^{T_3} = (I \otimes I \otimes Z_3)\rho(I \otimes I \otimes Z_3)^\dagger \quad (4.10)$$

with respect to the third subsystem gives $Z_3^{-1} = Z_3^*$.

The fact that ρ and ρ^{T_3} have the same standard form does not mean that either ρ or the standard form of ρ is symmetric under T_3 .

We can extend this relation to the invariants of ρ^{T_1} and ρ^{T_2} in the following way,

$$\rho^{T_2} = (Z^{-1}\rho^{T_3}(Z^{-1})^\dagger)^{T_2} = Z^{-1}\rho^{T_2T_3}(Z^{-1})^\dagger = Z^{-1}(\rho^{T_1})^*(Z^{-1})^\dagger \quad (4.11)$$

We see from this that the invariants of ρ^{T_1} and ρ^{T_2} have to be complex conjugates of each other, though they are not related to the invariants of ρ and ρ^{T_3} . The relation between the invariants and standard forms is illustrated in Figure 4.1.

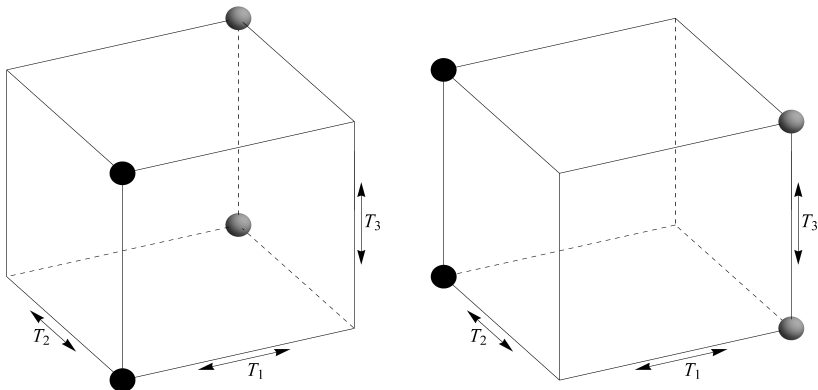


Figure 4.1: Relation between the invariants and standard forms of a type I state with $\rho \sim \rho^{T_3}$. The spheres with the same color have the same invariants and states with different colors have complex conjugated invariants.

About 5% of our states have the same properties as type I states, under partial transposition of two different subsystems. We call states of this kind type II states. Assume for the sake of the argument that

$$\rho^{T_3} = Z\rho Z^\dagger, \quad \rho^{T_2} = Y\rho Y^\dagger \quad (4.12)$$

with $Z = I \otimes I \otimes Z_3$ and $Y = I \otimes Y_2 \otimes I$. Then

$$\rho^* = \rho^T = \rho^{T_1T_2T_3} = (YZ\rho(YZ)^\dagger)^{T_1} = (YZ)\rho^{T_1}(YZ)^\dagger \quad (4.13)$$

with $YZ = I \otimes Y_2 \otimes Z_3$. So the invariants of ρ^{T_1} are the complex conjugates of the invariants of ρ . Note that this is a special case of the previous type. The relation between the invariants and standard forms is illustrated in Figure 4.2.

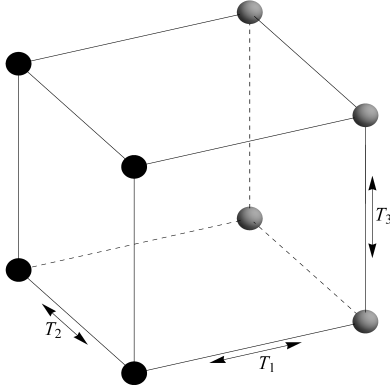


Figure 4.2: Relation between the invariants and standard forms of a type II state with $\rho \sim \rho^{T_2} \sim \rho^{T_3}$.

About 2 – 3% of our states are what we call type III. For these states doing any one of the partial transpositions complex conjugates the corresponding factor of the product vectors. The other factors are not conserved, but their invariants are complex conjugates of the invariants of ρ . Equivalently, their invariants are conserved under two concurrent partial transpositions. We transform ρ^{T_i} to standard form by applying transformations $V^{(i)} = V_1^{(i)} \otimes V_2^{(i)} \otimes V_3^{(i)}$ so that $\rho^{T_i} \rightarrow V^{(i)} \rho^{T_i} (V^{(i)})^\dagger$

We find empirically that the standard form of ρ^{T_i} is the complex conjugate of the standard form of ρ ,

$$V^{(i)} \rho^{T_i} (V^{(i)})^\dagger = (V^{(0)} \rho V^{(0)})^* \Rightarrow \rho^{T_i} = W^{(i)} \rho^* (W^{(i)})^\dagger \quad (4.14)$$

where $W_j^{(i)} = (V_j^{(i)})^{-1} (V_j^{(0)})^*$. Note that $W_i^{(i)} = I$, since that factor of the product vectors is conserved. The relation between the invariants and standard forms is illustrated in Figure 4.3.

Finally about 10 – 15% of our states have no discernible relation between their product vectors. We call these states type IV.

If we now define $A \sim B$ mean that $A = WBW^\dagger$ for some $W = W_1 \otimes W_2 \otimes W_3$ we get the following summary:

Summary of types of states

Type I: $\rho \sim \rho^{T_i}$ and $\rho^{T_j} \sim (\rho^{T_k})^*$

Type II: $\rho \sim \rho^{T_i} \sim \rho^{T_j}$ and $\rho \sim (\rho^{T_k})^*$

Type III: $\rho \sim (\rho^{T_i})^*$ for $i = 1, 2, 3$. Equivalently, $\rho \sim \rho^{T_i T_j}$

Type IV: None of the above

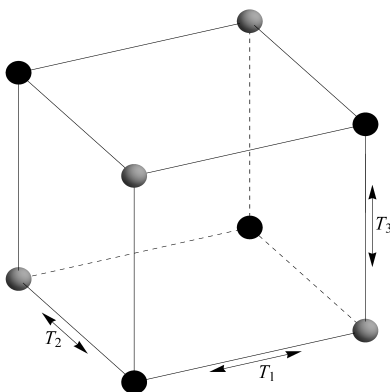


Figure 4.3: Relations between the invariants and standard forms of a type III state.

4.2.1 A note on separable states

A product vector $z = u \otimes v \otimes w$ defines a separable density matrix of rank 1111:

$$\rho = zz^\dagger = (uu^\dagger) \otimes (vv^\dagger) \otimes (ww^\dagger) \quad (4.15)$$

Doing a partial transposition on this separable state is the same as complex conjugating the corresponding factor of z .

A convex combination of n of these product density matrices is in general a state of rank $nnnn$, as long as all n product vectors and their partial conjugates are linearly independent.

We find six product vectors in the range of a generic rank 5555 state, and since the range is five dimensional one of these vectors is a linear combination of the other five. So the convex combination of the $n = 6$ density matrices is a rank five matrix. The linear dependence between the six vectors is generally broken when the vectors are partially conjugated, so the convex combination is rank 5666.

This means that in any generic rank five subspace there are six rank one states that form a simplex of separable states. The states on the surface of the simplex have rank $nnnn$, with $n = 1, 2, \dots, 5$, whereas the states in the interior have rank 5666.

4.3 Symmetric forms

In this section we will show how to use the invariants conserved under partial transpositions to transform a state to a form with symmetries under partial transpositions.

4.3.1 Types I and II

As we saw in Section 4.2 only one factor of the product vectors is changed under the relevant partial transposition, and it is still conserved up to an SL transformation. We want to try to transform that component of the system such that it is also conserved under the partial transposition.

We can derive a necessary condition for such a symmetric form to exist. If we start with a symmetric form $\tilde{\rho}^{T_3} = \tilde{\rho}$ and do a product transformation away from this form,

$$\rho = (A \otimes B \otimes C)\tilde{\rho}(A \otimes B \otimes C)^\dagger \quad (4.16)$$

then the partial transposition is the following:

$$\rho^{T_3} = (A \otimes B \otimes C^*)\tilde{\rho}(A \otimes B \otimes C^*)^\dagger = (I \otimes I \otimes (C^* C^{-1}))\rho(I \otimes I \otimes (C^* C^{-1}))^\dagger \quad (4.17)$$

Comparing this with our definition of a state which is of type I,

$$\rho^{T_3} = (Z_1 \otimes Z_2 \otimes Z_3)\rho(Z_1 \otimes Z_2 \otimes Z_3)^\dagger \quad (4.18)$$

gives that

$$Z_1 = Z_2 = I, \quad Z_3 = C^* C^{-1} \quad (4.19)$$

which agrees with our empirical result that the u and v factors of the product vectors are unchanged by partial transposition of the third system and the w factor is only changed by an SL transformation Z_3 , which has the property $Z_3^{-1} = Z_3^*$. Note that A and B is completely arbitrary, since it does not affect the relation between those factors of the product vectors.

This means that we will be able to transform the state to symmetric form if we can find a C that fulfils $Z_3 = C^* C^{-1}$.

We find the same type of problem when finding the symmetric form of type III states, and solve it by transforming the equivalent of Z_3 to the identity by Lorentz transformations. In the case of type I and II state we solved the problem another way, which is presented in the followng.

Partial transposition of any subsystem is in fact a transposition of sixteen 2×2 matrices, see Figure 4.4. Let us assume for simplicity that the state is SL-invariant under T_3 . So we are looking for a transformation $U = I \otimes I \otimes V$ so that:

$$\tilde{\rho} = U\rho U^\dagger, \quad \tilde{\rho}^{T_3} = \tilde{\rho} \quad (4.20)$$

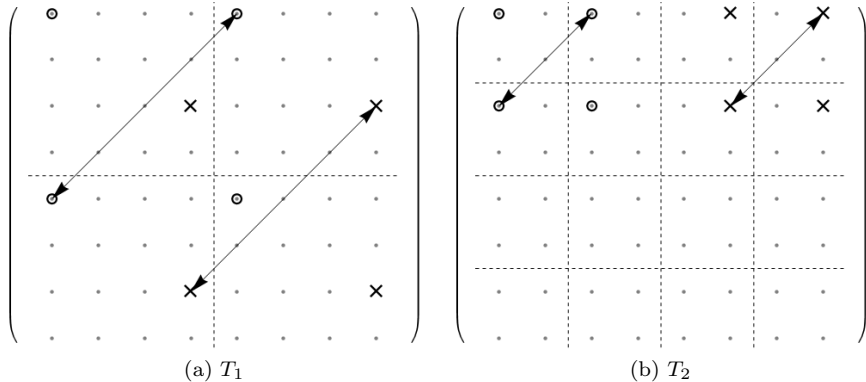


Figure 4.4: Partial transposition as 2×2 matrix transposition

Explicitly,

$$\tilde{\rho} = U\rho U^\dagger = \begin{pmatrix} V & 0 & 0 & 0 \\ 0 & V & 0 & 0 \\ 0 & 0 & V & 0 \\ 0 & 0 & 0 & V \end{pmatrix} \begin{pmatrix} A_1 & A_2 & A_3 & A_4 \\ A_5 & A_6 & A_7 & A_8 \\ A_9 & A_{10} & A_{11} & A_{12} \\ A_{13} & A_{14} & A_{15} & A_{16} \end{pmatrix} \begin{pmatrix} V^\dagger & 0 & 0 & 0 \\ 0 & V^\dagger & 0 & 0 \\ 0 & 0 & V^\dagger & 0 \\ 0 & 0 & 0 & V^\dagger \end{pmatrix} \quad (4.21)$$

$$= \begin{pmatrix} VA_1V^\dagger & VA_2V^\dagger & VA_3V^\dagger & VA_4V^\dagger \\ VA_5V^\dagger & VA_6V^\dagger & VA_7V^\dagger & VA_8V^\dagger \\ VA_9V^\dagger & VA_{10}V^\dagger & VA_{11}V^\dagger & VA_{12}V^\dagger \\ VA_{13}V^\dagger & VA_{14}V^\dagger & VA_{15}V^\dagger & VA_{16}V^\dagger \end{pmatrix} \quad (4.22)$$

That $\tilde{\rho}$ is symmetric under partial transposition means that

$$(VA_iV^\dagger)^T = VA_iV^\dagger \quad \forall i = 1, \dots, 16. \quad (4.23)$$

A_i will not be Hermitian in general, but can be split into two matrices B_i and C_i that are Hermitian:

$$A_i = B_i + iC_i, \quad B_i = A_i^\dagger + A_i, \quad C_i = i(A_i^\dagger - A_i) \quad (4.24)$$

$$M = \begin{pmatrix} t + z & x - iy \\ x + iy & t - z \end{pmatrix} \quad (4.25)$$

can be represented as a four-vector $a = (t, x, y, z)^T$. The condition in Equation 4.23 then means that VB_iV^\dagger and VC_iV^\dagger must be orthogonal to σ_y in the Minkowski inner product.

We find numerically that the 32 four-vectors that represent B_i and C_i span a three dimensional subspace, so that there is one vector a that is orthogonal to all of them

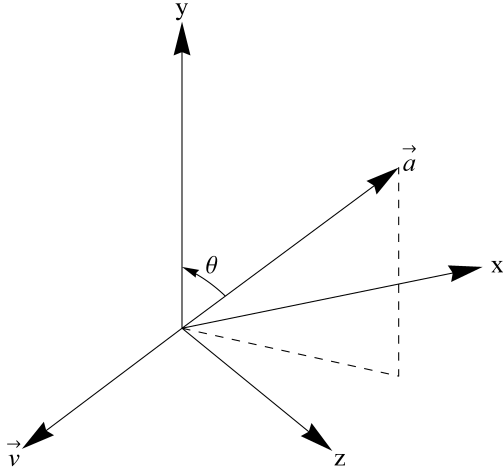


Figure 4.5: Rotation around an axis \vec{v} by θ radians

by the Minkowski inner product. We will transform this orthogonal vector a into σ_y through one SL transformation V . First turn a into a Hermitian matrix:

$$A = a^\mu \sigma_\mu = \begin{pmatrix} t + z & x - iy \\ x + iy & t - z \end{pmatrix} \quad (4.26)$$

To remove the x and z component, rotate around the axis

$$\vec{v} = \frac{1}{\sqrt{x^2 + z^2}} (-z, 0, x) \quad (4.27)$$

by θ radians, see Figure 4.5. The SU(2) rotation matrix is:

$$R = \cos\left(\frac{\theta}{2}\right) I + \sin\left(\frac{\theta}{2}\right) \vec{v} \cdot \vec{\sigma} \quad (4.28)$$

Applying the rotation matrix to A transforms it into:

$$A' = RAR^\dagger = \begin{pmatrix} t & -i\tilde{y} \\ i\tilde{y} & t \end{pmatrix} \quad (4.29)$$

To get rid of the time component do a Lorentz boost in the e_y direction. In the SL-formalism this boost is

$$B = I + b\sigma_y \quad (4.30)$$

This applied to A' gives

$$A'' = BA'B = \begin{pmatrix} tb^2 + 2yb + t & -i(yb^2 + 2tb + y) \\ i(yb^2 + 2tb + y) & tb^2 + 2yb + t \end{pmatrix} \quad (4.31)$$

We want the time component of A'' to be 0, so we solve the second order equation

$$tb^2 + 2yb + t = 0 \quad (4.32)$$

for b . The combined transformation

$$V = BR \quad (4.33)$$

transforms all B_i and C_i so that they become orthogonal to σ_y . The full transformation of ρ is

$$\tilde{\rho} = (I \otimes I \otimes V)\rho(I \otimes I \otimes V)^\dagger \quad (4.34)$$

This matrix is symmetric under T_3 , so $\tilde{\rho}^{T_2}$ must be the complex conjugate of $\tilde{\rho}^{T_1}$:

$$\tilde{\rho}^{T_1} = \tilde{\rho}^{T_3 T_2 T} = (\tilde{\rho}^{T_2})^* \quad (4.35)$$

A type II state has two partial transposes that are SL transforms of itself. We always find that it can be transformed to a form that is symmetric under two different partial transpositions. The transformation that transforms ρ to a symmetric form under one partial transposition is independent of the transformation that transforms ρ to a symmetric form under another transposition, since A and B in Equation 4.16 is arbitrary.

Type I and II states as biseparable states When we view a type I or II state as a bipartite state, i.e. 2×4 , $2 \times (2) \times 2$ or 4×2 we find empirically that it is separable when split into its symmetric part and the rest. So if, for instance, $\tilde{\rho}^{T_1} = \tilde{\rho}$ then ρ is separable as a 2×4 state. This agrees nicely with the result published by Kraus et al. (2000), where they show that a $2 \times N$ state ρ is separable if $\rho^{T_1} = \rho$. If it is symmetric under both T_1 and T_3 then it is separable in both 2×4 and 4×2 dimensions.

This observation has so far not enabled us to explicitly construct these states. It may not be very useful since there are infinitely many 2×4 product vectors in a five dimensional subspace, see Appendix F.

4.3.2 Type III

We have from Section 4.2 that a type III state has the following symmetries,

$$\rho^{T_i} = W^{(i)}(\rho)^* \left(W^{(i)}\right)^\dagger \quad \text{for } i = 1, 2, 3 \quad (4.36)$$

with $W^{(i)} = W_1^{(i)} \otimes W_2^{(i)} \otimes W_3^{(i)}$ and $W_i^{(i)} = I$. We want to transform the state ρ to a form $\tilde{\rho}$ so that $\tilde{\rho}^{T_i} = (\tilde{\rho})^*$ for $i = 1, 2, 3$.

We can derive a necessary condition for such a conjugate symmetric form to exist. If we write

$$\rho = (A \otimes B \otimes C)\tilde{\rho}(A \otimes B \otimes C)^\dagger \quad (4.37)$$

then the partial transposition of the first subsystem is the following:

$$\begin{aligned} \rho^{T_1} &= (A^* \otimes B \otimes C)\tilde{\rho}^{T_1}(A^* \otimes B \otimes C)^\dagger \\ &= (A^* \otimes B \otimes C)(\tilde{\rho})^*(A^* \otimes B \otimes C)^\dagger \\ &= (I \otimes (B(B^*)^{-1}) \otimes (C(C^*)^{-1}))\rho^*(I \otimes (B(B^*)^{-1}) \otimes (C(C^*)^{-1}))^\dagger \end{aligned} \quad (4.38)$$

Comparing this to Equation 4.36 gives

$$W_1^{(1)} = I, \quad W_2^{(1)} = B(B^*)^{-1}, \quad W_3^{(1)} = C(C^*)^{-1}. \quad (4.39)$$

The same argument for $i = 2$ and $i = 3$ gives:

$$W_1^{(2)} = A(A^*)^{-1}, \quad W_2^{(2)} = I, \quad W_3^{(2)} = C(C^*)^{-1} \quad (4.40)$$

$$W_1^{(3)} = A(A^*)^{-1}, \quad W_2^{(3)} = B(B^*)^{-1}, \quad W_3^{(3)} = I \quad (4.41)$$

so

$$\begin{aligned} W^{(1)} &= I \otimes W_2 \otimes W_3 \\ W^{(2)} &= W_1 \otimes I \otimes W_3 \\ W^{(3)} &= W_1 \otimes W_2 \otimes I \end{aligned} \quad (4.42)$$

$$(4.43)$$

which agrees with our empirical results for how the partial transposition changes the product vectors. Our problem is now to solve the equations

$$A^{-1}W_1A^* = B^{-1}W_2B^* = C^{-1}W_3C^* = I \quad (4.44)$$

for A , B and C . Let us start with $W = W_1$. It has the property $W^{-1} = W^*$. This implies that $|\det W| = 1$ so we may as well multiply by an overall phase factor such that $\det W = 1$

$$W = \begin{pmatrix} y + ix & i(z + t) \\ i(z - t) & y - ix \end{pmatrix} \quad (4.45)$$

with $t, x, y, z \in \mathbb{R}$. Its determinant,

$$\det W = -t^2 + x^2 + y^2 + z^2 = 1, \quad (4.46)$$

is conserved when W is acted upon by a matrix $A \in \text{SL}(2, \mathbb{C})$:

$$W \rightarrow A^{-1}WA^* \quad (4.47)$$

This is therefore another way of representing the Lorentz four-vector and transforming it.

The identity matrix can be represented as the four-vector $(0, 0, 1, 0)$ in this representation. So we need to transform the four-vector (t, x, y, z) into $(0, 0, 1, 0)$. To transform the matrix we must know the generators of the action in Equation 4.47.

The generators Consider an infinitesimal Lorentz transformation $U = I + \epsilon L$ acting on Equation 4.45:

$$W' = U^{-1} W U^* = (I + \epsilon L) W (I - \epsilon L^*) = W + \epsilon(LW - WL^*) + \mathcal{O}(2) \quad (4.48)$$

The change is

$$\delta W = LW - WL^* \quad (4.49)$$

Inserting $L = \frac{1}{2}\sigma_1$ gives

$$\delta W = \begin{pmatrix} -it & -ix \\ ix & it \end{pmatrix} \quad (4.50)$$

$$x \rightarrow x - \epsilon t \quad t \rightarrow t - \epsilon x \quad (4.51)$$

which is a boost in the negative x -direction, i.e. $-K_x$. Inserting the other normal generators of $SU(2, \mathcal{C})$: $\frac{1}{2}\sigma_i$ and $\frac{i}{2}\sigma_i$ gives in short:

$$L = \frac{1}{2}\sigma_1 \Rightarrow \delta W = \begin{pmatrix} -it & -ix \\ ix & it \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = -K_x \quad (4.52)$$

$$L = \frac{i}{2}\sigma_1 \Rightarrow \delta W = \begin{pmatrix} -z & iy \\ iy & -z \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = J_x \quad (4.53)$$

$$L = \frac{1}{2}\sigma_2 \Rightarrow \delta W = \begin{pmatrix} t & -iy \\ iy & t \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = -K_y \quad (4.54)$$

$$L = \frac{i}{2}\sigma_2 \Rightarrow \delta W = \begin{pmatrix} iz & -ix \\ -ix & -iz \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} = J_y \quad (4.55)$$

$$L = \frac{1}{2}\sigma_3 \Rightarrow \delta W = \begin{pmatrix} 0 & i(z-t) \\ -i(z+t) & 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = K_z \quad (4.56)$$

$$L = \frac{i}{2}\sigma_3 \Rightarrow \delta W = \begin{pmatrix} -x+iy & 0 \\ 0 & -x-iy \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = -J_z \quad (4.57)$$

First do a rotation around the vector $\vec{v} = \frac{1}{\sqrt{x^2+z^2}}(-z, 0, x)$ to get rid of the x and z components, see Figure 4.5.

$$R = \cos\left(\frac{\alpha}{2}\right)I + \sin\left(\frac{\alpha}{2}\right)\vec{v} \cdot \vec{J} \quad (4.58)$$

Now applying this matrix to W we get a matrix of with the form:

$$W' = RW R^* = \begin{pmatrix} \tilde{y} & -it \\ it & \tilde{y} \end{pmatrix} \quad (4.59)$$

to get rid of the time component do a boost in the e_y -direction:

$$T = I + bK_y \quad (4.60)$$

The combined transformation $A = TR$ transforms the W_1 to the identity. Repeating the transformation for W_2 and W_3 gives us B and C

$$\tilde{\rho} = (A^{-1} \otimes B^{-1})\rho P^\dagger \Rightarrow \tilde{\rho}^{T_i} = \tilde{\rho}^* \quad (4.61)$$

Chapter 5

Perturbing states

After finding different kinds of states we want to see if there are differences in the geometry of the different states. Specifically rank 5555 PPT states lie on surfaces of rank 5555 states, where some of the directions on the surface may preserve the range of the state. We determine the surfaces' dimensions (Section 5.1) and how they lie in relation the simplex of separable states (Section 5.2).

This section extends the work done by Hansen et al. (2012) to tripartite systems.

Let ρ be a rank 5555 density operator with orthonormal eigenvectors v_1, \dots, v_5 and define

$$V = (v_1 \quad \dots \quad v_5) \quad (5.1)$$

The orthogonal projection on the range of ρ is

$$P = VV^\dagger \quad (5.2)$$

and the orthogonal complement $Q = \mathbb{1} - P$ is the orthogonal projection on the kernel of ρ . These projection operators satisfy $P\rho P = \rho$ and $Q\rho Q = 0$. Consider a perturbation

$$\rho' = \rho + \epsilon A \quad (5.3)$$

with $\text{Tr } A = 0$. If $\text{Tr } A \neq 0$ replace A with $A - \text{Tr } A \rho$. If $PAP = A$ then $\text{Im}g \rho \subset \text{Im}g \rho'$ and $\text{Im}g \rho' = \text{Im}g \rho$ to first order in ϵ . And, to first order in ϵ , the zero eigenvalues of ρ become the eigenvalues of ϵQAQ , so the condition

$$QAQ = 0 \quad (5.4)$$

is enough to ensure that the rank of ρ' will be the same as the rank of ρ .

Projections are linear operators so we can define orthogonal projection operators

$\mathbf{I}, \mathbf{P}, \mathbf{Q}, \mathbf{S}$ on the real Hilbert space of Hermitian matrices:

$$\mathbf{I}\rho = \rho \quad (5.5)$$

$$\mathbf{P}\rho = P\rho P \quad (5.6)$$

$$\mathbf{Q}\rho = Q\rho Q = \rho - P\rho - \rho P + P\rho P \quad (5.7)$$

$$\mathbf{S}\rho = (\mathbf{I} - \mathbf{P} - \mathbf{Q})\rho = P\rho + \rho P - 2P\rho P \quad (5.8)$$

In the same way we define projections related to ρ^{T_i} :

$$\mathbf{P}_i X = (P_i X^{T_i} P_i)^{T_i} \quad (5.9)$$

$$\mathbf{Q}_i X = (Q_i X^{T_i} Q_i)^{T_i} \quad (5.10)$$

$$\mathbf{S}_i X = (\mathbf{I} - \mathbf{P}_i - \mathbf{Q}_i) X \quad (5.11)$$

Note that we defined $\rho = \rho^{T_0}$ so $\mathbf{P}_0 = \mathbf{P}$, $\mathbf{Q}_0 = \mathbf{Q}$ and $\mathbf{S}_0 = \mathbf{S}$. We can use these projections to impose various constraints on the perturbation matrix A . The perturbation conserves the rank and positivity of ρ if, and only if,

$$\mathbf{Q}A = 0 \leftrightarrow (\mathbf{I} - \mathbf{Q})A = A \quad (5.12)$$

and only conserves the image space if $\mathbf{P}A = A$. Defining $\mathbf{R}_i = \mathbf{I} - \mathbf{Q}_i$ and combining the constraints for ρ and its partial transposes we can set up an eigenvector equation for A :

$$\mathbf{G}A = (\mathbf{P}_0 + \mathbf{R}_1 + \mathbf{R}_2 + \mathbf{R}_3)A = 4A. \quad (5.13)$$

A perturbation matrix that satisfies Equation 5.13 will conserve the range of ρ and the rank of ρ^{T_i} for $i = 1, 2, 3$. Similarly we may set up matrix equations that will conserve other combinations of ranges and ranks.

For simplicity we denote conserving the range of ρ and the ranks of all its partial transposes as PRRR, conserving the ranges of ρ and ρ^{T_1} and the rank of ρ^{T_2} and ρ^{T_3} as PPRR, and so on.

5.1 Dimensions

Each eigenvector of \mathbf{G} that has eigenvalue 4 is a direction you can perturb in that results in a state with the same image space as ρ . All these directions form a surface that can be perturbed along. You can of course always perturb in the direction defined by ρ itself, so the dimension of the surface is:

$$D = N - 1 \quad (5.14)$$

where N is the number of eigenvectors of \mathbf{G} with eigenvalue 4. This argument was done for PRRR, but it is analogous for every combination.

We find that the different types of states, as defined in Section 4.2, lie on surfaces of different dimensions. As also may be expected it does not matter whether we conserve the range of ρ , ρ^{T_1} , ρ^{T_2} or ρ^{T_3} , all the partial transposes are equivalent.

We find that every state of type I or II lies on a 32 dimensional surface of rank 5555 states. When we impose another constraint, i.e. demand that the perturbation must preserve the range of one of ρ^{T_i} , the number of dimensions is reduced to two. Yet another constraint reduces the number of dimensions to zero.

The type III states lie on a 27 dimensional surface of rank 5555 states, and three of those dimensions also preserve the range of ρ .

Finally, the type of state with no symmetry between ρ and its partial transposes is on a 29 dimensional surface of rank 5555 states and it is not possible to perturb and conserve any range.

These results are summarised in Table 5.1.

Type	Dimensions				
	RRRR	PRRR	PPRR	PPPR	PPPP
I	32	2	0	0	0
II	32	2	0	0	0
III	27	3	0	0	0
IV	29	0	0	0	0

Table 5.1: Perturbing rank 5555 extremal states. All the partial transposes are equivalent in this list, i.e. the specific range we conserve does not matter

5.2 Walking on the surface

Once we have found the dimensions of these surfaces we would like to be able to walk on them. Interesting questions are if the type of the states is the same all over the surface, what is the edge of the surface and how are the surfaces situated relative to the simplex of separable states (see page 24).

Numerically walking on the surface requires successive perturbations like the one in Equation 5.3. The equation is exactly the Euler method for numerically solving the differential equation $D[\rho] = f(\rho)$ where f is the displacement along the surface. The Euler method is unfortunately inaccurate so we find ourselves far from the surface after only a hundred steps or so.

It is possible to project the state down unto the surface when this happens. Say for simplicity that we conserve the range of ρ and the ranks of the partial transposes. The image does not change so $\rho = P\rho P^\dagger$ gives the right image space. Projecting a partial transpose unto the range of its five dominant eigenvalues makes it rank five as well. Unfortunately these two operations does not work at the same time, but repeating it works to a certain degree, i.e. repeating

$$\rho \mapsto P(\rho + (P_1\rho^{T_1}P_1)^{T_1} + (P_2\rho^{T_2}P_2)^{T_2} + (P_3\rho^{T_3}P_3)^{T_3})P \quad (5.15)$$

several thousand times tends to get ρ nearer to the surface.

Unfortunately this approach has been prohibitively time consuming. So we have instead implemented a fourth order Runge-Kutta method (Section G.2). It is far more accurate and can do tens of thousands of steps of length 10^{-5} or less before straying far from the surface.

We found, by taking walks in random directions, that the type of state is conserved on the surface of states with the same image space, e.g. if you start with a state that is SL-invariant under T_3 the states on the surface around it are also SL-invariant under T_3 .

A fast way to get to the edge of the surface is to find the direction that leads to the largest decrease in the smallest non-zero eigenvalue. The change Δ in the eigenvalue associated with an eigenvector ψ is

$$\Delta = \epsilon \psi^\dagger A \psi \quad (5.16)$$

so to find the fastest way to the edge of the surface we want to minimize

$$f(x) = \psi^\dagger \left(\sum_i x_i M_i \right) \psi, \quad (5.17)$$

where M_i are the directions that preserves rank/image and ψ is the eigenvector with lowest non-zero eigenvalue, under the constraint

$$g(x) = \sum_i x_i^2 = c \quad (5.18)$$

Using Lagrange multipliers we know the minimum must be a solution of the system:

$$\begin{cases} \nabla f(x) &= \lambda \nabla g(x) \\ g(x) &= c \end{cases} \Rightarrow \begin{cases} \psi^\dagger M_1 \psi &= 2\lambda x_1 \\ \dots &\Rightarrow x_i \propto \psi^\dagger M_i \psi \\ g(x) &= c \end{cases} \quad (5.19)$$

Doing this for each perturbation step should give a fast way to the edge of the surface.

When we walk to the edge of a two dimensional surfaces of type I or type II states, we find either an extremal type 1 rank 4444 state or a separable state of rank less than or equal to two.

To check whether all the surfaces touch the simplex of separable states, we must aim towards it. Specifically, this means taking the difference between the state and one of the simplexes and projecting it down unto the surface each step.

In the case that the fastest way to the edge leads to a rank 4444 state, aiming specifically for the different vertices of the simplex works for some, but not all of the vertices. Additionally, we find that the surface touches rank two states on a straight line between some of the vertices. This makes it pretty obvious that a

part of the edge is touching some number of lines $p\rho_s^i + (1-p)\rho_s^j$ where $0 \leq p \leq 1$, $\rho_s^i = z_i^0$ and $\rho_s^j = z_j^0$. We find empirically that these lines form a connected curve which is never closed.

The situation for a surface of type III states is the same, though we may find rank three separable states at the edge.

All the surfaces have very small curvature.

Chapter 6

Finding states on a specified subspace

Another interesting question is whether there can be more than one kind of state on a specified subspace. Is it for instance possible to find a type I state in the range of one of the type IV states we have generated earlier?

Any five linearly independent vectors in the image space will span the space. So we can choose five of the product vectors and make any state in the image space by taking a linear combination of them:

$$\rho = \sum_{i,j=1}^5 x_{i,j} z_i z_j^\dagger \quad (6.1)$$

Let $\mu_i^{(j)}$ denote the eigenvalues of ρ^{T_j} in ascending order. Making ρ be rank 5555 can be formulated as a minimisation problem:

$$f(x) = \sum_{i=1}^3 \sum_{j=0}^3 \left(|\mu_i^{(j)}(x)|^2 \right) \quad (6.2)$$

When $f(x) = 0$ then Equation 6.1 is a state of rank 5555 or less.

This objective function works fine for finding rank 5555 states, but mostly converges to a non extremal states on the simplex of separable states. To prevent this we add a repulsive potential by dividing the function value by the volume of the six dimensional simplex with vertices consisting of the five product vectors and the proposed state ρ . This volume goes to zero as the proposed state approaches the simplex.

In Section 6.1 we present the implementation of the simulated annealing minimisation routine we have used. In Section 6.2 we present what kinds of states we find

on different subspaces. In Section 6.3 we discuss a property of the range of type III states.

6.1 Minimisation routine

We may use a random search algorithm to find the minimum of Equation 6.2, but it does not converge very well in general. Instead we implement a simulated annealing routine.

Simulated annealing is a variant of the Metropolis algorithm, which means it sometimes takes a step "uphill" so it should be less likely to converge to a local minimum. The algorithm requires 4 elements: the objective function f , the system state \mathbf{x} of N variables, the control parameter T (including an annealing schedule by which it is reduced) and some way to make random changes in the configuration.

The last point is the most problematic one. The method should be efficient in long narrow valleys, i.e. places where almost all directions lead uphill, and efficient independent of how near you get to the minimum. We have used the approach suggested by Press et al. (2007). They replace the system state \mathbf{x} by a simplex of $N + 1$ points. The possible changes to the configuration are reflections, expansions and contractions of the simplex. To implement the Metropolis algorithm we add a positive random variable, proportional to the control parameter T , to the function value associated with each vertex, and we subtract a similar random variable from the function value of every proposed replacement point. This approach will always accept a downhill move, but may sometimes accept uphill moves.

At a temperature T the simplex will expand to cover approximately the region reachable at that temperature. It then randomly samples points inside that region. As the temperature decreases the simplex shrinks into the region reachable at the decreased temperature, which is likely to contain the lowest minimum encountered so far.

The annealing schedule we have used is a variation of $T \rightarrow (1 - \epsilon)T$ every m moves. $\frac{\epsilon}{m}$ is determined by the relation between T and the best minimum value encountered so far. Specifically the further the temperature gets from the minimum value the slower it changes. This approach works in this case since we are looking for global minima with function value zero.

For our MATLAB implementation of simulated annealing, see Section G.3.

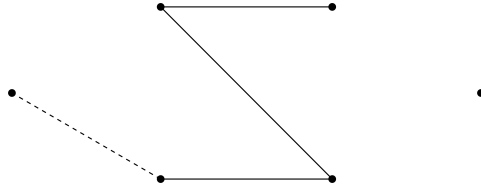


Figure 6.1: Edge of two different type I surfaces touching the simplex of separable states

6.2 Different rank 5555 states on the same subspace

On the range of a type I state there is generally another surface of type I states of another symmetry, and a surface of type II states with two corresponding symmetries.

Likewise on the range of a type II state we find two surfaces of type I with the corresponding symmetries. Notably we never find states with all three different symmetries on one range.

A type IV state, without symmetry, also has two surfaces of type I states on its range. Unlike the previous case we find no type II surface with the corresponding symmetries.

These twin surfaces of type I states are also present on the range of a type III state. In addition there is another three dimensional surface of type IV states. Like for the other type IV states any one of these lies on a 29 dimensional surface of rank 5555 states. Unlike the other type IV states three of those dimensions also conserve its range. It is also special since it cannot be perturbed in a way that conserves the range of its partial transposes. I.e. $PRRR=3$ and $RPRR=RRPR=RRRP=0$.

The disparity between these new IV states and any state we have examined earlier is a natural consequence of a special property of the range of a type III state and its partial transposes. The range of the type III state (and its partial transposes) contains three vectors that are E -orthogonal to the entire range. Such a new state of type IV has these vectors in its own range, but not in the range of its partial transposes.

Another question is how do these surfaces of states lie relative to each other. You cannot walk from a state with specific type and symmetry to another state with different type or symmetry while conserving the range.

The edges of the surface touches different parts of the simplex of separable states, see Figure 6.1. In the illustrated case we started with a state of type I, symmetric under T_3 , and found that it touches the simplex at four vertices and a line that

connects all of them (the solid line). In the same range we found a state symmetric under T_1 that touches the simplex at a line connecting two vertices (the dotted line). There is also a type II state, and its surface touches the vertices labeled 1,2 and 3, though not the line between them as far as we can tell.

6.3 E -orthogonal vectors of rank 5555 states

Let the set $\{v_1, \dots, v_5\}$ span the range of ρ and $x \in \mathbb{C}^5$. If

$$U = (v_1, v_2, v_3, v_4, v_5) \tag{6.3}$$

then Ux is a vector in this space. This vector is E -orthogonal to $\text{Im} \rho$ if

$$U^T E U x = 0 \tag{6.4}$$

so finding E -orthogonal vectors in a space boils down to finding the eigenvectors of $U^T E U$ with eigenvalue 0. $U^T E U$ is an antisymmetric 5×5 matrix so non-zero eigenvalues comes in pairs. That means that a 5 dimensional subspace can only contain one or three of these vectors. We can exclude five, because we know from the dimensional argument in Section 3.3.1 that there is not enough space in an eight dimensional vector space to support five vectors that are both orthonormal and E -orthogonal.

Searching the image spaces of all our states for these product vectors shows that the range of a generic type I, II or IV state contain one of these vectors. The range of a type III state on the other hand contains three vectors of these vectors.

In addition to symptomising the new states described in the previous section, it also has consequences for the rank 4444 states. We know that for a rank 4444 state to be type 2 its four eigenvectors must all be E -orthogonal, so any such state can only exist in the range of a type III state. Finding one of these states is easily done by the same method we used to find rank 5555 states, only now the four lowest eigenvalues are minimised.

Chapter 7

Conclusion and further work

Numerically generated rank 4444 and rank 5555 entangled PPT states have been investigated. We find that entangled rank 4444 states can be separated into two different classes. Entangled rank 4444 states must also be extremal, since they are the lowest rank states that can be entangled.

The first of these classes have a quadratic Lorentz invariant that is non-zero. We find that a state of this class is equivalent by an $SL \otimes SL \otimes SL$ transformation to a state that is symmetric under all partial transpositions, and we show how to construct it analytically.

UPB states and their equivalents are special non-generic states of this kind. A UPB state as an unextendable basis of orthogonal product vectors in its kernel. No other rank 4444 PPT states have product vectors in their kernel.

The second class of states have zero quadratic invariant. We show that this puts a strict condition on the range of the state. Rank 4444 PPT states are biseparable in three different ways and there are exactly four product vectors in the range for each of these three bipartitions. We can use these three sets of four vectors to construct these states analytically.

We are able to construct all known rank four entangled PPT states analytically. But UPB states have not been found with our numerical methods, so there may exist other non-generic types outside this classification.

The next step is to get a better understanding of extremal rank 5555 PPT states. The quadratic and quartic local Lorentz invariants that proved so useful for the rank 4444 states gave no useful information for our rank 5555 states. A special property of five dimensional subspaces is that there is a finite number of product vectors in them. We find six product vectors in the range of each state ρ and each

of its partial transposes, which we use to define local invariants of ρ and its partial transposes.

The Lorentz invariants are invariant under partial transposition, but this is not the case for the invariants defined by the product vectors in the range. We classify the states into four different types according to how their invariants are conserved under partial transpositions.

The invariants of a type I state are conserved under one specific partial transposition, and we find that the state is invariant under that partial transposition, up to an $SL \otimes SL \otimes SL$ transformation. A type II state is a type I state under two different partial transpositions. The invariants of a type III state are complex conjugated under all three partial transpositions, and we find that the state is complex conjugated under any partial transposition, up to an $SL \otimes SL \otimes SL$ transformation. A type IV state has no discernible relation between the invariants related to different partial transposes.

We have found empirically that a state of type I or II, for which one or two partial transpositions are SL transformations, is in the equivalence class of a state that is symmetric under the same partial transpositions. This implies that a type I or II state is biseparable in one and two partitions respectively, according to a result proved by Kraus et al. (2000).

A type III state, for which all partial transpositions are complex conjugations followed by SL-transformations, is also found to be in the equivalence class of a state that is conjugate symmetric under all partial transpositions. A general state of this type is not biseparable in any way.

The dimensions and geometry of surfaces of rank 5555 states have been examined. We have found that a type I and II state is on a 32 dimensional surface of rank 5555 states and that two of these dimensions also conserve the range of the state. A type III state is on a 27 dimensional surface of rank 5555 states and three of the dimensions conserve the range of the state as well. A general type IV state is on a 29 dimensional surface of rank 5555 states, none of which have the same range as the state.

On the edges of the surfaces that conserve the range we find rank 4444 extremal states and states of rank two or less and rank three or less, for type I/II and type III states respectively. The edge that touches the simplex of separable state forms a connected curve between some the rank one states.

We have looked for different kinds of of rank 5555 states on different subspaces, and found that there are two different two-dimensional surfaces of type I states and one two-dimensional surface of type II states on most subspaces. The states on the two different surfaces of type I states, each have one of the symmetries of the states of type II in the subspace. A general type IV state shares its range with two different two-dimensional surfaces of type I states, with two different symmetries. On the range of a type III state we find two different two-dimensional surfaces of type I states, with two different symmetries, but no type II states. Instead we

find a surface of special type IV states. In the range of ρ^{T_i} of one of the type IV states on this surface we find one single two-dimensional surface of type I states, symmetric under T_i .

We find that these different surfaces on the same range all touch the simplex of separable states in different ways, so it seems likely that the different separable states are actually not equivalent. It may be possible to use this to discover why surfaces of different types and symmetries occur on different subspaces, but we have not found such a connection yet.

Finally, we find that there are three vectors in the range of a type III state that are E -orthogonal to the whole range. This means that rank 4444 states of type 2 in the range of rank 5555 states only occur on this kind of subspace.

Further investigation is required to determine analytical forms for the rank 5555 states. The structure of the type IV states is still completely unknown to us.

Appendix A

Partial transpositions in $2 \otimes 2 \otimes 2$

Write a general 8×8 matrix as a 4×4 matrix of 2×2 matrices:

$$X = \begin{pmatrix} A & B & C & D \\ E & F & G & H \\ I & J & K & L \\ M & N & O & P \end{pmatrix}. \quad (\text{A.1})$$

The partial transposition T_1 moves 4×4 submatrices,

$$X^{T_1} = \begin{pmatrix} A & B & I & J \\ E & F & M & N \\ C & D & K & L \\ G & H & O & P \end{pmatrix}. \quad (\text{A.2})$$

T_2 moves 2×2 submatrices within 4×4 submatrices,

$$X^{T_2} = \begin{pmatrix} A & E & C & G \\ B & F & D & H \\ I & M & K & O \\ J & N & L & P \end{pmatrix}. \quad (\text{A.3})$$

T_3 transposes the 2×2 submatrices,

$$X^{T_3} = \begin{pmatrix} A^T & B^T & C^T & D^T \\ E^T & F^T & G^T & H^T \\ I^T & J^T & K^T & L^T \\ M^T & N^T & O^T & P^T \end{pmatrix}. \quad (\text{A.4})$$

Appendix B

$\text{SL}(2, \mathbb{C})$, Lorentz transformations, and Lorentz invariants

Let ϵ be the two dimensional Levi-Civita symbol,

$$\epsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (\text{B.1})$$

It is a square root of -1 , $\epsilon^2 = -1$. The Lie group $\text{SL}(2, \mathbb{C})$ consists of all 2×2 complex matrices with unit determinant. If $V \in \text{SL}(2, \mathbb{C})$,

$$V = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad (\text{B.2})$$

then

$$V^{-1} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = -\epsilon V^T \epsilon. \quad (\text{B.3})$$

Thus $V\epsilon V^T = \epsilon$, in this sense ϵ is an invariant tensor under $\text{SL}(2, \mathbb{C})$ transformations.

A general 2×2 Hermitian matrix may be written as

$$X = \begin{pmatrix} x^0 + x^3 & x^1 - ix^2 \\ x^1 + ix^2 & x^0 - x^3 \end{pmatrix} = x^\mu \sigma_\mu, \quad (\text{B.4})$$

where x^μ is a real fourvector, $\sigma_0 = \mathbb{1}$ is the unit matrix, and σ_j for $j = 1, 2, 3$ are the Pauli matrices. The determinant of X is

$$\det(X) = -\frac{1}{2} \text{Tr}(X^T \epsilon X \epsilon) = g_{\mu\nu} x^\mu x^\nu, \quad (\text{B.5})$$

where $g_{\mu\nu}$ is the metric tensor,

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (\text{B.6})$$

More generally, for $X = x^\mu \sigma_\mu$ and $Y = y^\mu \sigma_\mu$ we have

$$\text{Tr}(X^T \epsilon Y \epsilon) = -2g_{\mu\nu} x^\mu y^\nu = -2x^\mu y_\mu. \quad (\text{B.7})$$

The transformation $X \mapsto \tilde{X} = VXV^\dagger$ with $\det V = 1$ is a continuous Lorentz transformation. It leaves the determinant invariant, and leaves the scalar product between two fourvectors invariant because $\det V^T = \det V^\dagger = 1$, hence $V^T \epsilon V = V^\dagger \epsilon V^* = \epsilon$ and

$$\text{Tr}(\tilde{X}^T \epsilon \tilde{Y} \epsilon) = \text{Tr}(X^T (V^T \epsilon V) Y (V^\dagger \epsilon V^*)) = \text{Tr}(X^T \epsilon Y \epsilon). \quad (\text{B.8})$$

The parity inversion $\tilde{x}^2 = -x^2$ takes the form $\tilde{X} = X^T$ and leaves the scalar product invariant, although it is not of the form $\tilde{X} = VXV^\dagger$.

In $\mathbb{C}^8 = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ the antisymmetric tensor

$$E = \epsilon \otimes \epsilon \otimes \epsilon = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{B.9})$$

is invariant under $\text{SL} \otimes \text{SL} \otimes \text{SL}$ transformations, in the sense that $VEV^T = E$ when $V = V_1 \otimes V_2 \otimes V_3$ and $V_1, V_2, V_3 \in \text{SL}(2, \mathbb{C})$.

A general 8×8 Hermitian matrix may be written as

$$A = a^{\lambda\mu\nu} \sigma_\lambda \otimes \sigma_\mu \otimes \sigma_\nu \quad (\text{B.10})$$

with $4 \times 4 \times 4 = 64$ real coefficients

$$a^{\mu\nu\lambda} = \frac{1}{8} \text{Tr}(A(\sigma_\mu \otimes \sigma_\nu \otimes \sigma_\lambda)). \quad (\text{B.11})$$

A product transformation of the form $\tilde{A} = VAV^\dagger$ with $V = V_1 \otimes V_2 \otimes V_3$, as above, acts as three independent continuous Lorentz transformations on the three Lorentz indices. Note that the partial transpositions are discrete Lorentz transformations, since they are parity inversions.

For Hermitian matrices A, B the quantity

$$\text{Tr}(A^T E B E) = -8g_{\lambda\alpha}g_{\mu\beta}g_{\nu\gamma}a^{\lambda\mu\nu}b^{\alpha\beta\gamma} = -8a^{\lambda\mu\nu}b_{\lambda\mu\nu} \quad (\text{B.12})$$

is real and invariant under the product transformations $\tilde{A} = V A V^\dagger$, $\tilde{B} = V B V^\dagger$. It is also invariant under all three partial transpositions. Note that each Lorentz index on a tensor $a^{\lambda\mu\nu}$ represents its own subsystem and can therefore only be contracted against the corresponding index on the tensor $b^{\lambda\mu\nu}$.

A density matrix ρ in dimension $2 \times 2 \times 2$ has one quadratic Lorentz invariant

$$I_2 = \rho^{\mu\nu\lambda}\rho_{\mu\nu\lambda} = -\frac{1}{8} \text{Tr}(\rho^T E \rho E) \geq 0. \quad (\text{B.13})$$

For pure states $\rho_i = \psi_i \psi_i^\dagger$ we have that

$$\text{Tr}(\rho_i^T E \rho_j E) = [\psi_i^T E \psi_j][\psi_j^\dagger E \psi_i^*] = -[\psi_i^T E \psi_j][\psi_i^\dagger E \psi_j^*] = -|\psi_i^T E \psi_j|^2. \quad (\text{B.14})$$

The inequality $I_2 \geq 0$ follows because ρ is always a convex combination of pure states,

$$\rho = \sum_i \lambda_i \psi_i \psi_i^\dagger \quad \text{with} \quad \lambda_i > 0, \quad \sum_i \lambda_i = 1, \quad (\text{B.15})$$

and hence

$$\text{Tr}(\rho^T E \rho E) = -\sum_{i,j} \lambda_i \lambda_j |\psi_i^T E \psi_j|^2 \leq 0. \quad (\text{B.16})$$

There are five different fourth order invariants obtained by different combinations of index contractions, but one of these is simply the square of the second order invariant. The four new invariants can be written as

$$\begin{aligned} I_{41} &= \rho^{\mu\nu\lambda} \rho_{\mu\nu\gamma} \rho^{\alpha\beta\gamma} \rho_{\alpha\beta\lambda}, \\ I_{42} &= \rho^{\mu\nu\lambda} \rho_{\mu\beta\lambda} \rho^{\alpha\beta\gamma} \rho_{\alpha\nu\gamma}, \\ I_{43} &= \rho^{\mu\nu\lambda} \rho_{\mu\beta\gamma} \rho^{\alpha\beta\gamma} \rho_{\alpha\nu\lambda}, \\ I_{44} &= \rho^{\mu\nu\lambda} \rho_{\mu}^{\beta\gamma} \rho_{\nu\gamma}^{\alpha} \rho_{\alpha\beta\lambda}. \end{aligned} \quad (\text{B.17})$$

Note that all these Lorentz invariants are invariant under $\text{SL} \otimes \text{SL} \otimes \text{SL}$ transformations of a density matrix without subsequent normalization to unit trace. Division of the fourth order invariants by the square of the second order invariant gives true invariants that are also independent of the normalization of the density matrix. They may be used in order to test whether two density matrices belong to the same $\text{SL} \otimes \text{SL} \otimes \text{SL}$ equivalence class.

An alternative way to represent Lorentz transformation is by $\text{SL}(2, \mathbb{C})$ matrices acting on a matrix with the form,

$$X = \begin{pmatrix} y + ix & i(z - t) \\ i(z + t) & y - ix \end{pmatrix} \quad (\text{B.18})$$

as

$$X \mapsto \tilde{X}VXV^{(-1)*} \quad (\text{B.19})$$

It also leaves the determinant invariant and the scalar product between fourvectors invariant, since $\det V^{(-1)*} = 1$

$$\text{Tr}(\tilde{X}^T \epsilon \tilde{Y} \epsilon) = \text{Tr}(X^T (V^T \epsilon V) Y (V^{-1*} \epsilon (V^{-1*})^T)) = \text{Tr}(X^T \epsilon Y^T \epsilon) \quad (\text{B.20})$$

B.1 The Generators

$$S_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (\text{B.21})$$

$$S_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad (\text{B.22})$$

$$S_3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{B.23})$$

$$K_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{B.24})$$

$$K_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{B.25})$$

$$K_3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad (\text{B.26})$$

Appendix C

Standard forms of sets of vectors

Given four vectors $x_i \in \mathbb{C}^2$, $i = 1, 2, 3, 4$. We write

$$x = (x_1, x_2, x_3, x_4) = \begin{pmatrix} a & c & e & g \\ b & d & f & h \end{pmatrix}. \quad (\text{C.1})$$

We consider here the generic case with $\det(x_i, x_j) \neq 0$ for $i \neq j$. Multiplication by the matrix

$$U = \begin{pmatrix} d & -c \\ -b & a \end{pmatrix} \quad (\text{C.2})$$

and a subsequent normalization of the vectors gives the form

$$y = \begin{pmatrix} 1 & 0 & 1 & t_2 \\ 0 & 1 & t_1 & 1 \end{pmatrix}, \quad (\text{C.3})$$

with $\det(y_i, y_j) \neq 0$ for $i \neq j$, which means that $t_1 t_2 \neq 0, 1$. Multiplication by

$$V = \begin{pmatrix} -t_1 & 0 \\ 0 & 1 \end{pmatrix} \quad (\text{C.4})$$

and normalization now gives the standard form

$$z = \begin{pmatrix} 1 & 0 & 1 & t \\ 0 & 1 & -1 & 1 \end{pmatrix}, \quad (\text{C.5})$$

with one variable parameter $t = -t_1 t_2 \neq 0, -1$. Since

$$t = -\frac{\det(z_1, z_3) \det(z_2, z_4)}{\det(z_1, z_4) \det(z_2, z_3)}, \quad (\text{C.6})$$

and this ratio of determinants is invariant under nonsingular linear transformations and vector normalizations, we have that

$$t = -\frac{\det(x_1, x_3) \det(x_2, x_4)}{\det(x_1, x_4) \det(x_2, x_3)} = -\frac{(af - be)(ch - dg)}{(ah - bg)(cf - de)}. \quad (\text{C.7})$$

We see that t will be complex in the generic case. In the special case where t is real and positive, we may multiply by

$$W = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{t} \end{pmatrix} \quad (\text{C.8})$$

and normalize so as to obtain the standard form

$$w = \begin{pmatrix} 1 & 0 & 1 & \sqrt{t} \\ 0 & 1 & -\sqrt{t} & 1 \end{pmatrix}, \quad (\text{C.9})$$

where the vectors are real and pairwise orthogonal, $w_i^\dagger w_j = w_i^T w_j = 0$ for $i, j = 1, 2$ and $i, j = 3, 4$.

Instead of equation (C.5) we might have chosen one of two alternative standard forms,

$$z' = \begin{pmatrix} 1 & 1 & 0 & t' \\ 0 & -1 & 1 & 1 \end{pmatrix}, \quad (\text{C.10})$$

or

$$z'' = \begin{pmatrix} 1 & 1 & t'' & 0 \\ 0 & -1 & 1 & 1 \end{pmatrix}. \quad (\text{C.11})$$

The invariant formula for t , equation (C.5), gives that

$$t = -1 - t', \quad t = -\frac{1}{1 + t''}, \quad (\text{C.12})$$

or inversely,

$$t' = -1 - t, \quad t'' = -1 - \frac{1}{t}. \quad (\text{C.13})$$

In the case where t is real we see that $t > 0$ gives $t' < 0$, $t'' < 0$, whereas $-1 < t < 0$ gives $t' < 0$, $t'' > 0$, and $t < -1$ gives $t' > 0$, $t'' < 0$. Thus, if t is real and $t \neq 0, -1$, there is always exactly one pairing of the four vectors, either $(x_1 x_2)(x_3 x_4)$, $(x_1 x_3)(x_2 x_4)$, or $(x_1 x_4)(x_2 x_3)$, such that there exists a linear transformation which will make both pairs real and orthogonal.

Appendix D

A problem of finding product vectors in a subspace

Given four vectors $\psi_j \in \mathbb{C}^8$ with components ψ_{ij} , $i = 1, \dots, 8$, $j = 1, \dots, 4$. We write a linear combination of them as a matrix product,

$$\phi = \sum_{j=1}^4 \alpha_j \psi_j = \psi \alpha \quad (\text{D.1})$$

with $\alpha \in \mathbb{C}^4$. Assume that ϕ is a tensor product

$$\phi = \begin{pmatrix} a \\ b \end{pmatrix} \otimes \begin{pmatrix} c \\ d \end{pmatrix} \otimes \begin{pmatrix} e \\ f \end{pmatrix} = \begin{pmatrix} ace \\ acf \\ ade \\ adf \\ bce \\ bcf \\ bde \\ bdf \end{pmatrix}. \quad (\text{D.2})$$

The presence of the first factor in the tensor product implies the equation

$$(A - \mu B)\alpha = 0, \quad (\text{D.3})$$

where $\mu = a/b$, and A and B are the following 4×4 matrices,

$$A = \begin{pmatrix} \psi_{11} & \psi_{12} & \psi_{13} & \psi_{14} \\ \psi_{21} & \psi_{22} & \psi_{23} & \psi_{24} \\ \psi_{31} & \psi_{32} & \psi_{33} & \psi_{34} \\ \psi_{41} & \psi_{42} & \psi_{43} & \psi_{44} \end{pmatrix}, \quad B = \begin{pmatrix} \psi_{51} & \psi_{52} & \psi_{53} & \psi_{54} \\ \psi_{61} & \psi_{62} & \psi_{63} & \psi_{64} \\ \psi_{71} & \psi_{72} & \psi_{73} & \psi_{74} \\ \psi_{81} & \psi_{82} & \psi_{83} & \psi_{84} \end{pmatrix}. \quad (\text{D.4})$$

The presence of the second factor implies the equation

$$(C - \mu D)\alpha = 0, \quad (\text{D.5})$$

where $\mu = c/d$, and where

$$C = \begin{pmatrix} \psi_{11} & \psi_{12} & \psi_{13} & \psi_{14} \\ \psi_{21} & \psi_{22} & \psi_{23} & \psi_{24} \\ \psi_{51} & \psi_{52} & \psi_{53} & \psi_{54} \\ \psi_{61} & \psi_{62} & \psi_{63} & \psi_{64} \end{pmatrix}, \quad D = \begin{pmatrix} \psi_{31} & \psi_{32} & \psi_{33} & \psi_{34} \\ \psi_{41} & \psi_{42} & \psi_{43} & \psi_{44} \\ \psi_{71} & \psi_{72} & \psi_{73} & \psi_{74} \\ \psi_{81} & \psi_{82} & \psi_{83} & \psi_{84} \end{pmatrix}. \quad (\text{D.6})$$

The presence of the third factor implies the equation

$$(E - \mu F)\alpha = 0, \quad (\text{D.7})$$

where $\mu = e/f$, and where

$$E = \begin{pmatrix} \psi_{11} & \psi_{12} & \psi_{13} & \psi_{14} \\ \psi_{31} & \psi_{32} & \psi_{33} & \psi_{34} \\ \psi_{51} & \psi_{52} & \psi_{53} & \psi_{54} \\ \psi_{71} & \psi_{72} & \psi_{73} & \psi_{74} \end{pmatrix}, \quad F = \begin{pmatrix} \psi_{21} & \psi_{22} & \psi_{23} & \psi_{24} \\ \psi_{41} & \psi_{42} & \psi_{43} & \psi_{44} \\ \psi_{61} & \psi_{62} & \psi_{63} & \psi_{64} \\ \psi_{81} & \psi_{82} & \psi_{83} & \psi_{84} \end{pmatrix}. \quad (\text{D.8})$$

Equation (D.3) is a generalized eigenvalue equation, having in the generic case four different complex eigenvalues μ_i with corresponding eigenvectors α_i , defining four vectors that are product vectors in dimension 2×4 of the form

$$\phi_i = \psi\alpha_i = x_i \otimes u_i \quad \text{with} \quad x_i = \begin{pmatrix} \mu_i \\ 1 \end{pmatrix}, \quad u_i = B\alpha_i. \quad (\text{D.9})$$

Similarly, equation (D.5) gives four eigenvalues μ_i with corresponding eigenvectors α_i , defining four vectors that are product vectors when we use the split tensor product defined in Appendix E,

$$\phi_i = \psi\alpha_i = y_i \otimes_s v_i \quad \text{with} \quad y_i = \begin{pmatrix} \mu_i \\ 1 \end{pmatrix}, \quad v_i = D\alpha_i. \quad (\text{D.10})$$

Finally, equation (D.7) gives four eigenvalues μ_i with corresponding eigenvectors α_i , defining four vectors that are product vectors in dimension 4×2 ,

$$\phi_i = \psi\alpha_i = w_i \otimes z_i \quad \text{with} \quad z_i = \begin{pmatrix} \mu_i \\ 1 \end{pmatrix}, \quad w_i = F\alpha_i. \quad (\text{D.11})$$

If the two equations (D.3) and (D.7) have a common eigenvector α , then $\phi = \psi\alpha$ is a product vector in two ways, both in dimension 2×4 and in 4×2 . This means that it is a product vector in dimension $2 \times 2 \times 2$, and the same α is an eigenvector of equation (D.5).

Note that the standard method for solving the generalized eigenvalue equations (D.3), (D.5), and (D.7) depends on the non singularity of the matrices B , D , and F . If one or more of these matrices are singular, we may usually avoid the problem simply by making a random product transformation $\psi \mapsto \tilde{\psi} = V\psi$ with $V = V_1 \otimes V_2 \otimes V_3$, then solving the problem with $\tilde{\psi}$ instead of ψ and transforming back in the end.

Appendix E

The split tensor product

We find it useful to define a split tensor product so as to be able to take out the middle factor in a tensor product of three factors. Thus we define

$$x \otimes y \otimes z = y \otimes_s (x \otimes z) . \tag{E.1}$$

For $y = (c, d)^T \in \mathbb{C}^2$ and $v = (p, q, r, s)^T \in \mathbb{C}^4 = \mathbb{C}^2 \otimes \mathbb{C}^2$ we define

$$y \otimes_s v = \begin{pmatrix} cp \\ cq \\ dp \\ dq \\ cr \\ cs \\ dr \\ ds \end{pmatrix} . \tag{E.2}$$

This corresponds to equation (D.2) with $p = ae$, $q = af$, $r = be$, $s = bf$.

Appendix F

Linear combinations of product vectors

We have six product vectors in a generic rank five subspace. We may transform five them to a standard form

$$v_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad v_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad v_3 = \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \\ -1 \\ 1 \\ 1 \\ -1 \end{pmatrix}, \quad v_4 = \begin{pmatrix} r_1 s_1 t_1 \\ r_1 s_1 \\ r_1 t_1 \\ r_1 \\ s_1 t_1 \\ s_1 \\ t_1 \\ 1 \end{pmatrix}, \quad v_5 = \begin{pmatrix} r_2 s_2 t_2 \\ r_2 s_2 \\ r_2 t_2 \\ r_2 \\ s_2 t_2 \\ s_2 \\ t_2 \\ 1 \end{pmatrix} \quad (\text{F.1})$$

and they will in general span the subspace. I.e. an arbitrary vector v in the subspace can be written as

$$v = \alpha v_1 + \beta v_2 + \gamma v_3 + \delta v_4 + v_5 \quad (\text{F.2})$$

up to some normalisation. For v to be a 2×4 product vector it must fulfil the following equations:

$$\frac{v(1)}{v(5)} = \frac{v(2)}{v(6)} = \frac{v(3)}{v(7)} = \frac{v(4)}{v(8)} \quad (\text{F.3})$$

where $v(i)$ is the i th component of the vector. We may solve these equations for α, β and γ .

$$\alpha = \frac{\delta(r_1 - r_2)(s_1(t_1 + 1)t_2 - s_2(t_1(s_1 + t_2 + 1) - s_1 t_2))}{\delta(s_1 - t_1) + s_2 - t_2} \quad (\text{F.4})$$

$$\beta = \frac{\delta(r_1 - r_2)(-s_1(t_2 + 1) + s_2 t_1 + s_2 + t_1 - t_2)}{\delta r_1(s_1 - t_1) + r_2(s_2 - t_2)} \quad (\text{F.5})$$

$$\gamma = -\frac{\delta(r_1 - r_2)(s_2 t_1 - s_1 t_2)}{-\delta(r_1 + 1)(s_1 - t_1) - (r_2 + 1)s_2 + (r_2 + 1)t_2} \quad (\text{F.6})$$

which gives an analytical expression for the 2×4 product vectors in the subspace.

Appendix G

MATLAB code

Matlab code for the various algorithms discussed in the preceding sections is provided.

G.1 Symmetric forms

G.1.1 Type I

Matlab implementation of algorithm in Section 4.3.1

```
function [transform] = typelSymmetricTransform(rho0, n)
% TYPE1SYMMETRICTRANSFORM, function that finds the
% transformation of rho to symmetric form.
% Input:
% - rho0
% - n, which partial transposition rho0 is invariant
  under

% Partial transposition as 2-by-2 transpositions
if n == 1
    kk = 0;
    for jj = 1:4
        for ii = 1:4
            kk = kk+1;
            AAA{kk} = [rho0(ii, jj), rho0(ii, jj+4);
                      rho0(ii+4, jj), rho0(ii+4, jj+4)];
        end
    end
elseif n == 2
```

```

kk = 0;
for jj = [1,2,5,6]
    for ii = [1,2,5,6]
        kk = kk+1;
        AAA{kk} = [rho0(ii,jj),rho0(ii,jj+2);
                  rho0(ii+2,jj),rho0(ii+2,jj+2)];
    end
end
elseif n == 3
    kk = 0;
    for jj = 1:2:7
        for ii = 1:2:7
            kk = kk+1;
            AAA{kk} = [rho0(ii,jj),rho0(ii,jj+1);
                      rho0(ii+1,jj),rho0(ii+1,jj+1)];
        end
    end
end
end

AAAv = zeros(4,32);
ll = 0;
for kk = 1:16
    BBB = AAA{kk}' + AAA{kk};
    CCC = i*(AAA{kk}' - AAA{kk});
    ll = ll+1;
    AAAv(1,ll) = BBB(1,1)+BBB(2,2);
    AAAv(2,ll) = BBB(1,2)+BBB(2,1);
    AAAv(3,ll) = i*(BBB(1,2)-BBB(2,1));
    AAAv(4,ll) = BBB(1,1)-BBB(2,2);
    ll = ll+1;
    AAAv(1,ll) = CCC(1,1)+CCC(2,2);
    AAAv(2,ll) = CCC(1,2)+CCC(2,1);
    AAAv(3,ll) = i*(CCC(1,2)-CCC(2,1));
    AAAv(4,ll) = CCC(1,1)-CCC(2,2);
end
svd(AAAv)

% Find the orthogonal vector
gmat = diag([1,-1,-1,-1]);
gAAAv = gmat*AAAv;

[eve,evam] = eig(gAAAv*gAAAv');

ortV4 = eve(:,1);
ortV3 = ortV4(2:4);

```



```

ortV3 = ortV3/sqrt(ortV3'*ortV3);

% t*s0+x*s1+y*s2+z*s3
AAAort = [ortV4(1)+ortV4(4), ortV4(2)-i*ortV4(3);
          ortV4(2)+i*ortV4(3),ortV4(1)-ortV4(4)];

rotAx = [-ortV3(3);0;ortV3(1)];

rotAng = atan2(sqrt(rotAx'*rotAx),ortV3(2))

rotAx = rotAx/sqrt(rotAx'*rotAx);

cos1 = cos(rotAng/2);
sin1 = sin(rotAng/2);xs

% Rotation to make spatial coordinates propto e_y
rotMat = cos1*eye(2)-i*sin1*[rotAx(3),rotAx(1);rotAx(1),-
    rotAx(3)];

AAAort1 = rotMat*AAAort*rotMat'

xx = real(AAAort1(1,1))
yy = -imag(AAAort1(1,2))
bb = 0.0;
for ii = 1:20000
    bb = 0.5*(1+bb^2)*xx/yy;
end

% Boost to get rid of time coordinate
boostMat = [1,i*bb;-i*bb,1];

totTrans = boostMat*rotMat;

transform = totTrans;
end

```

G.1.2 Type III

Matlab implementation of algorithm in Section 4.3.2

```

function [transform] = type3symmetricTransform(U)
    % TYPE3SYMMETRICTRANSFORM, Transforms U to the identity
    % Input: U

    t = 0.5*imag(U(1,2)-U(2,1));

```

```

x = 0.5*imag(U(1,1)-U(2,2));
y = 0.5*real(U(1,1)+U(2,2));
z = 0.5*imag(U(2,1)+U(1,2));

salfa = sqrt((x^2+z^2)/(x^2+y^2+z^2));
calfa = y/sqrt(x^2+y^2+z^2);
alfa = atan2(salfa,calfa);

nx = -z/sqrt(x^2+z^2);
nz = x/sqrt(x^2+z^2);

rotMat = cos(0.5*alfa)*eye(2) + i*sin(0.5*alfa)*[-nz,nx;
  nx,nz];

% Rotation to get rid of x and z components
Urot = rotMat*U*conj(rotMat^-1);

yy = 0.5*real(Urot(1,1)+Urot(2,2));
tt = 0.5*imag(Urot(1,2)-Urot(2,1));
bb = 0.0;
aa = 1.0;
for ii = 1:20000
  bb = -0.5*((1+bb^2)*tt)/yy;
end

% Boost to get rid of y component
boostMat = (eye(2)+bb*[0,i;-i,0])/sqrt(1+bb^2)

transform = boostMat*rotMat;
end %end function

```

G.2 4th order Runge Kutta

```

function [rhoNew] = RK4(rho0,direction,h,dims)
% RK4 4th order Runge Kutta step that preserves
% img(rho0) & the rank of its partial transposes
% h - step length
% direction - "direction" along the image preserving
% surface
% dims - #directions that preserves img(rho0) and rank(
% rho^(Ti))

dims = 65-dims;

```

```

% (P+R+R+R)x=1x
[evePRRR,evaPRRR] = PRRRc(rho0);

% Directions with (P+R+R+R)x=4x
surface = evePRRR(:,dims:64);

% Projection of direction unto the surface
Acoeff = direction'*surface;
A = surface*Acoeff';
Am = rvec2hmat(A,8);
Am = Am - trace(Am)*rho0;
k1 = Am;

%----k2----
[evePRRR,evaPRRR] = PRRRc(rho0 + h*k1/2);

surface = evePRRR(:,dims:64);

Acoeff = direction'*surface;
A = surface*Acoeff';
Am = rvec2hmat(A,8);
Am = Am - trace(Am)*rho0;
k2 = Am;

%----k3----
[evePRRR,evaPRRR] = PRRRc(rho0 + h*k2/2);

surface = evePRRR(:,dims:64);

Acoeff = direction'*surface;
A = surface*Acoeff';
Am = rvec2hmat(A,8);
Am = Am - trace(Am)*rho0;
k3 = Am;

%----k4----
[evePRRR,evaPRRR] = PRRRc(rho0 + h*k3);

surface = evePRRR(:,dims:64);

Acoeff = direction'*surface;
A = surface*Acoeff';
Am = rvec2hmat(A,8);
Am = Am - trace(Am)*rho0;
k4 = Am;

```

```

rhoNew = stateNorm(rho0 + (h/6)*(k1+2*k2+2*k3+k4));
end

```

G.3 Simulated annealing

This is our implementation of the algorithm described in Section 6.1.

Example objective function

```

function OUT = minf(x)
    % MINF, target function for finding rank5555 states
    % Input:
    % x: 50 real variables
    % (global)zzz05: 5 product vectors in img(rho)
    % (global)volMat: matrix for comp. volume of simpl+rho
    % (global)rvec16: product vectors as real 64 vector
    global zzz05 volMat rvec16;

    AA = zzz05*(reshape(x(1:25),5,5)+1i*reshape(x(26:50)
        ,5,5));
    rho0 = AA*AA';
    rho0 = rho0+rho0';
    rho0 = rho0/trace(rho0);
    ss = 0.0;
    rho1 = dt38(rho0,1);
    eval = eig(rho1);
    eval = sort(real(eval));
    % ss += square sum of three lowest eigenvalues of rho1
    ss = ss+eval(1:3)'*eval(1:3);
    rho2 = dt38(rho0,2);
    eva2 = eig(rho2);
    eva2 = sort(real(eva2));
    % ss += square sum of three lowest eigenvalues of rho2
    ss = ss+eva2(1:3)'*eva2(1:3);
    rho3 = dt38(rho0,3);
    eva3 = eig(rho3);
    eva3 = sort(real(eva3));
    % ss += square sum of three lowest eigenvalues of rho3
    ss = ss+eva3(1:3)'*eva3(1:3);
    % Repulsive potential to get away from separable states
    rho0v = hmat2rvec8(rho0);
    for ii = 2:7

```

```

    rdiff = rho0v - rvec16(:,ii-1);
    volMat(8,ii) = rdiff'*rdiff;
    volMat(ii,8) = volMat(8,ii);
end
vv = abs(det(volMat));
ss = ss/(vv)^2;

OUT = ss;
end%end function

```

Simulated annealing implementation

```

function [yflu,p,y,psum,yhi] = amotsa(p,y,psum,ihi,yhi,tt,
    fac)
    % Extrapolates by a factor fac through the face of the
    % simplex
    % across from the high point, tries it, and replaces
    % the high point if the new point is better
    global yb pb;
    %
    ndim = length(p(:,1));
    fac1 = (1.0-fac)/ndim;
    fac2 = fac1 - fac;
    ptry = psum*fac1-p(:,ihi)*fac2;
    ytry = minf(ptry);
    if ytry <= yb % Save the best-ever
        pb = ptry;
        yb = ytry;
    end
    yflu = ytry-tt*log(rand(1)); % NOTE: subtract
    if yflu < yhi

        y(ihi) = ytry;
        yhi = yflu;
        psum = psum + ptry - p(:,ihi);
        p(:,ihi) = ptry;
    end
end

end %function

function [p] = anneal(iter, T, p)
%ANNEAL, function for simulated annealing.
% Input:
% - iter: number of iterations
% - T:    temperature
% - p:    simplex

```

```

ndim = length(p(:,1));
tt = -T;

psum = sum(p,2);
y = zeros(length(p(1,:)),1);
for ii = 1:length(p(1,:))
    y(ii) = minf(p(:,ii));
end

while true
    yt = y + tt*log(rand(size(y))); % Give a thermal
        fluctuation

    [ySort, indSort] = sort(yt);
    yhi = ySort(end);
    ihi = indSort(end);
    ynhi = ySort(end-1);
    ylo = ySort(1);
    ilo = indSort(1);

    if iter < 0
        % If returning put the best guess in slot 1
        ybest = y(ilo);
        y(ilo) = y(1);
        y(1) = ybest;
        pbest = p(:,ilo);
        p(:,ilo) = p(:,1);
        p(:,1) = pbest;

        conv = false;
        return;
    end

    iter = iter - 2;

    % Begin a new iteration.
    % First extrapolate by a factor -1 through the
    % face of the simplex across from the high point, i.e
    % '
    % reflect the simplex from the high point.

    [ytry,p,y,psum,yhi] = amotsa(p,y,psum,ihi,yhi,tt,-1.0)
    ;
    if ytry <= ylo
        % Gives a result better than the best point,

```

```

        % so try an additional extrapolation by a factor
        % of 2.
        [ytry,p,y,psum,yhi] = amotsa(p,y,psum,ihi,yhi,tt
        ,2.0);
elseif ytry >= ynhi
        % The reflected point is worse than the second-
        % highest,
        % so look for an intermediate lower point, i.e.,
        % do a one-dimensional contraction.
        ysave = yhi;

        [ytry,p,y,psum,yhi] = amotsa(p,y,psum,ihi,yhi,tt
        ,0.5);
if ytry >= ysave
        % Can't seem to get rid of the high point.
        % Better contract around the lowest (best)
        % point.
        for ii = 1:length(p(1,:))
            if ii ~= ilo
                psum = 0.5*(p(:,ii)+p(:,ilo));
                p(:,ii) = psum;
                y(ii) = minf(psum);
            end
        end
        iter = iter - ndim;
        psum = sum(p,2);
    end
else
        iter = iter + 1;
end
end

```


Bibliography

- John S Bell et al. On the einstein-podolsky-rosen paradox. *Physics*, 1(3):195–200, 1964.
- Charles H. Bennett, David P. DiVincenzo, Tal Mor, Peter W. Shor, John A. Smolin, and Barbara M. Terhal. Unextendible product bases and bound entanglement. *Phys. Rev. Lett.*, 82:5385–5388, Jun 1999. doi: 10.1103/PhysRevLett.82.5385. URL <http://link.aps.org/doi/10.1103/PhysRevLett.82.5385>.
- Lin Chen and Yi-Xin Chen. Rank-three bipartite entangled states are distillable. *Phys. Rev. A*, 78:022318, Aug 2008. doi: 10.1103/PhysRevA.78.022318. URL <http://link.aps.org/doi/10.1103/PhysRevA.78.022318>.
- A. Einstein, B. Podolsky, and N. Rosen. Can quantum-mechanical description of physical reality be considered complete? *Phys. Rev.*, 47:777–780, May 1935. doi: 10.1103/PhysRev.47.777. URL <http://link.aps.org/doi/10.1103/PhysRev.47.777>.
- Øyvind S. Garberg. Positive partial transpose states in multipartite quantum systems. Master’s thesis, Norwegian University of Science and Technology, June 2012.
- Øyvind S. Garberg, Børge Irgens, and Jan Myrheim. Extremal states of positive partial transpose in a system of three qubits. *Phys. Rev. A*, 87:032302, Mar 2013. doi: 10.1103/PhysRevA.87.032302. URL <http://link.aps.org/doi/10.1103/PhysRevA.87.032302>.
- D. M. Greenberger, M. A. Horne, and A. Zeilinger. Going Beyond Bell’s Theorem. *ArXiv e-prints*, December 2007.
- Leif Ove Hansen, Andreas Hauge, Jan Myrheim, and Per Øyvind Sollid. Low-rank positive-partial-transpose states and their relation to product vectors. *Phys. Rev. A*, 85:022309, Feb 2012. doi: 10.1103/PhysRevA.85.022309. URL <http://link.aps.org/doi/10.1103/PhysRevA.85.022309>.
- Micha Horodecki, Pawe Horodecki, and Ryszard Horodecki. Separability of mixed states: necessary and sufficient conditions. *Physics Letters A*, 223(12):

- 1 – 8, 1996. ISSN 0375-9601. doi: [http://dx.doi.org/10.1016/S0375-9601\(96\)00706-2](http://dx.doi.org/10.1016/S0375-9601(96)00706-2). URL <http://www.sciencedirect.com/science/article/pii/S0375960196007062>.
- Pawel Horodecki, John A Smolin, Barbara M Terhal, and Ashish V Thapliyal. Rank two bipartite bound entangled states do not exist. *Theoretical Computer Science*, 292(3):589 – 596, 2003. ISSN 0304-3975. doi: [http://dx.doi.org/10.1016/S0304-3975\(01\)00376-0](http://dx.doi.org/10.1016/S0304-3975(01)00376-0). URL <http://www.sciencedirect.com/science/article/pii/S0304397501003760>. jce:title;Algorithms in Quantum Information Prcoessing;ce:title;.
- Siniša Karnas and Maciej Lewenstein. Separability and entanglement in $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^N$ composite quantum systems. *Phys. Rev. A*, 64:042313, Sep 2001. doi: 10.1103/PhysRevA.64.042313. URL <http://link.aps.org/doi/10.1103/PhysRevA.64.042313>.
- B. Kraus, J. I. Cirac, S. Karnas, and M. Lewenstein. Separability in $2 \times n$ composite quantum systems. *Phys. Rev. A*, 61:062302, May 2000. doi: 10.1103/PhysRevA.61.062302. URL <http://link.aps.org/doi/10.1103/PhysRevA.61.062302>.
- J. M. Leinaas, J. Myrheim, and E. Ovrum. Extreme points of the set of density matrices with positive partial transpose. *Phys. Rev. A*, 76:034304, Sep 2007. doi: 10.1103/PhysRevA.76.034304. URL <http://link.aps.org/doi/10.1103/PhysRevA.76.034304>.
- Jon Magne Leinaas, Jan Myrheim, and Eirik Ovrum. Geometrical aspects of entanglement. *Phys. Rev. A*, 74:012313, Jul 2006. doi: 10.1103/PhysRevA.74.012313. URL <http://link.aps.org/doi/10.1103/PhysRevA.74.012313>.
- Jon Magne Leinaas, Jan Myrheim, and Per Øyvind Sollid. Low-rank extremal positive-partial-transpose states and unextendible product bases. *Phys. Rev. A*, 81:062330, Jun 2010a. doi: 10.1103/PhysRevA.81.062330. URL <http://link.aps.org/doi/10.1103/PhysRevA.81.062330>.
- Jon Magne Leinaas, Jan Myrheim, and Per Øyvind Sollid. Numerical studies of entangled positive-partial-transpose states in composite quantum systems. *Phys. Rev. A*, 81:062329, Jun 2010b. doi: 10.1103/PhysRevA.81.062329. URL <http://link.aps.org/doi/10.1103/PhysRevA.81.062329>.
- N. David Mermin. What’s wrong with these elements of reality? *Print edition*, 43 (6), 1990.
- Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information (Cambridge Series on Information and the Natural Sciences)*. Cambridge University Press, 1 edition, January 2004. ISBN 0521635039. URL <http://www.amazon.com/exec/obidos/redirect?tag=citeulike07-20&path=ASIN/0521635039>.

- Jian-Wei Pan, Dik Bouwmeester, Matthew Daniell, Harald Weinfurter, and Anton Zeilinger. Experimental test of quantum nonlocality in three-photon greenberger-horne-zeilinger entanglement. *Nature*, 403(6769):515–519, Feb 2000. ISSN 0028-0836. doi: 10.1038/35000514. URL <http://dx.doi.org/10.1038/35000514>.
- Asher Peres. Separability criterion for density matrices. *Phys. Rev. Lett.*, 77:1413–1415, Aug 1996. doi: 10.1103/PhysRevLett.77.1413. URL <http://link.aps.org/doi/10.1103/PhysRevLett.77.1413>.
- William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery. *Numerical Recipes 3rd Edition: The Art of Scientific Computing*. Cambridge University Press, New York, NY, USA, 3 edition, 2007. ISBN 0521880688, 9780521880688.
- E. Schrödinger. Die gegenwärtige Situation in der Quantenmechanik. *Naturwissenschaften*, 23:807–812, November 1935. doi: 10.1007/BF01491891.
- Per Øyvind Sollid, Jon Magne Leinaas, and Jan Myrheim. Unextendible product bases and extremal density matrices with positive partial transpose. *Phys. Rev. A*, 84:042325, Oct 2011. doi: 10.1103/PhysRevA.84.042325. URL <http://link.aps.org/doi/10.1103/PhysRevA.84.042325>.