IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

State space structure and entanglement of rotationally invariant spin systems

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2005 J. Phys. A: Math. Gen. 38 9019

(http://iopscience.iop.org/0305-4470/38/41/013)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.94
The article was downloaded on 03/06/2010 at 04:00

Please note that terms and conditions apply.

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) 9019–9037 doi:10.1088/0305-4470/38/41/013

State space structure and entanglement of rotationally invariant spin systems

Heinz-Peter Breuer

Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

E-mail: breuer@physik.uni-freiburg.de

Received 29 June 2005, in final form 30 June 2005
Published 28 September 2005
Online at stacks.iop.org/JPhysA/38/9019

Abstract
We investigate the structure of $SO(3)$-invariant quantum systems which are composed of two particles with spins j_1 and j_2. The states of the composite spin system are represented by means of two complete sets of rotationally invariant operators, namely by the projections P_J onto the eigenspaces of the total angular momentum J, and by certain invariant operators Q_K which are built out of spherical tensor operators of rank K. It is shown that these representations are connected by an orthogonal matrix whose elements are expressible in terms of Wigner's 6-j symbols. The operation of the partial time reversal of the combined spin system is demonstrated to be diagonal in the Q_K-representation. These results are employed to obtain a complete characterization of spin systems with $j_1 = 1$ and arbitrary $j_2 \geqslant 1$. We prove that the Peres–Horodecki criterion of positive partial transposition (PPT) is necessary and sufficient for separability if j_2 is an integer, while for half-integer spins j_2 there always exist entangled PPT states (bound entanglement). We construct an optimal entanglement witness for the case of half-integer spins and design a protocol for the detection of entangled PPT states through measurements of the total angular momentum.

PACS numbers: 03.67.Mn, 03.65.Ud, 03.65.Yz

1. Introduction

Entanglement is a basic feature of composite quantum systems connected to the tensor product structure of the underlying Hilbert space of states. A mixed state of a bipartite quantum system described by some density matrix ρ is said to be entangled or inseparable if ρ cannot be written as a convex linear combination of product states. Otherwise it is called classically correlated or separable [1]. The properties of entangled states are responsible for many of the fascinating and curious aspects of the quantum world and lie at the core of many proposed applications in quantum information processing [2–4].

The general characterization and quantification of entanglement in mixed quantum states is a highly non-trivial problem. It is even very difficult, in general, to formulate simple operational criteria which allow a unique identification of all separable states of a given composite system. There do exist, however, many necessary separability criteria [5–13]. A simple and, in fact, very strong criterion is the Peres–Horodecki criterion [5, 6] which states that a necessary condition for a given density matrix ρ to be separable is that it has a positive partial transposition (PPT states). It is known that this criterion is necessary and sufficient for certain low-dimensional systems, while it is only necessary in higher dimensions [6].

The analysis of the entanglement structure is greatly facilitated through the introduction of symmetries, i.e., if one restricts oneself to those states of the composite system which are invariant under certain groups of symmetry transformations. Important examples in this context are the manifolds of the Werner states [1], of the isotropic states [7, 14] and of the orthogonal states [15]. Here, we investigate entanglement under the symmetry group $SO(3)$ of proper three-dimensional rotations of the coordinate axes. More precisely, we consider the problem of mixed state entanglement of systems which are composed of two particles with spins j_1 and j_2, and which are invariant under product representations of the group $SO(3)$ or, equivalently, of the covering group $SU(2)$. A basic tool of our analysis is the work of Vollbrecht and Werner [15] which provides a general scheme for the treatment of entanglement under given symmetry groups.

Mixed $SO(3)$-invariant states of composite systems arise, for example, from the interaction of open systems [16] with isotropic environments [17]. Their analysis is of great importance and leads to many applications. As examples we mention investigations on the connection between quantum phase transitions and the behaviour of entanglement measures (see, e.g., [18, 19]), the analysis of entanglement of $SU(2)$-invariant multiphoton states generated by the parametric down-conversion [20], and studies of the entanglement of formation [21]. The technique of this paper could also be relevant for the characterization of quantum correlations in Fermionic or Bosonic systems developed recently [22, 23].

The Hilbert space of a system which is composed of two particles with spins j_1 and j_2 is given by the tensor product $\mathbb{C}^{N_1} \otimes \mathbb{C}^{N_2}$, where $N_1 = 2j_1 + 1$ and $N_2 = 2j_2 + 1$ are the dimensions of the local spin spaces. We call such a system an $N_1 \otimes N_2$ system. Throughout the paper we will assume that $j_1 \leqslant j_2$, i.e., $N_1 \leqslant N_2$.

According to the Peres–Horodecki criterion [5, 6] the cases of $2 \otimes 2$ and $2 \otimes 3$ systems are trivial: it is known that in these cases the PPT criterion is necessary and sufficient for all states, i.e., even for states which are not invariant under rotations. Schliemann [24] has shown recently that the PPT criterion is also necessary and sufficient for $SO(3)$-invariant $2 \otimes N_2$ systems with arbitrary N_2. The case of $3 \otimes 3$ systems has been treated by Vollbrecht and Werner [15], who proved that the PPT criterion is again necessary and sufficient for separability. For $4 \otimes 4$ systems a qualitatively new situation arises. It has been demonstrated in [25] that the PPT criterion is not sufficient and that the entangled PPT states form a three-dimensional manifold which is isomorphic to a prism. In the present work, we investigate the important special case of $3 \otimes N_2$ systems with arbitrary N_2.

The method developed in [25] enables the treatment of the case of equal spins $j_1 = j_2$. In this paper we extend this method to arbitrary spins j_1 and j_2. For the analysis of entanglement under $SO(3)$-symmetry it is advantageous to replace the transposition used in the PPT criterion by another unitarily equivalent operation, namely by the antiunitary transformation of the time reversal. The reason for this fact is that the operation of the time reversal commutes with the representations of the rotation group.

There are two natural representations of rotationally invariant states. The first one uses the fact that any invariant state can be written as a unique convex linear combination of the projections P_J onto the eigenspaces of the total angular momentum J of the composite spin system. The advantage of this representation is that it leads to very simple conditions expressing the positivity and the normalization of physical states. However, the set of the PPT states is most easily determined in another representation which employs the irreducible spherical tensor operators of spin-j particles. We will construct a complete system of invariant operators Q_K which are built out of the spherical tensors of rank K. Any invariant state of the composite spin system can then be written as a unique linear combination of the Q_K. The introduction of the invariant operators Q_K generalizes the ideas of Schliemann [24, 26], who has developed a representation of $SU(2)$-invariant states by means of spin–spin correlators and has formulated various separability conditions and sum rules in terms of these correlators.

The paper is organized as follows. The representations of $SO(3)$-invariant states in terms of the invariant operators P_J and Q_K are constructed in section 2. We also derive in this section the linear transformation which connects these representations, and show that it is given by an orthogonal matrix whose elements are determined by Wigner's 6-j symbols. The behaviour of states under partial time reversal and the construction of the set of the invariant separable states are discussed in section 3.

The general theory is then applied in section 4 to the case of $3 \otimes N_2$ systems with arbitrary N_2. We prove that the PPT criterion represents a necessary and sufficient separability condition for $3 \otimes N_2$ systems if and only if N_2 is odd. Thus, for integer spins j_2 all PPT states are separable, while for half-integer spins j_2 there always exist entangled PPT states. This fact has already been conjectured by Hendriks [27] on the basis of a detailed numerical investigation. We also show that for half-integer j_2 the boundary of the separability region is curved. Finally, section 5 contains a discussion of the results and some conclusions. In particular, we construct an optimal entanglement witness for the case of half-integer spins and exploit this witness to design a protocol which allows the detection of entangled PPT states through measurements of the total angular momentum.

2. Representations of $SO(3)$-invariant states

We consider two particles with spins j_1 and j_2 and corresponding angular momentum operators $\hat{\boldsymbol{j}}^{(1)}$ and $\hat{\boldsymbol{j}}^{(2)}$. The Hilbert space $\mathbb{C}^{N_1}$ of the first particle is spanned by the common eigenstates $|j_1, m_1\rangle$ of the square of $\hat{\boldsymbol{j}}^{(1)}$ and of $\hat{\boldsymbol{j}}_z^{(1)}$, where $N_1 \equiv 2j_1 + 1$ and $m_1 = -j_1, \ldots, +j_1$. Correspondingly, the Hilbert space $\mathbb{C}^{N_2}$ of the second particle is spanned by the eigenstates $|j_2, m_2\rangle$, where $N_2 \equiv 2j_2 + 1$ and $m_2 = -j_2, \ldots, +j_2$.

The Hilbert space of the total system composed of both particles is given by the tensor product $\mathbb{C}^{N_1} \otimes \mathbb{C}^{N_2}$. The angular momentum operator of the composite system is defined by

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{j}}^{(1)} \otimes I + I \otimes \hat{\boldsymbol{j}}^{(2)}, \tag{2.1}$$

where I denotes the unit matrix. A state of the composite system is described by a density matrix on the product space, i.e., by a positive operator ρ on $\mathbb{C}^{N_1} \otimes \mathbb{C}^{N_2}$ with unit trace: $\rho \geqslant 0, \operatorname{tr} \rho = 1$.

The irreducible unitary representation of the group $SO(3)$ of proper rotations R on the state space of a particle with spin j will be denoted by $D^{(j)}(R)$. The transformation of the states of the composite spin system is then given by the product representation $D^{(j_1)}(R) \otimes D^{(j_2)}(R)$. A state ρ of the combined system is said to be rotationally invariant or $SO(3)$-invariant if the relation

$$[D^{(j_1)}(R) \otimes D^{(j_2)}(R)]\rho[D^{(j_1)}(R) \otimes D^{(j_2)}(R)]^\dagger = \rho$$

holds true for all proper rotations $R \in SO(3)$.

We shall use two different representations of rotationally invariant states. The first one employs the projection operators

$$P_J = \sum_{M=-J}^{+J} |JM\rangle\langle JM|, \tag{2.2}$$

where $|JM\rangle$ denotes the common eigenstate of the square of the total angular momentum $\hat{\boldsymbol{J}}$ and of its z-component $\hat{J}_z$, i.e., we have $\hat{\boldsymbol{J}}^2|JM\rangle = J(J+1)|JM\rangle$ and $\hat{J}_z|JM\rangle = M|JM\rangle$. The operator P_J projects onto the manifold which is spanned by the eigenstates belonging to a fixed value J of the total angular momentum. According to the triangular inequality J takes on N_1 different values which may be integer or half-integer valued:

$$J = j_2 - j_1, j_2 - j_1 + 1, \ldots, j_2 + j_1. \tag{2.3}$$

It follows from Schur's lemma that any invariant state ρ can be written as a linear combination of the P_J:

$$\rho = \frac{1}{\sqrt{N_1 N_2}} \sum_J \frac{\alpha_J}{\sqrt{2J+1}} P_J. \tag{2.4}$$

Here, the α_J are real parameters and we have introduced convenient normalization factors of $\sqrt{N_1 N_2}$ and $\sqrt{2J+1}$. In order for equation (2.4) to represent a true density matrix the α_J must of course be positive and normalized appropriately:

$$\alpha_J \geqslant 0, \tag{2.5}$$

$$\operatorname{tr}\rho = \sum_J \sqrt{\frac{2J+1}{N_1 N_2}} \alpha_J = 1. \tag{2.6}$$

Any invariant state ρ is thus uniquely characterized by a real vector $\boldsymbol{\alpha}$ in an N_1-dimensional parameter space $\mathbb{R}^{N_1}$ which will be referred to as α-space. The conditions of the positivity and of the normalization of ρ are expressed by the relations (2.5) and (2.6). We denote the set of all vectors $\boldsymbol{\alpha}$ whose components α_J satisfy these relations by S^α. Being isomorphic to the set of invariant states, S^α is of course a convex set. We infer from equations (2.5) and (2.6) that S^α represents an $(N_1 - 1)$-dimensional simplex.

A useful alternative representation of the invariant states is obtained by use of a complete system of irreducible spherical tensor operators (see, e.g., [28, 29]). The tensor operators which act on the state space of the particle with spin j_i are written as $T^{(i)}_{K_i q_i}$, where $i = 1, 2$. The index $K_i = 0, 1, \ldots, 2j_i$ denotes the rank of the tensor operator. For a given rank K_i the index q_i takes on the values $q_i = -K_i, -K_i + 1, \ldots, +K_i$. We thus have $(2K_i + 1)$ tensor operators $T^{(i)}_{K_i q_i}$ of rank K_i which transform under rotations according to an irreducible representation of the rotation group. The explicit definitions of the tensors and a brief summary of their properties are given in appendix A.

Using the tensor operators one defines Hermitian operators Q_K acting on the state space of the composite spin system:

$$Q_K = \sum_{q=-K}^{+K} T^{(1)}_{Kq} \otimes T^{(2)\dagger}_{Kq}, \tag{2.7}$$

where the index K takes on N_1 different integer values:

$$K = 0, 1, \ldots, 2j_1. \tag{2.8}$$

It follows from the transformation properties of the tensor operators that all Q_K are invariant under rotations. For instance, the operator Q_0 is proportional to the identity, $Q_0 = \frac{1}{\sqrt{N_1 N_2}} I \otimes I$, while Q_1 is proportional to the invariant scalar product $\hat{\boldsymbol{j}}^{(1)} \cdot \hat{\boldsymbol{j}}^{(2)}$ of the spin vectors.

The Q_K defined by equation (2.7) form a complete system of operators. This means that any rotationally invariant Hermitian operator can be represented as a unique linear combination of the Q_K in a way analogous to equation (2.4):

$$\rho = \frac{1}{\sqrt{N_1 N_2}} \sum_K \frac{\beta_K}{\sqrt{2K+1}} Q_K. \tag{2.9}$$

Here, we have again introduced appropriate normalization factors and real parameters β_K which form a vector $\boldsymbol{\beta}$ in an N_1-dimensional parameter space $\mathbb{R}^{N_1}$ referred to as β-space. The operators Q_K satisfy $\mathrm{tr}\{Q_K Q_{K'}\} = (2K+1)\delta_{KK'}$. This fact follows directly from the orthogonality relation (A.1) for the spherical tensors. The Q_K for $K \neq 0$ are therefore traceless which leads to the normalization condition

$$\mathrm{tr}\,\rho = \beta_0 = 1. \tag{2.10}$$

The sets $\{P_J\}$ and $\{Q_K\}$ represent complete systems of invariant operators. The corresponding parameter vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ must, therefore, be related by a linear transformation $\mathbb{R}^{N_1} \mapsto \mathbb{R}^{N_1}$. We write

$$\boldsymbol{\beta} = L\boldsymbol{\alpha}, \tag{2.11}$$

where L is an $(N_1 \times N_1)$ matrix. To find the elements of this matrix we use equations (2.4) and (2.9) to get

$$\sum_J \frac{\alpha_J}{\sqrt{2J+1}} P_J = \sum_K \frac{\beta_K}{\sqrt{2K+1}} Q_K. \tag{2.12}$$

Multiplying this equation by $Q_{K'}$ and taking the trace we find that the elements of L are given by

$$L_{KJ} = [(2K+1)(2J+1)]^{-1/2}\,\mathrm{tr}\{Q_K P_J\}. \tag{2.13}$$

This can be expressed as

$$L_{KJ} = \sqrt{(2K+1)(2J+1)}(-1)^{j_1+j_2+J} \begin{Bmatrix} j_1 & j_2 & J \\ j_2 & j_1 & K \end{Bmatrix}. \tag{2.14}$$

The curly brackets denote a 6-j symbol introduced by Wigner [30] into the quantum theory of angular momentum. A proof of the relation (2.14) is given in appendix B. The 6-j symbols are scalar quantities which are defined through invariant sums over products of Clebsch–Gordan coefficients. They describe the transformation between different coupling schemes for the addition of three angular momenta [28]. Their properties have been studied in great detail and many closed formulae, recursion relations and sum rules are known. In particular, it follows from the sum rules that L represents an orthogonal $(N_1 \times N_1)$ matrix.

The above results lead to the conclusion that the set of $SO(3)$-invariant states is represented in β-space by the set

$$S^{\beta} = LS^{\alpha}. \tag{2.15}$$

The set S^{β} is again an $(N_1 - 1)$-dimensional simplex which may be constructed by determining the images of the extreme points of S^{α} under the orthogonal transformation L.

The introduction of two parameter spaces is motivated by the following observations. On the one hand, the set of states is most easily constructed as a subset in α-space. This is due to the fact that the representation of equation (2.4) corresponds to the spectral decomposition of ρ and, therefore, the requirement of the positivity of ρ immediately leads to the simple condition (2.5). On the other hand, the representation (2.9) of states in β-space is much more suitable for the construction of the set of separable states, which is due to the fact that the operation of the partial time reversal is diagonal in the Q_K-representation.

3. Invariant separable states

A state ρ of the composite spin system is said to be separable if it is possible to write this state as a convex linear combination of product states:

$$\rho = \sum_i \lambda_i \rho_i^{(1)} \otimes \rho_i^{(2)}, \qquad \lambda_i \geqslant 0, \qquad \sum_i \lambda_i = 1, \tag{3.1}$$

where the $\rho_i^{(1)}$ and $\rho_i^{(2)}$ are normalized states of the first and second spins, respectively [1]. It is clear that the set in β-space which represents the invariant and separable states is a convex subset of S^β. This subset will be denoted by $S^\beta_{\rm sep}$.

Following the work of Vollbrecht and Werner [15] we define a projection super-operator ($SO(3)$ twirling) by means of

$$\Pi\rho = \int {\rm d}R\, U(R)\rho U(R)^\dagger, \tag{3.2}$$

where $U(R) \equiv D^{(j_1)}(R) \otimes D^{(j_2)}(R)$ and the integration is extended over all group elements $R \in SO(3)$. The twirl operation maps any state ρ of the composite spin system to an $SO(3)$-invariant state $\Pi\rho$. Moreover, if ρ is separable then $\Pi\rho$ also is separable. In terms of the invariant operators P_J or Q_K the action of the twirl operation may be expressed by

$$\Pi\rho = \sum_J \frac{{\rm tr}\{P_J\rho\}}{2J+1} P_J = \sum_K \frac{{\rm tr}\{Q_K\rho\}}{2K+1} Q_K. \tag{3.3}$$

It is known that any invariant separable state is a convex linear combination of Π-projections of pure product states. Given a pure product state

$$\rho = |\varphi^{(1)}\varphi^{(2)}\rangle\langle\varphi^{(1)}\varphi^{(2)}|, \tag{3.4}$$

equation (3.3) shows that the corresponding parameters α_J and β_K of its projection $\Pi\rho$ are given by

$$\alpha_J = \sqrt{\frac{N_1N_2}{2J+1}} \langle\varphi^{(1)}\varphi^{(2)}|P_J|\varphi^{(1)}\varphi^{(2)}\rangle, \tag{3.5}$$

$$\beta_K = \sqrt{\frac{N_1N_2}{2K+1}} \langle\varphi^{(1)}\varphi^{(2)}|Q_K|\varphi^{(1)}\varphi^{(2)}\rangle. \tag{3.6}$$

We introduce into equation (3.6) the definition (2.7) of the Q_K and define the functions

$$\tilde\beta_K[\varphi^{(1)},\varphi^{(2)}] = \sqrt{\frac{N_1N_2}{2K+1}} \sum_{q=-K}^{+K} \langle\varphi^{(1)}|T^{(1)}_{Kq}|\varphi^{(1)}\rangle\langle\varphi^{(2)}|T^{(2)\dagger}_{Kq}|\varphi^{(2)}\rangle. \tag{3.7}$$

Let us further define W^β as the range of the parameter vector $\boldsymbol\beta$ whose components are given by these functions, where $|\varphi^{(1)}\rangle \in \mathbb{C}^{N_1}$ and $|\varphi^{(2)}\rangle \in \mathbb{C}^{N_2}$ run independently over all normalized states of the first and second spins, respectively:

$$W^\beta = \{\boldsymbol\beta \mid \beta_K = \tilde\beta_K[\varphi^{(1)},\varphi^{(2)}], \|\varphi^{(1,2)}\| = 1\}. \tag{3.8}$$

The set of separable states is then equal to the convex hull of W^β:

$$S^\beta_{\rm sep} = {\rm hull}(W^\beta). \quad (3.9)$$

This means that $S^\beta_{\rm sep}$ is equal to the smallest convex set which contains W^β.

Within this formulation the problem of constructing $S^\beta_{\rm sep}$ reduces to the determination of the convex hull of the range of the functions $\tilde{\beta}_K$. Even for the present case of a highly symmetric state space this is, in general, an extremely difficult task. A strong necessary condition for separability is the Peres–Horodecki criterion [5, 6]. According to this criterion a necessary condition for a given state ρ to be separable is that its partial transposition is a positive operator: $T_2\rho \equiv (I \otimes T)\rho \geqslant 0$. Here, $TB = B^T$ denotes the transposition of the operator B on $\mathbb{C}^{N_2}$ which is defined in terms of the basis states of the second spin by means of $\langle j_2, m_2|B^T|j_2, m_2'\rangle = \langle j_2, m_2'|B|j_2, m_2\rangle$. The partial transposition T_2 is then defined by $T_2(A \otimes B) = A \otimes B^T$.

The operation of taking the partial transposition destroys the rotational invariance of states, i.e., if ρ is invariant under rotations the partially transposed state $T_2\rho$ is generally not $SO(3)$-invariant. However, there exists another operation which is unitarily equivalent to T_2 and which does map rotationally invariant operators to rotationally invariant operators. This operation will be denoted by $\vartheta_2 = I \otimes \vartheta$. It involves the antiunitary time reversal transformation ϑ of the second spin and will therefore be referred to as partial time reversal.

According to Wigner's representation theorem [30], the action of the time reversal transformation ϑ on an operator B can be expressed as

$$\vartheta B = V B^T V^\dagger = \tau B^\dagger \tau^{-1}. \quad (3.10)$$

In the first expression, T denotes again the transposition and V is a unitary matrix which represents a rotation of the coordinate system about the y-axis by the angle π. In the second expression of equation (3.10) τ denotes the operator $\tau = V\tau_0$ which comprises the π-rotation V and the operator τ_0 of the complex conjugation. The operator τ is antiunitary and satisfies

$$\tau^2 = (-1)^{2j_2}. \quad (3.11)$$

ϑ is a positive but not completely positive map. It is unitarily equivalent to the transposition T and, hence, the Peres–Horodecki criterion can be expressed by

$$\vartheta_2\rho \equiv (I \otimes \vartheta)\rho \geqslant 0. \quad (3.12)$$

A great advantage of the representation of states in β-space is that the operators Q_K have a very simple behaviour under the map ϑ_2. Namely, as is shown in appendix A, they are eigenoperators of the partial time reversal: $\vartheta_2 Q_K = (-1)^K Q_K$. In β-space the map ϑ_2 therefore induces a reflection of the coordinate axes corresponding to the odd values of K:

$$\vartheta_2 : \beta_K \mapsto (-1)^K \beta_K. \quad (3.13)$$

We thus get the image $\vartheta_2 S^\beta$ of S^β by reversing the signs of the odd coordinates.

We define $S^\beta_{\rm ppt}$ as the set of states which are positive under ϑ_2 or, equivalently, under T_2 (PPT states). This set is equal to the intersection of S^β with its image $\vartheta_2 S^\beta$. According to the Peres–Horodecki criterion the set of separable states is a subset of the set of PPT states. Hence, we have

$$S^\beta_{\rm sep} \subset S^\beta_{\rm ppt} = S^\beta \cap \vartheta_2 S^\beta. \quad (3.14)$$

We note three properties which turn out to be useful in the construction of the set of separable states.

(1) The functions defined by equation (3.7) are invariant under simultaneous rotations of the input arguments:

$$\tilde{\beta}_K[D^{(j_1)}(R)\varphi^{(1)}, D^{(j_2)}(R)\varphi^{(2)}] = \tilde{\beta}_K[\varphi^{(1)}, \varphi^{(2)}]. \tag{3.15}$$

This property is an immediate consequence of the rotational invariance of the operators Q_K.

(2) The range W^β defined in equation (3.8) is obviously invariant under the partial time reversal ϑ_2. This means that $\boldsymbol{\beta} \in W^\beta$ implies $\vartheta_2\boldsymbol{\beta} \in W^\beta$.

(3) There exist two distinguished separable states. These are the states given by the parameter vector $\boldsymbol{\alpha}$ with components

$$\alpha_J = \sqrt{\frac{N_1 N_2}{2J_{\max}+1}}\delta_{J,J_{\max}}, \qquad J_{\max} \equiv j_1 + j_2, \tag{3.16}$$

and the partially time reversed state given by $\boldsymbol{\alpha}' = \vartheta_2\boldsymbol{\alpha}$. To proof this statement we consider a pure product state ρ of the form of equation (3.4) with $|\varphi^{(1)}\rangle = |j_1, +j_1\rangle$ and $|\varphi^{(2)}\rangle = |j_2, +j_2\rangle$. We then have the obvious relation $|J = J_{\max}, M = +J_{\max}\rangle = |\varphi^{(1)}\varphi^{(2)}\rangle$ and, hence,

$$\langle\varphi^{(1)}\varphi^{(2)}|P_J|\varphi^{(1)}\varphi^{(2)}\rangle = \delta_{J,J_{\max}}. \tag{3.17}$$

Equation (3.5) then immediately leads to equation (3.16). This means that the pure product state ρ is mapped under the twirl operation to the separable state $\Pi\rho = \frac{1}{2J_{\max}+1}P_{J_{\max}}$ corresponding to the maximal value of the total angular momentum $J_{\max}$. It follows from point (2) that the partially time reversed state also is separable.

The point $\boldsymbol{\alpha}$ given by equation (3.16) is an extreme point of the simplex S^α and its image $\boldsymbol{\alpha}'$ is an extreme point of $\vartheta_2 S^\alpha$. Thus, $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}'$ are extreme points of S^α_{ppt}. It follows that the corresponding points $\boldsymbol{\beta} = L\boldsymbol{\alpha}$ and $\boldsymbol{\beta}' = L\boldsymbol{\alpha}'$ in β-space belong to W^β and represent extreme points of S^β_{ppt}.

As an illustration of the above analysis consider a $2\otimes N_2$ system for which $j_1 = \frac{1}{2}$ and j_2 is arbitrary. As has been demonstrated by Schliemann [24], the PPT criterion is a necessary and sufficient separability condition in this case. Within the present formulation this statement can be proven as follows. We first note that the index K takes on the two values $K = 0, 1$ such that $\boldsymbol{\beta}$ is a two-dimensional vector. Because of the normalization condition (2.10) we only need a single parameter β_1 to characterize uniquely an invariant state of a $2\otimes N_2$ system. It follows that S^β can be represented by an interval of the β_1-axis, and S^β_{ppt} by a sub-interval of this interval. Since an interval has exactly two extreme points (its endpoints), we conclude with the help of point (3) above that the extreme points of S^β_{ppt} belong to W^β. By the relation (3.9) the sets S^β_{ppt} and S^β_{sep} therefore coincide. This shows that the PPT criterion is indeed necessary and sufficient for separability.

4. $3\otimes N$ systems

Let us now consider the case $j_1 = 1$ ($N_1 = 3$) and j_2 arbitrary, i.e. the case of $3\otimes N_2$ systems. For convenience we write $N \equiv N_2 = 2j_2 + 1$. Since J takes on the values $J = j_2 - 1, j_2$ and $j_2 + 1$, $\boldsymbol{\alpha}$ is a three-vector

$$\boldsymbol{\alpha} = \begin{pmatrix} \alpha_{j_2-1} \\ \alpha_{j_2} \\ \alpha_{j_2+1} \end{pmatrix}. \tag{4.1}$$

The set S^α of invariant states is given by the relations:

$$\alpha_{j_2-1}, \alpha_{j_2}, \alpha_{j_2+1} \geqslant 0 \tag{4.2}$$

and

$$\sqrt{\frac{N-2}{3N}}\alpha_{j_2-1} + \sqrt{\frac{1}{3}}\alpha_{j_2} + \sqrt{\frac{N+2}{3N}}\alpha_{j_2+1} = 1. \tag{4.3}$$

We observe that S^α is a 2-simplex, i.e. a triangle whose vertices are given by the following parameter vectors $\boldsymbol{\alpha}$:

$$\begin{pmatrix} 0 \\ 0 \\ \sqrt{\frac{3N}{N+2}} \end{pmatrix}, \qquad \begin{pmatrix} \sqrt{\frac{3N}{N-2}} \\ 0 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 \\ \sqrt{3} \\ 0 \end{pmatrix}. \tag{4.4}$$

In order to transform to β-space we first determine the matrix L by means of the formulae (B.3)–(B.5):

$$L = \begin{bmatrix} \sqrt{\frac{N-2}{3N}} & \sqrt{\frac{1}{3}} & \sqrt{\frac{N+2}{3N}} \\ -\sqrt{\frac{(N-2)(N+1)}{2N(N-1)}} & -\sqrt{\frac{2}{(N-1)(N+1)}} & \sqrt{\frac{(N-1)(N+2)}{2N(N+1)}} \\ \sqrt{\frac{(N+1)(N+2)}{6N(N-1)}} & -\sqrt{\frac{2(N-2)(N+2)}{3(N-1)(N+1)}} & \sqrt{\frac{(N-1)(N-2)}{6N(N+1)}} \end{bmatrix}.$$

The extreme points of S^β are found by applying this matrix to the vectors given in equation (4.4). Since β_0 is identically equal to 1 by the normalization condition (2.10), we can represent points in β-space by two coordinates (β_1, β_2). One finds that S^β is a triangle in the (β_1, β_2)-plane with the vertices:

$$A = \left(\sqrt{\frac{3(N-1)}{2(N+1)}}, \sqrt{\frac{(N-1)(N-2)}{2(N+1)(N+2)}}\right), \tag{4.5}$$

$$B = \left(-\sqrt{\frac{3(N+1)}{2(N-1)}}, \sqrt{\frac{(N+1)(N+2)}{2(N-1)(N-2)}}\right), \tag{4.6}$$

$$C = \left(-\sqrt{\frac{6}{(N-1)(N+1)}}, -\sqrt{\frac{2(N-2)(N+2)}{(N-1)(N+1)}}\right). \tag{4.7}$$

The image $\vartheta_2 S^\beta$ of S^β under the partial time reversal is obtained by reversing the sign of the coordinate β_1. Consequently, S^β_{ppt} is a polygon with the four vertices A, A', D and E, where A is given by equation (4.5) and

$$A' = \left(-\sqrt{\frac{3(N-1)}{2(N+1)}}, \sqrt{\frac{(N-1)(N-2)}{2(N+1)(N+2)}}\right), \tag{4.8}$$

$$D = \left(0, -\sqrt{\frac{2(N-1)(N-2)}{(N+1)(N+2)}}\right), \tag{4.9}$$

$$E = \left(0, \sqrt{\frac{(N+1)(N-1)}{2(N+2)(N-2)}}\right). \tag{4.10}$$

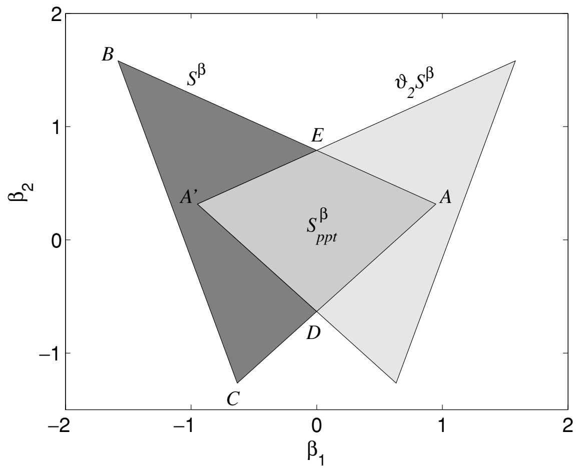

Figure 1. State space structure of a system composed of two particles with spins $j_1 = 1$ and $j_2 = \frac{3}{2}$ ($N = 4$). The triangle ABC represents the set S^β of invariant states, while the triangle $\vartheta_2 S^\beta$ is its image under the partial time reversal. The polygon $AA'DE$ represents the set S^β_{ppt} of the PPT states.

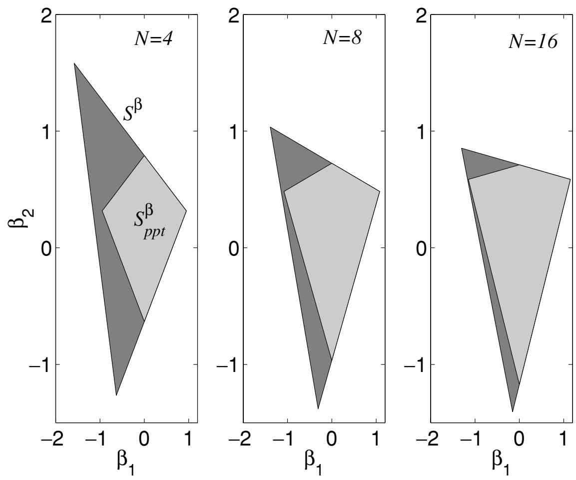

Figure 2. The sets of the invariant states S^β and of the invariant PPT states S^β_{ppt} for three different values of N.

Here, $A' = \vartheta_2 A$ is the image of A under ϑ_2, while D and E are the intersections of the lines AC and AB with the β_2-axis, respectively. The case $N = 4$ is illustrated in figure 1. Similar pictures are obtained for other values of N. Examples are shown in figure 2. Note that the origin of the (β_1, β_2)-plane describes the state $\rho = \frac{1}{3N} I \otimes I$ of maximal entropy.

To construct the set S^β_{sep} of separable states we have to investigate the functions

$$\tilde{\beta}_1[\varphi^{(1)}, \varphi^{(2)}] = \sqrt{N} \sum_{q=-1}^{+1} \langle \varphi^{(1)} | T^{(1)}_{1q} | \varphi^{(1)} \rangle \langle \varphi^{(2)} | T^{(2)\dagger}_{1q} | \varphi^{(2)} \rangle \qquad (4.11)$$

and

$$\tilde{\beta}_2[\varphi^{(1)},\varphi^{(2)}] = \sqrt{\frac{3N}{5}} \sum_{q=-2}^{+2} \langle\varphi^{(1)}|T_{2q}^{(1)}|\varphi^{(1)}\rangle\langle\varphi^{(2)}|T_{2q}^{(2)\dagger}|\varphi^{(2)}\rangle. \tag{4.12}$$

We distinguish two cases, namely the cases of odd and of even N.

Theorem 1. *For integer spins $j_2 = 1, 2, 3, \ldots$ one has $S_{\mathrm{ppt}}^{\beta} = S_{\mathrm{sep}}^{\beta}$. Hence, for all $3 \otimes N$ systems with odd N the PPT criterion represents a necessary and sufficient condition for the separability of rotationally invariant states.*

To proof this theorem we show that the vertices A, A', D and E of the polygon S_{ppt}^{β} belong to W^{β}. The statement $S_{\mathrm{ppt}}^{\beta} = S_{\mathrm{sep}}^{\beta}$ then follows immediately from equation (3.9).

The point A corresponds to the parameter vector $\boldsymbol{\alpha}$ given by equation (3.16). It follows that this point as well as the point $A' = \vartheta_2 A$ belongs to W^{β}. Hence, it suffices to verify that $D, E \in W^{\beta}$.

To show that $E \in W^{\beta}$ we choose the states

$$|\varphi^{(1)}\rangle = |1, m_1 = 0\rangle, \qquad |\varphi^{(2)}\rangle = |j_2, m_2 = 0\rangle. \tag{4.13}$$

According to the selection rules for the matrix elements of the tensor operators (A.3) and to equation (A.8) we have that $\langle\varphi^{(1)}|T_{1q}^{(1)}|\varphi^{(1)}\rangle = 0$ for $q = 0, \pm 1$ and, therefore,

$$\tilde{\beta}_1 = 0. \tag{4.14}$$

On the other hand, the non-vanishing matrix elements of the second-rank tensors are given by (see equation (A.10))

$$\langle\varphi^{(1)}|T_{20}^{(1)}|\varphi^{(1)}\rangle = -\tfrac{2}{\sqrt{6}}, \tag{4.15}$$

and

$$\langle\varphi^{(2)}|T_{20}^{(2)}|\varphi^{(2)}\rangle = \frac{-2\sqrt{5}j_2(j_2+1)}{\sqrt{(N+2)(N+1)N(N-1)(N-2)}}, \tag{4.16}$$

which yields

$$\begin{aligned}\tilde{\beta}_2 &= \sqrt{\frac{3N}{5}}\langle\varphi^{(1)}|T_{20}^{(1)}|\varphi^{(1)}\rangle\langle\varphi^{(2)}|T_{20}^{(2)}|\varphi^{(2)}\rangle \\ &= \sqrt{\frac{(N+1)(N-1)}{2(N+2)(N-2)}}.\end{aligned} \tag{4.17}$$

We see from equations (4.14), (4.17) and (4.10) that $(\tilde{\beta}_1, \tilde{\beta}_2) = E$ and, hence, that the point E belongs to W^{β}.

To show that D also belongs to W^{β} we take the states

$$|\varphi^{(1)}\rangle = |1, 0\rangle, \qquad |\varphi^{(2)}\rangle = |j_2, +j_2\rangle. \tag{4.18}$$

Since the state $|\varphi^{(1)}\rangle$ is the same as before, equations (4.14) and (4.15) hold true. Instead of equation (4.16), however, we get

$$\langle\varphi^{(2)}|T_{20}^{(2)}|\varphi^{(2)}\rangle = \frac{2\sqrt{5}\left[3j_2^2 - j_2(j_2+1)\right]}{\sqrt{(N+2)(N+1)N(N-1)(N-2)}}. \tag{4.19}$$

This gives

$$\begin{aligned}\tilde{\beta}_2 &= \sqrt{\frac{3N}{5}}\langle\varphi^{(1)}|T_{20}^{(1)}|\varphi^{(1)}\rangle\langle\varphi^{(2)}|T_{20}^{(2)}|\varphi^{(2)}\rangle \\ &= -\sqrt{\frac{2(N-1)(N-2)}{(N+1)(N+2)}}.\end{aligned} \tag{4.20}$$

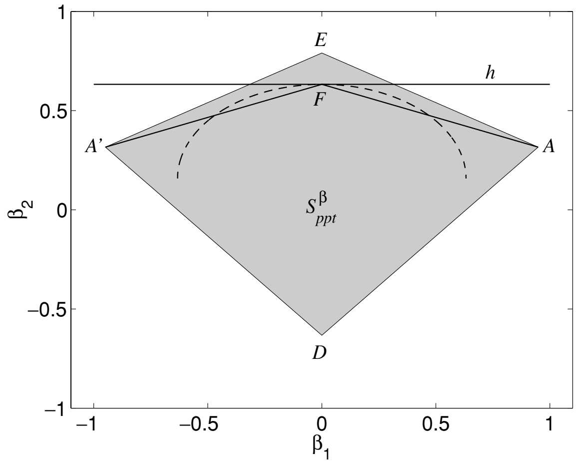

Figure 3. The set of PPT states $S^{\beta}_{\rm ppt}$ for $N = 4$. The set $S^{\beta}_{\rm sep}$ lies entirely below the straight line h through F which is parallel to the β_1-axis. The broken line shows the curve defined by equations (4.37) and (4.38).

A comparison with equation (4.9) shows that $(\tilde\beta_1, \tilde\beta_2) = D \in W^{\beta}$. This concludes the proof of the theorem.

Let us now turn to the case of half-integer spins j_2, i.e., we assume that N is even. Of course, we again have that A and A' belong to W^{β}. But also $D \in W^{\beta}$ because the state $|j_2, +j_2\rangle$ exists for integer as well as for half-integer spins j_2. The argument following equation (4.18) can thus also be applied in the present case. It follows that $S^{\beta}_{\rm sep}$ contains at least the triangle $AA'D$ (see figure 3).

On the other hand, the state $|j_2, m_2 = 0\rangle$ exists, of course, only for integer spins j_2. Instead of (4.13) we consider the states

$$|\varphi^{(1)}\rangle = |1, 0\rangle, \qquad |\varphi^{(2)}\rangle = |j_2, +1/2\rangle, \tag{4.21}$$

which lead to

$$\tilde\beta_1 = 0, \qquad \tilde\beta_2 = \sqrt{\frac{(N+2)(N-2)}{2(N+1)(N-1)}}. \tag{4.22}$$

This shows that the point

$$F = \left(0, \sqrt{\frac{(N+2)(N-2)}{2(N+1)(N-1)}}\right) \tag{4.23}$$

belongs to W^{β}. Hence, $S^{\beta}_{\rm sep}$ contains at least the polygon with the vertices A, A', D and F.

We introduce the straight line h which intersects the point F and which is parallel to the β_1-axis (see figure 3). We are going to demonstrate that $S^{\beta}_{\rm sep}$ lies entirely below this line. The line h is thus tangential to $S^{\beta}_{\rm sep}$ and corresponds to an optimal entanglement witness (see section 5). To show this we employ the rotational invariance of the functions $\tilde\beta_K$ (see equation (3.15)) to obtain a suitable parametrization of the states of the first spin $j_1 = 1$. Namely, by an appropriate rotation R, any state of this spin can be brought into the following form:

$$|\varphi^{(1)}\rangle = \sqrt{r}|1, +1\rangle + \sqrt{1-r}|1, -1\rangle, \tag{4.24}$$

where we omit an irrelevant overall phase factor and r is a real parameter taken from the interval [0, 1]. Invoking the rotational invariance we may assume without restriction that $|\varphi^{(1)}\rangle$ is of this form. The state space of the first spin j_1 has thus only a single relevant parameter $r \in [0, 1]$.

By use of the representation (4.24) the quantities $\tilde{\beta}_1$ and $\tilde{\beta}_2$ become functions of the parameter r and of the state vector $|\varphi^{(2)}\rangle$ of the second spin. Inserting equation (4.24) into equation (4.11) and using equations (A.8) and (A.9) of appendix A, we get

$$\tilde{\beta}_1[r, \varphi^{(2)}] = \sqrt{\frac{N}{2}}(2r-1)\langle\varphi^{(2)}|T_{10}^{(2)}|\varphi^{(2)}\rangle. \tag{4.25}$$

The function $\tilde{\beta}_2$ is found by substituting expression (4.24) into equation (4.12) and by using equations (A.10)–(A.12). One finds that $\tilde{\beta}_2$ can be written as the expectation value

$$\tilde{\beta}_2[r, \varphi^{(2)}] = \langle\varphi^{(2)}|H(\lambda)|\varphi^{(2)}\rangle \tag{4.26}$$

of the Hermitian $(N \times N)$ matrix

$$H(\lambda) \equiv H_0 + \lambda H_1. \tag{4.27}$$

Here, we have defined

$$H_0 = \sqrt{\frac{N}{10}}T_{20}^{(2)}, \qquad H_1 = \frac{1}{2}\sqrt{\frac{3N}{5}}\left(T_{22}^{(2)} + T_{22}^{(2)\dagger}\right),$$

and introduced the parameter

$$\lambda = 2\sqrt{r(1-r)}, \qquad 0 \leqslant \lambda \leqslant 1. \tag{4.28}$$

For a given value of λ the function $\tilde{\beta}_2$ defined by equation (4.26) is certainly smaller than or equal to the largest eigenvalue of $H(\lambda)$ which we denote by $\varepsilon_0(\lambda)$. We are going to demonstrate below that $\varepsilon_0(\lambda)$ is a monotonically increasing function of λ and attains its maximum at $\lambda = 1$:

$$\varepsilon_0(1) = \sqrt{\frac{(N+2)(N-2)}{2(N+1)(N-1)}}. \tag{4.29}$$

Hence, we have

$$\tilde{\beta}_2[r, \varphi^{(2)}] \leqslant \varepsilon_0(1) \tag{4.30}$$

for all r and $|\varphi^{(2)}\rangle$. Note that $\varepsilon_0(1)$ is equal to the β_2-coordinate of the point F (see equation (4.23)). This shows that, as claimed, all points of W^{β} and, hence, all points of $S^{\beta}_{\rm sep}$ lie below the line h.

To prove that $\varepsilon_0(\lambda)$ is a monotonically increasing function of λ we denote the eigenvalues of $H(\lambda)$ by $\varepsilon_n(\lambda)$, where $n = 0, 1, 2, \ldots$, and $n = 0$ labels the largest eigenvalue. With the help of equation (A.6) one verifies that $H(\lambda)$ is invariant under time reversal. It follows that if $|\varphi\rangle$ is an eigenstate of $H(\lambda)$ then also the time reversed state $\tau|\varphi\rangle$ is an eigenstate with the same eigenvalue. Since j_2 is half-integer valued the states $|\varphi\rangle$ and $\tau|\varphi\rangle$ are orthogonal. In fact, using the antiunitarity of τ and equation (3.11) we get

$$\langle\tau\varphi|\varphi\rangle = \langle\tau^2\varphi|\tau\varphi\rangle^* = (-1)^{2j_2}\langle\tau\varphi|\varphi\rangle = -\langle\tau\varphi|\varphi\rangle,$$

which shows that $\langle\tau\varphi|\varphi\rangle = 0$.

All eigenvalues $\varepsilon_n(\lambda)$ are thus two-fold degenerate and we write the corresponding eigenstates as $|\varphi_{n,k}(\lambda)\rangle$, where the index $k = 1, 2$ labels the eigenstates corresponding to the same eigenvalue: $|\varphi_{n,2}(\lambda)\rangle = \tau|\varphi_{n,1}(\lambda)\rangle$. We remark that the two-fold degeneracy is analogous to the Kramers degeneracy according to which the energy levels of an invariant system of an odd number of spin-$\frac{1}{2}$ particles are at least two-fold degenerate (see, e.g., [31]).

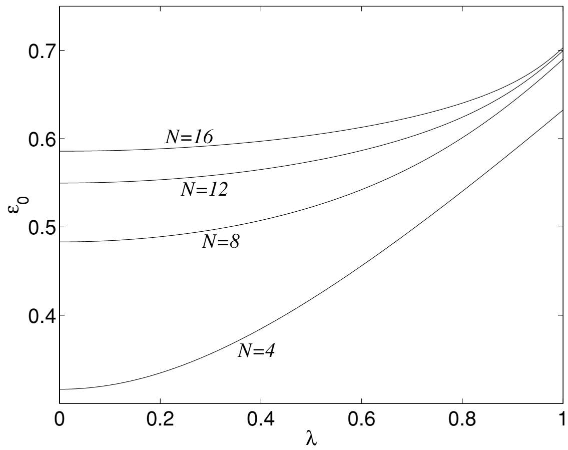

Figure 4. The largest eigenvalue $\varepsilon_0(\lambda)$ of the matrix $H(\lambda)$ defined by equation (4.27) for different values of N.

The Hellman–Feynman theorem now yields

$$\frac{\mathrm{d}\varepsilon_0}{\mathrm{d}\lambda} = \langle\varphi_{0,1}(\lambda)|H_1|\varphi_{0,1}(\lambda)\rangle. \tag{4.31}$$

In particular, we have

$$\left.\frac{\mathrm{d}\varepsilon_0}{\mathrm{d}\lambda}\right|_{\lambda=0} = 0. \tag{4.32}$$

On differentiating equation (4.31) once again we find

$$\frac{\mathrm{d}^2\varepsilon_0}{\mathrm{d}\lambda^2} = 2\sum_{n\neq 0,k}\frac{|\langle\varphi_{n,k}(\lambda)|H_1|\varphi_{0,1}(\lambda)\rangle|^2}{\varepsilon_0(\lambda)-\varepsilon_n(\lambda)} \geqslant 0. \tag{4.33}$$

This shows that $\varepsilon_0(\lambda)$ is a convex function of λ with zero derivative at $\lambda = 0$. It follows that $\varepsilon_0(\lambda)$ increases monotonically. Some examples of the behaviour of this function are shown in figure 4.

It remains to verify equation (4.29). We first note that $H(1)$ can be written with the help of equations (A.10) and (A.12) in terms of the spin operator $\hat{\boldsymbol{j}}^{(2)}$ as

$$H(1) = 2\sqrt{\frac{2}{(N+2)(N+1)(N-1)(N-2)}}\left([\hat{\boldsymbol{j}}^{(2)}]^2 - 3\big[\hat{j}_y^{(2)}\big]^2\right). \tag{4.34}$$

The largest eigenvalue of this matrix is given by

$$\varepsilon_0(1) = 2\sqrt{\frac{2}{(N+2)(N+1)(N-1)(N-2)}}\left(j_2(j_2+1)-\frac{3}{4}\right). \tag{4.35}$$

Using $N = 2j_2 + 1$ one shows that this equation coincides with equation (4.29).

We finally demonstrate that the boundary of S^{β}_{sep} is differentiable at the point F (see equation (4.23)). To this end, we construct a smooth curve which belongs to W^{β} and passes the point F. Consider the following fixed state of the second spin:

$$|\varphi^{(2)}\rangle = \frac{1}{\sqrt{2}}\big|\hat{j}_y^{(2)} = +1/2\big\rangle + \frac{\mathrm{i}}{\sqrt{2}}\big|\hat{j}_y^{(2)} = -1/2\big\rangle. \tag{4.36}$$

This is an eigenstate of the matrix $H(1)$ [equation (4.34)] corresponding to the largest eigenvalue $\varepsilon_0(1)$. Since $|\varphi^{(2)}\rangle$ is fixed, the functions $\tilde{\beta}_1$ and $\tilde{\beta}_2$ depend only on the parameter r and describe a curve in the (β_1, β_2)-plane. Writing $r \equiv (1+\mu)/2$ and determining the matrix elements one finds

$$\tilde{\beta}_1 = \sqrt{\frac{3N^2}{8(N+1)(N-1)}}\mu, \tag{4.37}$$

$$\tilde{\beta}_2 = \frac{\varepsilon_0(1)}{4}\left(1 + 3\sqrt{1-\mu^2}\right), \tag{4.38}$$

where $-1 \leqslant \mu \leqslant +1$. The curve described by these equations represents the upper half of an ellipse in the (β_1, β_2)-plane (see figure 3). It intersects the point F and lies entirely in W^β. Since F is the only point of h belonging to W^β, it follows that the boundary of the separability region must be curved and that it is differentiable at the extreme point F, the line h being the tangent. Summarizing, we have shown:

Theorem 2. *For half-integer spins $j_2 = \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \ldots$, the set $S^\beta_{\rm sep}$ of separable states is a true subset of the set of PPT states. Hence, for all $3 \otimes N$ systems with even N the PPT criterion is only necessary and there always exist entangled PPT states. The line h represents the tangent to $S^\beta_{\rm sep}$ at the extreme point F. The set $S^\beta_{\rm sep}$ is bounded by the straight lines AD and $A'D$ and by a concave curve which passes the points A, A' and F.*

5. Discussion and conclusions

The state space structure of rotationally invariant spin systems has been analysed in this paper. The set of invariant states has been represented by means of two systems of invariant operators, namely by the projections P_J onto the total angular momentum manifolds and by the invariant operators Q_K composed of the spherical tensors. The transformation between both representations was found to be given by a matrix L which is determined by certain 6-j symbols of Wigner. The Q_K-representation is particularly useful in applying the PPT criterion for separability because the Q_K are eigenoperators of the partial time reversal. The method has been demonstrated to lead to a complete classification of separability of $3 \otimes N$ systems. We have shown that the PPT criterion is necessary and sufficient for all systems with odd N, while entangled PPT states exist for systems with even N.

Some remarks on the structure of the state space in the limit $N \to \infty$ might be of interest. In this limit the value of the second spin j_2 becomes arbitrary large. We infer from equations (4.6)–(4.9) that the point B then converges to the point A', and C to D. At the same time F converges to E (see equations (4.10) and (4.23)). Hence, as N increases the set $S^\beta_{\rm ppt}$ approaches the set S^β and $S^\beta_{\rm sep}$ approaches $S^\beta_{\rm ppt}$. This behaviour is also indicated in figure 2. The limit $N \to \infty$ thus corresponds to a kind of classical limit in which all invariant states have a positive partial transpose and are separable.

The line h constructed in section 4 leads to an entanglement witness which we denote by $\mathcal{W}$. An entanglement witness is a Hermitian operator which satisfies $\mathrm{tr}\{\mathcal{W}\sigma\} \geqslant 0$ for any separable state σ, and $\mathrm{tr}\{\mathcal{W}\rho\} < 0$ for at least one non-separable state ρ [6, 12]. The hyperplane h corresponding to an entanglement witness $\mathcal{W}$ is defined by $\mathrm{tr}\{\mathcal{W}\rho\} = 0$. In the case of $3 \otimes N$ systems h is a one-dimensional line and the witness is, in fact, optimal [13] because h is tangential to the region of separable states. We have formulated the witness in β-space. Transforming back to α-space one easily shows that the entanglement witness corresponding to h may be written in terms of the projections P_J as

$$\mathcal{W} = -\frac{1}{N-2}P_{j_2-1} + P_{j_2} + \frac{1}{N+2}P_{j_2+1}. \tag{5.1}$$

This expression leads to the following physical interpretation of $\mathcal{W}$. Suppose one carries out a measurement of the total angular momentum J on some invariant state ρ. If ρ is separable the inequality

$$-\frac{p_{j_2-1}}{N-2} + p_{j_2} + \frac{p_{j_2+1}}{N+2} \geqslant 0 \tag{5.2}$$

must be satisfied, where $p_J = \mathrm{tr}\{P_J\rho\}$ denotes the probability of finding the value J. In other words, if the inequality (5.2) is violated the state ρ must necessarily be entangled.

We exploit the witness (5.1) to design a prescription for the detection of entangled PPT states in $3 \otimes N$ systems with even N (bound entanglement [32]). A given state ρ is positive under partial transposition if and only if the corresponding point (β_1, β_2) lies below the line through A' and E, and above the line through A' and D (see figure 1). If we transform to α-space this yields the conditions

$$-\frac{2p_{j_2-1}}{N-1} + \frac{(N^2-5)p_{j_2}}{(N+1)(N-1)} + \frac{2p_{j_2+1}}{N+1} \geqslant 0 \tag{5.3}$$

and

$$\frac{2p_{j_2-1}}{(N-1)(N-2)} - \frac{2p_{j_2}}{N-1} + p_{j_2+1} \geqslant 0. \tag{5.4}$$

These inequalities are equivalent to the PPT condition (3.12). Hence, entangled PPT states can be detected in the following way. Suppose again that a total angular momentum measurement is performed on some state ρ. If one finds that the measurement outcomes, i.e. the probabilities p_J, satisfy the inequalities (5.3) and (5.4) *and violate* the inequality (5.2) then the state ρ must be an entangled PPT state.

The witness $\mathcal{W}$ defined in equation (5.1) does not detect all entangled PPT states. As has been shown in section 4, a part of the boundary of the region of the separable states is curved and, therefore, one needs an infinite number of linear entanglement witnesses. The upper boundary of S^{β}_{sep} can, of course, be described by means of a suitable nonlinear equation. A possible way to derive the latter is to construct the envelope of appropriate families of curves of the type given by equations (4.37) and (4.38).

The considerations of section 4 reveal that for $3 \otimes N_2$ systems half-integer spins are crucial for the emergence of entangled PPT states. The entanglement structure of systems involving half-integer spins is thus quite different from those with integer spins. It seems that this is closely connected to the fact that pure states which are invariant under time reversal only exist for integer spins, while for half-integer spins a given pure state is always orthogonal to its time reversed state. A clear physical interpretation of this result and its generalization to arbitrary $N_1 \otimes N_2$ systems is of great interest. The next step to further investigate this point could be to study $4 \otimes N_2$ systems, which is possible by the method developed in this paper.

Acknowledgments

The author would like to thank J Schliemann and F Petruccione for helpful comments and stimulating discussions.

Appendix A. Spherical tensor operators

We define here the irreducible spherical tensor operators T_{Kq} acting on the state space $\mathbb{C}^N$ of a particle with spin j, where $N = 2j+1$, $K = 0, 1, \ldots, 2j$, and $q = -K, \ldots, +K$. The tensor operators $T^{(i)}_{K_i q_i}$ for $i = 1, 2$ used in the main text are obtained by setting $j = j_1$ or $j = j_2$.

The spherical tensor operators T_{Kq} represent a complete system of operators on $\mathbb{C}^N$. This means that any operator on the state space of the spin-j particle may be written as a unique linear combination of the T_{Kq}. Moreover, the tensors are orthonormal with respect to the Hilbert–Schmidt inner product:

$$\mathrm{tr}\left\{T^{\dagger}_{K'q'} T_{Kq}\right\} = \delta_{KK'}\delta_{qq'}. \tag{A.1}$$

For a fixed K the $(2K+1)$ operators T_{Kq} represent the spherical components of a tensor of rank K. They transform according to an irreducible representation of $SO(3)$ which corresponds to the angular momentum K:

$$D^{(j)}(R) T_{Kq} D^{(j)}(R)^{\dagger} = \sum_{q'=-K}^{+K} D^{(K)}_{q'q}(R) T_{Kq'}. \tag{A.2}$$

For instance, the T_{1q} behave as components of a vector, and the T_{2q} as components of a second-rank tensor.

The matrix elements of the tensors may be defined in terms of Wigner's 3-j symbols as [28, 30]

$$\langle j, m|T_{Kq}|j, m'\rangle = \sqrt{2K+1}(-1)^{j-m}\begin{pmatrix} j & j & K \\ m & -m' & -q \end{pmatrix}. \tag{A.3}$$

The 3-j symbols are closely related to the Clebsch–Gordan coefficients:

$$\langle j_1, m_1; j_2, m_2|JM\rangle = \sqrt{2J+1}(-1)^{j_1-j_2+M}\begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & -M \end{pmatrix}. \tag{A.4}$$

According to the selection rules for the 3-j symbols the matrix element (A.3) is equal to zero for $m - m' - q \neq 0$. In particular, we have $T_{00} = \frac{1}{\sqrt{N}} I$.

The matrix elements (A.3) of the tensor operators are real and one has $T^{\dagger}_{Kq} = T^{T}_{Kq} = (-1)^q T_{K,-q}$. It follows that the T_{Kq} are eigenoperators of the time reversal transformation ϑ which was defined in equation (3.10). In fact, using the transformation behaviour (A.2) of the tensors and the fact that a rotation by π about the y-axis is represented by the unitary matrix

$$D^{(K)}_{q'q}(\pi) = (-1)^{K-q'}\delta_{q',-q}, \tag{A.5}$$

one finds

$$\vartheta T_{Kq} = V T^{T}_{Kq} V^{\dagger} = (-1)^K T_{Kq}. \tag{A.6}$$

As a consequence, the operators Q_K which have been introduced in equation (2.7) are eigenoperators of the partial time reversal $\vartheta_2 = I \otimes \vartheta$:

$$\vartheta_2 Q_K = (-1)^K Q_K. \tag{A.7}$$

We finally list the non-vanishing matrix elements of the tensor operators needed in section 4:

$$\langle j, m|T_{10}|j, m\rangle = 2m\sqrt{\frac{3}{N(N-1)(N+1)}}, \tag{A.8}$$

$$\langle j, m|T_{11}^{\dagger}|j, m+1\rangle = -\sqrt{\frac{6(j-m)(j+m+1)}{N(N-1)(N+1)}}, \tag{A.9}$$

$$\langle j, m|T_{20}|j, m\rangle = \frac{2\sqrt{5}[3m^2 - j(j+1)]}{\sqrt{(N+2)(N+1)N(N-1)(N-2)}}, \tag{A.10}$$

$$\langle j, m|T_{21}^{\dagger}|j, m+1\rangle = -\sqrt{5}(1+2m)\sqrt{\frac{6(j-m)(j+m+1)}{(N+2)(N+1)N(N-1)(N-2)}}, \tag{A.11}$$

$$\langle j, m|T_{22}^{\dagger}|j, m+2\rangle = \sqrt{5}\sqrt{\frac{6(j-m-1)(j-m)(j+m+1)(j+m+2)}{(N+2)(N+1)N(N-1)(N-2)}}. \tag{A.12}$$

Appendix B. Proof of relation (2.14)

The starting point is given by equation (2.13). We insert into this equation the definitions (2.2) and (2.7) for the invariant operators P_J and Q_K, and introduce complete sets of product basis states $|j_1, m_1; j_2, m_2\rangle$. This yields a multiple sum over products of two Clebsch–Gordan coefficients and two matrix elements of the tensor operators. By use of equations (A.3) and (A.4) the Clebsch–Gordan coefficients as well as the matrix elements of the spherical tensors can be written in terms of the 3-j symbols. We also use the selection rules for the 3-j symbols and their symmetry properties. This procedure leads to the following sum over 4-fold products of 3-j symbols:

$$\begin{aligned} L_{KJ} = {}& \sqrt{(2K+1)(2J+1)}(-1)^{j_1+j_2+J} \sum_{\{m_i\}} \chi(\{m_i\}) \\ & \times \begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_1 & K \\ -m_1 & m_5 & -m_6 \end{pmatrix} \\ & \times \begin{pmatrix} j_2 & j_2 & K \\ -m_4 & -m_2 & m_6 \end{pmatrix} \begin{pmatrix} j_2 & j_1 & J \\ m_4 & -m_5 & -m_3 \end{pmatrix}, \end{aligned} \tag{B.1}$$

where $\chi(\{m_i\})$ is a phase factor:

$$\chi(\{m_i\}) = (-1)^{j_1+m_1}(-1)^{j_2+m_2}(-1)^{J+m_3}(-1)^{j_2+m_4}(-1)^{j_1+m_5}(-1)^{K+m_6}.$$

The sum over the quantum numbers $m_1, \ldots, m_6$ in equation (B.1) exactly corresponds to a certain 6-j symbol of Wigner [30]. A general 6-j symbol involves six angular momenta and is written as

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix}. \tag{B.2}$$

The sum of equation (B.1) is equal to the 6-j symbol (B.2) with $j_3 = J$, $j_4 = j_2$, $j_5 = j_1$ and $j_6 = K$. Hence, we see that equation (B.1) reduces to equation (2.14). We remark that a similar technique has been used in [25] in order to derive an expression for the matrix which represents the partial time reversal ϑ_2 in the P_J-representation.

By use of the formulae for the 6-j symbols [28] we find that the first three rows of L are given by

$$L_{0J} = \sqrt{\frac{2J+1}{N_1 N_2}}, \tag{B.3}$$

and

$$L_{1J} = -2\sqrt{3(2J+1)}\frac{j_1(j_1+1)+j_2(j_2+1)-J(J+1)}{\sqrt{(N_1-1)N_1(N_1+1)(N_2-1)N_2(N_2+1)}}, \tag{B.4}$$

$$L_{2J} = 2\sqrt{5(2J+1)} \times \frac{3X(X-1)-4j_1(j_1+1)j_2(j_2+1)}{\sqrt{(N_1-2)(N_1-1)N_1(N_1+1)(N_1+2)(N_2-2)(N_2-1)N_2(N_2+1)(N_2+2)}}, \tag{B.5}$$

where

$$X \equiv j_1(j_1+1)+j_2(j_2+1)-J(J+1).$$

References

[1] Werner R F 1989 *Phys. Rev.* A **40** 4277

[2] Eckert K, Gühne O, Hulpke F, Hyllus P, Korbicz J, Mompart J, Bruß D, Lewenstein M and Sanpera A 2005 *Quantum Information Processing* ed G Leuchs and T Beth (Berlin: Wiley-VCH)

[3] Alber G, Beth T, Horodecki M, Horodecki P, Horodecki R, Rötteler M, Weinfurter H, Werner R and Zeilinger A 2001 *Quantum Information* (Berlin: Springer)

[4] Nielsen M A and Chuang I L 2000 *Quantum Computation and Quantum Information* (Cambridge: Cambridge University Press)

[5] Peres A 1996 *Phys. Rev. Lett.* **77** 1413

[6] Horodecki M, Horodecki P and Horodecki R 1996 *Phys. Lett.* A **223** 1

[7] Horodecki M and Horodecki P 1999 *Phys. Rev.* A **59** 4206

[8] Cerf N J, Adami C and Gingrich R M 1999 *Phys. Rev.* A **60** 898

[9] Nielsen M A and Kempe J 2001 *Phys. Rev. Lett.* **86** 5184

[10] Rudolph O 2003 *Phys. Rev.* A **67** 032312

[11] Chen K and Wu L-A 2003 *Quantum Inf. Comput.* **3** 193

[12] Terhal B M 2000 *Phys. Lett.* A **271** 319

[13] Lewenstein M, Kraus B, Cirac J I and Horodecki P 2000 *Phys. Rev.* A **62** 052310

[14] Rains E M 1999 *Phys. Rev.* A **60** 179

[15] Vollbrecht K G H and Werner R F 2001 *Phys. Rev.* A **64** 062307

[16] Breuer H P and Petruccione F 2002 *The Theory of Open Quantum Systems* (Oxford: Oxford University Press)

[17] Verri M and Gorini V 1978 *J. Math. Phys.* **19** 1803

[18] Osterloh A, Amico L, Falci G and Fazio R 2002 *Nature* **416** 608

[19] Osborne T J and Nielsen M A 2002 *Phys. Rev.* A **66** 032110

[20] Durkin G A, Simon C, Eisert J and Bouwmeester D 2004 *Phys. Rev.* A **70** 062305

[21] Manne K K and Caves C M 2005 *Preprint* quant-ph/0506151

[22] Schliemann J, Cirac J I, Kuś M, Lewenstein M and Loss D 2001 *Phys. Rev.* A **64** 022303

[23] Eckert K, Schliemann J, Bruß D and Lewenstein M 2002 *Ann. Phys., NY* **299** 88

[24] Schliemann J 2003 *Phys. Rev.* A **68** 012309

[25] Breuer H P 2005 *Phys. Rev.* A **71** 062330

[26] Schliemann J 2005 *Phys. Rev.* A **72** 012307

[27] Hendriks B 2002 *Diploma Thesis* University of Braunschweig

[28] Edmonds A R 1957 *Angular Momentum in Quantum Mechanics* (Princeton, NJ: Princeton University Press)

[29] Schwinger J 1965 *Quantum Theory of Angular Momentum* ed L C Biedenharn and H Van Dam (New York: Academic) p 229

[30] Wigner E P 1959 *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra* (New York: Academic)

[31] Sakurai J J 1994 *Modern Quantum Mechanics* (Reading, MA: Addison-Wesley)

[32] Horodecki M, Horodecki P and Horodecki R 1998 *Phys. Rev. Lett.* **80** 5239