International Journal of Theoretical Physics, Vol. 38, No. 6, 1999

The State Space of a Pair of Spin-1/2 Particles

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Received February 2, 1999

The state space of a quantum mechanical system consisting of more than one particle exhibits some unusual features giving rise to interesting phenomena, such as the Einstein–Rosen–Podolsky paradox. In order to get a feel for the structure of such a state space, it is useful to study the spin component of a pair of spin-1/2 particles, whose associated state space is clearly the simplest example occurring within the context of quantum mechanical systems of more than one particle. In a series of papers R. Horodecki *et al.* did just that and they found some beautiful results, which are certainly of interest to the mathematical physicist. In the present note, in a different context and using somewhat different methods of proof, we rederive some of the results obtained by Horodecki. Furthermore, using these methods we are able to prove some additional results which to our knowledge have never been published.

1. INTRODUCTION

According to the usual axioms of quantum mechanics the spin observables are in one-to-one correspondence with the real part:

$$A_h := \{a \in A \big| a^* = a\} \tag{1}$$

of the C*-algebra of all linear operators

$$A := L(H) \tag{2}$$

in a finite-dimensional Hilbert space H and the set of all spin states is in one-to-one correspondence with the set of all positive-semidefinite operators of trace one:

$$S := \{a \in A_h \big| a \geq 0 \ \& \ \text{trace}(a) = 1\} \tag{3}$$

We adopt the notation H_n, A_n, and S_n for the spin component of the

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0020-7748/99/0600-174 1$16.00/0

Hilbert space, the *C*-algebra*, and the *state space*, respectively, of a system consisting of n spin-1/2 particles. By U_n we shall denote the unitary group of A_n.

In the case of a single spin-1/2 particle, the spin component of the Hilbert space is two-dimensional, i.e., we have

$$H_1 := C^2 \tag{4}$$

We shall denote by $\{e_1, e_2\}$ the *standard basis* for H_1. A_{1h} is the carrier space of the adjoint representation $u \mapsto adj(u)$: $a \mapsto aua^*$, $u \in U_1$, $a \in A_{1h}$ of the unitary group U_1. It decomposes into *two* irreducible constituents, the identity representation spanned by the identity matrix σ_0 and the representation by rotation matrices, whose carrier space is spanned by the three Pauli matrices

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

The Pauli matrices satisfy the anticommutation relations

$$\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}\sigma_0, \qquad i, j = 1, 2, 3 \tag{5}$$

The relations imply that for $\mathbf{x}, \mathbf{y} \in \mathcal{R}^3$

$$(\mathbf{x} \cdot \sigma)(\mathbf{y} \cdot \sigma) + (\mathbf{y} \cdot \sigma)(\mathbf{x} \cdot \sigma) = 2(\mathbf{x}, \mathbf{y})\sigma_0 \tag{6}$$

Here $\mathbf{x} \cdot \sigma$ stands for the expression

$$\mathbf{x} \cdot \sigma = (x_1\sigma_1 + x_2\sigma_2 + x_3\sigma_3) \tag{7}$$

It follows that the map

$$\mathbf{x} \mapsto \mathbf{x} \cdot \sigma, \qquad \mathbf{x} \in \mathcal{R}^3 \tag{8}$$

is a linear *isometry* of $\mathcal{R}^3$ onto A_{1h}. Furthermore, to each unitary operator u in H there corresponds a rotation $R(u)$ of $\mathcal{R}^3$ via the formula

$$R(u)\mathbf{x} \cdot \sigma = u(\mathbf{x} \cdot \sigma)u^* \tag{9}$$

and the map $u \mapsto R(u)$ is a homomorphism of the unitary group U_1 onto the rotation group $SO(3)$, whose kernel is the center of U_1.

Let $x = 1/2(x_0\sigma_0 + \mathbf{x} \cdot \sigma) \in A_{1h}$ be an arbitrary self-adjoint one-particle operator. Then trace$(x) = x_0$ and $det(x) = 1/4(x_0^2 - \|\mathbf{x}\|^2)$. Therefore $x \in S_1$ iff $x_0 = 1$ and $\|\mathbf{x}\| \leq 1$.

Thus we can state the following lemma:

Lemma 1. A one-density operator

$$P(\mathbf{x}) := 1/2(\sigma_0 + \mathbf{x} \cdot \sigma) \tag{10}$$

is a one-dimensional projection in H_1 (and hence an extreme point of S_1), precisely if $\mathbf{x}$ is a unit vector.

Examples. The one-dimensional projections in H_1 associated with $\pm$ the members of the standard basis ($\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$) in $\mathcal{R}^3$, i.e., the operators

$$P_{i\pm} := P(\pm\mathbf{e}_i) = 1/2(\sigma_0 \pm \sigma_i), \qquad i = 1, 2, 3 \tag{11}$$

will subsequently play an important role (cf. Theorem 2).

Turning now to a pair of spin-1/2 particles, the spin component of the Hilbert space is given by the tensor product

$$H_2 = H_1 \otimes H_1 \tag{12}$$

Similarly the spin component of the C*-algebra is given by the tensor product

$$A_2 = A_1 \otimes A_1 \tag{13}$$

The symbol $\otimes$ also stands for a bilinear map $\otimes$: $H_1 \times H_1 \rightarrow H_2$, whose range spans H_2. A vector which lies in the range of this map is called *decomposable* . Given two elements $a, b \in A_1$, we can form the tensor product $a \otimes b$ by the requirement that for all ϕ, $\chi \in H_1$ the equation

$$(a \otimes b)(\phi \otimes \chi) = a\phi \otimes b\chi \tag{14}$$

holds. In this way we construct again a bilinear map $\otimes$, this time from $A_1 \times A_1$ into A_2. Again we shall call an element in A_2 of the form $a \otimes b$, with $a, b \in A_1$, *decomposable* . The assignment $u \mapsto u \otimes u$ ($u \in U_1$) defines a faithful representation of U_1 in H_2 which has two irreducible constituents, corresponding to the total spin 0 and 1, respectively, of the pair of particles, i.e., H_2 splits into an orthogonal sum

$$H_2 = H^0 \oplus H^1 \tag{15}$$

where H^0 is one-dimensional and spanned by the *singlet state*

$$\psi_0 = 1/\sqrt{2}(e_1 \otimes e_2 - e_2 \otimes e_1) \tag{16}$$

and H_1 is three-dimensional and spanned by the three *triplet states*

$$\begin{aligned} \psi_1 &= 1/\sqrt{2}(e_1 \otimes e_1 - e_2 \otimes e_2) \\ \psi_2 &= 1/\sqrt{2}(e_1 \otimes e_1 + e_2 \otimes e_2) \\ \psi_3 &= 1/\sqrt{2}(e_1 \otimes e_2 + e_2 \otimes e_1) \end{aligned} \tag{17}$$

The basis $\{\psi_0, \psi_1, \psi_2, \psi_3\}$ of H_2 is adapted to the direct sum decomposition into the irreducible U_1-modules H^0 and H^1. In physical literature this basis is called the *Bell basis*, in honor of J. S. Bell, the discoverer of Bell's inequality.

Here H^0 and H^1 are eigenspaces of the square $\mathbf{S}^2$ of the total spin, defined by

$$\mathbf{S}^2 := 1/2\left(3(\sigma_0 \otimes \sigma_0) + \sum_{i=1}^{3} (\sigma_i \otimes \sigma_i) \right) \tag{18}$$

More precisely, one easily verifies that for i, j = 1, 2, 3

$$(\sigma_i \otimes \sigma_i)\psi_0 = -\psi_0 \tag{19}$$

and

$$(\sigma_i \otimes \sigma_i)\psi_j = (-1)^{\delta_{ij}}\psi_j \tag{20}$$

For the sequel it is important to observe that A_{2h} is a real Hilbert space if endowed with the inner product

$$\langle a, b\rangle = \text{trace}(ab), \qquad (a, b \in A_{2h}) \tag{21}$$

and that it is also the carrier space of a representation of the subgroup $U_1 \otimes U_1 \subset U_2$ defined by the formula

$$a \mapsto a' = (u_1 \otimes u_2)a(u_1^* \otimes u_2^*), \qquad (a \in A_{2h}, \quad u_1, u_2 \in U_1) \tag{22}$$

A_{2h} decomposes into an orthogonal sum of four irreducible subspaces:

$$A_{2h} = A^0 \oplus A^1 \oplus A^{1'} \oplus A^2 \tag{23}$$

An orthogonal basis of A_{2h} adapted to this decomposition is given by the products

$$\{\sigma_0 \otimes \sigma_0, \sigma_0 \otimes \sigma_i, \sigma_i \otimes \sigma_0, \sigma_i \otimes \sigma_j | i, j = 1, 2, 3\} \tag{24}$$

Here $\{\sigma_0 \otimes \sigma_0\}$ spans A_0, $\{\sigma_i \otimes \sigma_0 | i = 1, 2, 3\}$ is a basis for A^1, $\{\sigma_0 \otimes \sigma_i | i = 1, 2, 3\}$ is a basis for $A^{1'}$, and finally $\{\sigma_i \otimes \sigma_j | i, j = 1, 2, 3\}$ is a basis for A^2.

Equations (19) and (20) allow us to express the projection operators $P_i := P_{\psi_i}$ corresponding to the members of the Bell basis in term of the basis (24):

$$\begin{aligned}
P_0 &= 1/4(\sigma_0 \otimes \sigma_0 - \sigma_1 \otimes \sigma_1 - \sigma_2 \otimes \sigma_2 - \sigma_3 \otimes \sigma_3) \\
P_1 &= 1/4(\sigma_0 \otimes \sigma_0 - \sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2 + \sigma_3 \otimes \sigma_3) \\
P_2 &= 1/4(\sigma_0 \otimes \sigma_0 + \sigma_1 \otimes \sigma_1 - \sigma_2 \otimes \sigma_2 + \sigma_3 \otimes \sigma_3) \\
P_3 &= 1/4(\sigma_0 \otimes \sigma_0 + \sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2 - \sigma_3 \otimes \sigma_3)
\end{aligned} \tag{25}$$

2. THE STRUCTURE OF THE SET OF ALL TWO-PARTICLE DENSITY OPERATORS

In this section we shall analyze the set S_2 of all density operators of a pair of spin-1/2 particles. Any density operator $\rho \in S_2$, when expanded with respect to the basis (24), yields an expression of the following form:

$$\rho = \rho(\mathbf{r}, \mathbf{s}, T)$$

$$:= 1/4(\sigma_0 \otimes \sigma_0 + \mathbf{r} \cdot \sigma \otimes \sigma_0 + \sigma_0 \otimes \mathbf{s} \cdot \sigma + \sum_{i,j=1}^{3} t_{ij}\sigma_i \otimes \sigma_j) \quad (26)$$

Definition 1. The 3×3 matrix

$$T_\rho = T = (t_{ij}) = \langle \sigma_i \otimes \sigma_j, \rho \rangle$$

is called the correlation matrix. Its singular values,

$$\mu_1 \geq \mu_2 \geq \mu_3$$

i.e., the eigenvalues of

$$[T_\rho] = (T_\rho^* T_\rho)^{1/2}$$

are called the *correlation values* of ρ.

The significance of the correlation matrix T_ρ is that the expectation value of a decomposable spin observable [i.e., one whose corresponding operator has the form $(\mathbf{a}\sigma \otimes \mathbf{c}\sigma)$], in the state represented by ρ, has the simple form

$$\varepsilon_\rho(\mathbf{a}, \mathbf{c}) := \langle (\mathbf{a}\sigma \otimes \mathbf{c}\sigma), \rho \rangle = (\mathbf{a}, T_\rho \mathbf{c}) \quad (27)$$

Examples. From equation (25) we can read off the correlation matrices of the projectors corresponding to the members of the Bell basis. They are given by the following *diagonal* matrices:

$$T_{P_0} = diag(-1, -1, -1)$$
$$T_{P_1} = diag(-1, +1, +1) \quad (28)$$
$$T_{P_2} = diag(+1, -1, +1)$$
$$T_{P_3} = diag(+1, +1, -1)$$

Our first problem is to characterize the convex set $\mathscr{C}$ of all correlation marices. For this purpose it is useful to observe that S_2 remains invariant under the action of the group $U_1 \otimes U_1$ on A_{2h}, defined by equation (22).

Formula (9) entails that density operators transform under this group as follows:

$$\rho' := (u_1 \otimes u_2)\rho(\mathbf{s}, \mathbf{r}, T)(u_1^* \otimes u_2^*) = \rho\, (R(u_1)\mathbf{r}, R(u_2)\mathbf{s}, R(u_1)TR(u_2)^*), \tag{29}$$

where $u_1, u_2 \in U_1$, from which we extract the following transformation law for correlation matrices:

$$T_{\rho'} = R(u_1)T_\rho R(u_2)^* \tag{30}$$

The group $U_1 \otimes U_1$ induces an equivalence relation on the sets of all density operators and correlation matrices, respectively.

Definition 2. Two density operators ρ, ρ' are said to be 1-*equivalent* (in symbols: $\rho' \simeq \rho$) provided $\rho' = (u_1 \otimes u_2)\rho(u_1^* \otimes u_2^*)$.

Two correlation matrices are said to be 1-*equivalent* (in symbols: $T' \simeq T$) provided there exist rotation matrices R_1, R_2 such that $T' = R_1 TR_2^*$.

One consequence of the transformation formula (30) is that the correlation values of ρ are *invariants* under the action of the group $U_1 \otimes U_1$.

Another consequence of the formula (30) is that each orbit of $U_1 \otimes U_1$ in S_2 contains a density operator ρ with a *diagonal* correlation matrix T_ρ. Thus we can state the following lemma:

Lemma 2. Given $\rho \in S_2$, there exists $\rho' \in S_2$ such that $\rho' \simeq \rho$ and

$$T_{\rho'} = \begin{cases} +diag(\mu_1, \mu_2, \mu_3) & \text{if} \quad detT_\rho \geq 0 \\ -diag(\mu_1, \mu_2, \mu_3) & \text{if} \quad detT_\rho < 0 \end{cases} \tag{31}$$

Remark. Observe that a necessary condition for the minus sign in equation (31) to hold is that T_ρ and therefore $[T_\rho]$ has full rank; in other words, none of the singular values is zero.

Proof of the Lemma. By the polar decomposition theorem there exists a rotation matrix R_ρ such that

$$T_\rho = \begin{cases} R_\rho[T_\rho] & \text{if} \quad detT_\rho \geq 0 \\ -R_\rho[T_\rho] & \text{if} \quad detT_\rho < 0 \end{cases} \tag{32}$$

Now let R be a rotation matrix such that

$$R[T_\rho]R^* = diag(\mu_1, \mu_2, \mu_3)$$

Then we have

$$RR_\rho^* T_\rho R^* = \begin{cases} +diag(\mu_1, \mu_2, \mu_3) & \text{if} \quad detT_\rho \geq 0 \\ -diag(\mu_1, \mu_2, \mu_3) & \text{if} \quad detT_\rho < 0 \end{cases} \tag{33}$$

Now let $u_1, u_2 \in U_1$ be such that $R(u_1) = RR_\rho^*$ and $R(u_2) = R$. Then $\rho' = (u_1 \otimes u_2)\rho(u_1^* \otimes u_2^*)$ has the desired property. QED

The following proposition is a well-known consequence of the the Cauchy–Schwarz inequality:

Proposition 1. If **a** and **c** are unit vectors in $\mathcal{R}^3$, then

$$\left|\varepsilon_\rho(\mathbf{a}, \mathbf{c})\right| = \left|(\mathbf{a}, T_\rho \mathbf{c})\right| \leq \mu_1 \tag{34}$$

Moreover, equality holds iff **c** is an eigenvector of T_ρ belonging to the greatest eigenvalue u_1 and **a** is of the form $O\mathbf{c}$, where $O = \pm R_\rho$ is the orthogonal matrix occurring in a polar decomposition of T_ρ [cf. equation (32)].

As a particular instance of inequality (34) we obtain

$$\left|t_{ij}\right| \leq \mu_1 \qquad \text{for} \quad i, j = 1, 2, 3$$

The following theorem is due to Horodecki *et al.*[4] It characterizes the set Δ of all *diagonal* correlation matrices.

Theorem 1. The set Δ of all diagonal correlation matrices considered as a subset of the three-dimensional space of all diagonal 3×3 matrices coincides with the tetrahedron with the vertices T_{P_k} [compare equations (28)].

Proof. Let $\mathcal{T}$ denote the tetrahedron with vertices T_{P_k}, $k = 0, 1, 2, 3$, within the space of all diagonal 3×3 matrices identified with $\mathcal{R}^3$. Then it easily seen that the dual tetrahedron of $\mathcal{T}$ within $\mathcal{R}^3$, i.e., the set

$$\mathcal{T}^0 = \{X \big| \langle X, T \rangle \leq 1 \ \forall T \in \mathcal{T}\}$$

coincides with $-\mathcal{T}$, i.e, using the bipolar theorem,

$$\mathcal{T} = (-\mathcal{T})^0 \tag{35}$$

Now let $\rho = \rho(\mathbf{r}, \mathbf{s}, T)$ be a density operator with diagonal correlation matrix $T = T_\rho = diag(t_1, t_2, t_3)$. Then the condition that $\langle \rho, P_k \rangle \geq 0$ for $k = 0, 1, 2, 3$ implies that T_ρ belongs to $(-\mathcal{T})^0$. Thus we have $\Delta \subset (-\mathcal{T})^0$. Since on the other hand $\mathcal{T} \subset \Delta$, the conclusion follows from equation (35). QED

Remark. Note that the theorem represents $\mathcal{T}$ as the intersection of the following four half-spaces:

$$\begin{aligned} t_1 + t_2 + t_3 &\leq 1 \\ t_1 - t_2 - t_3 &\leq 1 \\ -t_1 + t_2 - t_3 &\leq 1 \\ -t_1 - t_2 + t_3 &\leq 1 \end{aligned} \tag{36}$$

Theorem 2. The set $\mathcal{C}$ of all correlation matrices is given by

$$\mathcal{C} = -convSO(3)$$

whereby the set of extreme points of $\mathcal{C}$ coincides with $-SO(3)$.

Proof. The group $SO(3) \times SO(3)$ acts on $\mathcal{C}$ via the rule

$$(R_1, R_2)T = R_1 T R_2^*, \qquad T \in \mathcal{C}, \quad (R_1, R_2) \in SO(3) \times SO(3)$$

Since $-I = T_{P_0} \in \mathcal{C}$, it follows that for any $R \in SO(3)$, $- R = (R, I)(-I) \in \mathcal{C}$. Since $\mathcal{C}$ is convex we conclude that $-convSO(3) \subset \mathcal{C}$. To show the converse inclusion, observe that any correlation matrix T is 1-equivalent to a *diagonal* correlation matrix and that by Theorem 1 a diagonal correlation matrix clearly belongs to $-convSO(3)$. That the set of extreme points of $\mathcal{C}$ agrees with $SO(3)$ follows from the obvious fact that the identity matrix cannot be obtained as a weighted mean of two *different* rotation matrices. QED

Among all two-particle density operators $\rho \in S_2$ there are those which correspond to states in which the spins of the two particles are *classically* correlated.

Definition 3. A density operator $\rho \in S_2$ is said to be *separable*, provided it belongs to the convex hull of the set $\mathcal{P}_0$ of all density operators of the form $P \otimes Q$ where $P, Q \in S_1$ are one-dimensional projectors in H_1. A correlation matrix $T \in C$ is called *separable* if it is of the form $T = T_\rho$ for some separable density operator ρ.

Remark. A density operator can well have a separable correlation marix without being separable itself; see Example 1 given at the end of the paper.

Since $\mathcal{P}_0$ is compact, it follows from a theorem of Minkowski that the set $S_2^0 = conv\mathcal{P}_0$ of all separable density operators is compact and therefore the extreme points of S_2^0 must belong to $\mathcal{P}_0$. The converse is also true. Indeed $\mathcal{P}_0$, being a set of one-dimensional projections in H_2, consists of extreme points of S_2 and therefore it certainly consists of extreme points of the subset S_2^0.

Thus we can state the following proposition:

Proposition 2. The set of extreme points of S_2^0 coincides with $\mathcal{P}_0$.

Using the expression for a one-dimensional projection in H_1 given by Lemma 1, we can easily find the form of the correlation matrix $T_{P(\mathbf{x})\otimes Q(\mathbf{y})}$ of an element $P(\mathbf{x}) \otimes Q(\mathbf{y})$ of $\mathcal{P}_0$. We can state the following result:

Lemma 3. We have

$$P(\mathbf{x}) \otimes Q(\mathbf{y}) = \rho(\mathbf{x}, \mathbf{y}, T_{P(\mathbf{x})\otimes Q(\mathbf{y})})$$

where

$$T_{P(\mathbf{x})\otimes Q(\mathbf{y})} = \begin{bmatrix} x_1 y_1 & x_1 y_2 & x_1 y_3 \\ x_2 y_1 & x_2 y_2 & x_2 y_3 \\ x_3 y_1 & x_3 y_2 & x_3 y_3 \end{bmatrix}$$

Let Δ_0 denote the set of all separable and *diagonal* correlation matrices. The following theorem is also due to Horodecki *et al.*[4] However, their proof differs from the one given here.

Theorem 3. As a subset of the three-dimensional space of all diagonal 3×3 matrices, Δ_0 coincides with the octahedron $\mathcal{O}$ with the vertices

$$\begin{aligned} T_{P_{1+}\otimes P_{1\pm}} &= diag(\pm 1\ 0\ 0) \\ T_{P_{2+}\otimes P_{2\pm}} &= diag(0\ \pm 1\ 0) \\ T_{P_{3+}\otimes P_{3\pm}} &= diag(0\ 0\ \pm 1) \end{aligned} \tag{37}$$

whereby the projectors $P_{i\pm}$, $i = 1, 2, 3$, in H_1 are associated with the standard basis vectors in $\mathcal{R}^3$ [cf. formulas (10) and (11)].

Note that $\mathcal{O}$ is characterized by the inequality

$$|t_1| + |t_2| + |t_3| \leq 1 \tag{38}$$

Proof. Since the extreme points of $\mathcal{O}$ belong to Δ_0 and Δ_0 is convex, we have $\mathcal{O} \subset \Delta_0$. To show the reverse inclusion, observe that if $\rho = \rho(\mathbf{r}, \mathbf{s}, T)$ is a separable density operator, then also $\rho' = \rho(-\mathbf{r}, \mathbf{s}, -T)$ is a (separable) density operator. Hence if $T \in \Delta_0$ is, then $T \in \mathcal{T} \cap -\mathcal{T} = \mathcal{O}$. QED

Combining this theorem with the fact that each correlation matrix T is 1-equivalent to $\pm diag(\mu_1, \mu_2, \mu_3)$, we obtain the following corollaries:

Corollary 1. A correlation matrix T is separable iff $\mu_1 + \mu_2 + \mu_3 \leq 1$.

Corollary 2. If a correlation matrix T is nonseparable, then $det T < 0$.

Proof. Let $D = \pm diag(\mu_1, \mu_2, \mu_3) \in \Delta$ with $D \simeq T$. If the + sign holds, then the first inequality of the system (36) implies $\mu_1 + \mu_2 + \mu_3 \leq 1$ and the correlation matrix T is separable. Thus $T \simeq D = -diag(\mu_1, \mu_2, \mu_3)$ and $detT = detD = -\mu_1\mu_2\mu_3 < 0$. (Cf. Remark after Lemma 2.) QED

Remark. The condition that $detT < 0$ is only necessary but not sufficient for nonseparability of T. Indeed the correlation matrix $T = -1/3I$ belongs to the octahedron $\mathbb{O}$ and therefore is separable; however, $detT < 0$ (see also Example 2 at the end of the paper).

Corollary 3. Let $\mu_1 \geq \mu_2 \geq \mu_3$ be the three singular values of a nonseparable correlation marix in descending order. Then

$$(1)\ \mu_1 + \mu_2 + \mu_3 > 1$$

$$(2)\ \mu_1 + \mu_2 \leq 1 + \mu_3 \tag{39}$$

Conversely, given any three numbers $\mu_1, \mu_2, \mu_3 \in (0, 1]$ in descending order and satisfying inequalities (1) and (2) of the Corollary, then

$$\rho = 1/2[(\mu_1 + \mu_2 + \mu_3 - 1)P_0 + (1 + \mu_1 - \mu_2 - \mu_3)P_{1+} \otimes P_{1-} + (1 - \mu_1 + \mu_2 - \mu_3)P_{2+} \otimes P_{2-} + (1 - \mu_1 - \mu_2 + \mu_3)P_{3+} \otimes P_{3-}] \tag{40}$$

is a (nonseparable) density operator with nonseparable correlation matrix $T_\rho = -diag(\mu_1, \mu_2, \mu_3)$.

Proof. Since T_ρ is nonseparable, it follows from Corollary 1 that its singular values satisfy inequality (1). Furthermore, since $T_\rho \simeq -diag(\mu_1, \mu_2, \mu_3) \in \Delta$ (cf. Proof of Corollary 2), the third inequality of the system (36) yields inequality (2) of Corollary 3. Conversely if (μ_1, μ_2, μ_3) is a triple of numbers from the interval (0,1], in descending order, which satisfies the two inequalities of Corollary 3, then ρ as defined by equation (40) is a density operator and a short computation shows that its correlation matrix coincides with $-diag(\mu_1, \mu_2, \mu_3)$. QED

3. CLASSIFICATION OF THE SET OF PURE STATES OF A TWO-SPIN SYSTEM

The set of all pure states of a system of two spin-1/2 particles is in one-to-one correspondence with the set $\mathcal{P}$ of one-dimensional projections in H_2. The set $\mathcal{P}$ coincides with the set of extreme points of S_2. Also note that $\mathcal{P}$ is *invariant* under the group $U_1 \otimes U_1$. In this section we are going to describe the orbits of $\mathcal{P}$ under the action of this group. It turns out that they can be parametrized by a single number ξ varying over the interval [0, 1]. If $\mathcal{P}_\xi$

denotes the orbit corresponding to $\xi \in [0, 1]$, then a representative of $\mathcal{P}_\xi$, whose correlation matrix is diagonal, is given by

$$Q(\xi) := 1/4(\sigma_0 \otimes \sigma_0 + \sqrt{1-\xi^2}\,(\sigma_1 \otimes \sigma_0) - \sqrt{1-\xi^2}\,(\sigma_0 \otimes \sigma_1) - \sigma_1 \otimes \sigma_1 - \xi(\sigma_2 \otimes \sigma_2) - \xi(\sigma_3 \otimes \sigma_3)) \quad (41)$$

Thus, in particular, $Q(0) = P_{1+} \otimes P_{1-}$ and $Q(1) = P_0$. More generally, $\mathcal{P}_0$ consists of all *decomposable* projections, whereas $\mathcal{P}_1$ coincides with the set of all projections of the form

$$P = \rho(0, 0, R) = 1/4(\sigma_0 \otimes \sigma_0 - \sum_{i,j=1}^{3} r_{i,j}(\sigma_i \otimes \sigma_j)) \quad (42)$$

where $R = (r_{i,j}) \in SO(3)$ is a rotation matrix. It follows that $\mathcal{P}_0$ is diffeomorphic to $S^2 \times S^2$ and $\mathcal{P}_1$ is diffeomorphic to the group of rotations $SO(3)$. For $\xi \in (0, 1)$, $\mathcal{P}_\xi$ turns out to be diffeomorphic to the five-dimensional manifold $S^2 \times SO(3)$.

In order to arrive at all these insights, we start by characterizing the one-dimensional projections among the general two-particle density operators.

Theorem 4. Let

$$\rho = \rho(\mathbf{r}, \mathbf{s}, T) := 1/4\,(\sigma_0 \otimes \sigma_0 + \mathbf{r}\cdot\sigma \otimes \sigma_0 + \sigma_0 \otimes \mathbf{s}\cdot\sigma + \sum_{i,j=1}^{3} t_{ij}\sigma_i \otimes \sigma_j) \in S_2 \quad (43)$$

be a two-particle density operator. Then ρ is a one-dimensional projection iff the following conditions are satisfied:

(1) $\|\mathbf{r}\|^2 + \|\mathbf{s}\|^2 + trace(T^*T) = 3$.
(2) $T^*\mathbf{r} = \mathbf{s}$ & $T\mathbf{s} = \mathbf{r}$.
(3) $det(T)I + T^*T = \|\mathbf{s}\|^2 E_{\mathbf{s}}$.

Here I stands for the identity matrix and $E_{\mathbf{s}}$ denotes the orthogonal projector in $\mathcal{R}^3$ onto the one-dimensional subspace generated by $\mathbf{s}$, in case $\mathbf{s} \neq \mathbf{0}$.

Making use of the observation that $\rho \in \mathcal{P}$ iff $\rho^2 = \rho$, the theorem follows immediately from the following proposition, which in turn can be verified by direct computation.

Proposition 3. Let $\rho = \rho(\mathbf{r}, \mathbf{s}, T)$ be as in the theorem. Then

$$\rho^2 = 1/16[(1 + \|\mathbf{r}\|^2 + \|\mathbf{s}\|^2 + trace(T^*T))(\sigma_0 \otimes \sigma_0) + 2(\mathbf{r} + T\mathbf{s})\cdot\sigma \otimes \sigma_0 + \sigma_0 \otimes 2(\mathbf{s} + T^*\mathbf{r})\cdot\sigma + 2\sum_{i,j=1}^{3}(t_{ij} + r_i s_j - (adT)_{ji})(\sigma_i \otimes \sigma_j)] \quad (44)$$

Here *adT* stands for the *adjoint* (or *adjugate*) matrix whose (j, i)th entry is the cofactor of t_{ij}.

Next we consider some consequences of conditions (1)–(3) of Theorem 4.

Lemma 4. For any $P \in \mathcal{P}$ the inequality

$$-1 \leq det(T_P) \leq 0 \tag{45}$$

holds.

Proof. Condition (2) implies that

$$\|\mathbf{r}\|^2 = (\mathbf{r}, T\mathbf{s}) = (T^*\mathbf{r}, \mathbf{s}) = \|\mathbf{s}\|^2 \tag{46}$$

and thus condition (1) simplifies to

$$2\|\mathbf{s}\|^2 + \mathrm{trace}(T^*T) = 3 \tag{47}$$

Furthermore, taking the trace in condition (3) yields

$$detT + \mathrm{trace}(T^*T) = \|\mathbf{s}\|^2 \tag{48}$$

Combining these two equations leads to

$$det(T) = \|\mathbf{s}\|^2 - 1 \tag{49}$$

Equation (49) implies in particular that $det(T) \geq -1$. On the other hand, condition (3) of Theorem 4 makes $det(T) > 0$ impossible, since otherwise the left-hand side of the condition would have rank 3, whereas the right hand side has rank at most one. QED

Lemma 4 implies that if we put

$$\xi := \sqrt{-det(T)} \tag{50}$$

then $\xi \in [0, 1]$. Observe that for each $\xi \in [0, 1]$ the set

$$\mathcal{P}_\xi := \{P \in \mathcal{P} \,|\, det(T_P) = -\xi^2\} \tag{51}$$

is invariant under $U_1 \otimes U_1$. Let us look at the special cases where $\xi = 0$ and $\xi = 1$, respectively. If $\xi = 0$, it follows from equation (49) that $\mathbf{s}$ and therefore by equation (46) also $\mathbf{r}$ are unit vectors. Moreover condition (3) of Theorem 1 becomes

$$T^*T = E_{\mathbf{s}} \tag{52}$$

an equation which shows that in this case T is a *partial isometry* between the one-dimensional subspaces of $\mathcal{R}^3$ generated by **s** and $\mathbf{r} = T\mathbf{s}$. Thus we have

$$\mathrm{P} = \rho(\mathbf{r},\mathbf{s},T) := P(\mathbf{r}) \otimes P(\mathbf{s}) \tag{53}$$

This argument justifies in retrospect the notation $\mathcal{P}_0$ for the set of all *decomposable* projections which we used in Section 2.

If $\xi = 1$, it follows from equation (49) that $\mathbf{s} = 0$. Condition (3) of Theorem 4 then implies that T is an (improper!) *orthogonal* matrix and therefore that P is of the form (42). Let us say of a projection of this kind (and the corresponding pure state) that it is of *orthogonal type*. Using this terminology, we can say that $\mathcal{P}_1$ comprises precisely the set of all projections of orthogonal type. It is obvious that the group $U_1 \otimes U_1$ acts transitively on $\mathcal{P}_0$ and on $\mathcal{P}_1$, i.e., $\mathcal{P}_0$ and $\mathcal{P}_1$ are *orbits*. The next theorem shows that this is true for *every* value of ξ.

Theorem 5. Given any $P \in \mathcal{P}_\xi$, P is 1-equivalent to the projection $Q(\xi)$ as defined by equation (41). Thus $\mathcal{P}_\xi$ is an orbit under the group $U_1 \otimes U_1$.

Proof. Throughout the proof we fix a particular projection $P := \rho(T\mathbf{s}, \mathbf{s}, T) \in \mathcal{P}_\xi$. Since the theorem obviously holds in the case where $\xi = 0, 1$, we may assume that $\xi \in (0, 1)$. Then $det(T) = -\xi^2 < 0$ and $\|\mathbf{s}\| = \sqrt{1 - \xi^2} \neq 0$. Condition (2) of Theorem 4 now implies that **s** is an eigenvector of $[T]$ belonging to the eigenvalue 1. Thus the greatest correlation value μ_1 of P is 1. We assert that $\mu_2 = \mu_3 = \xi$. Indeed from equation (47) we obtain

$$1 + \mu_2^2 + \mu_3^2 = \mathrm{trace}(T^*T) = 1 + 2\xi^2 \tag{54}$$

Moreover, since

$$\sqrt{\mu_2^2\,\mu_3^2} = det\,(T^*T)^{1/2} = \left|det\,(T)\right| = \xi^2 \tag{55}$$

we see that the geometric and the arithmetic means of the numbers μ_2^2, μ_3^2 coincide and equal ξ^2 and thus both numbers must also agree with ξ^2.

Next observe that since $det(T) < 0$, there exists a unique matrix $R \in SO(3)$ such that

$$T = -R[T] \tag{56}$$

It follows that

$$P = \rho(T\mathbf{s},\mathbf{s}, T) = \rho(-R\mathbf{s},\mathbf{s}, -R[T]) \simeq \rho(-\mathbf{s}, \mathbf{s}, -[T]) \tag{57}$$

Now let $R_1 \in SO(3)$ be such that $R_1[T]R_1^* = diag(1,\xi,\xi) =: D$. Then

$$\rho(-\mathbf{s},\mathbf{s}, -[T]) \simeq \rho(-R_1\mathbf{s},R_1\mathbf{s}, -D) \tag{58}$$

Since $R_1\mathbf{s}$ must be an eigenvector of D of length $\sqrt{1 - \xi^2}$ belonging to the eigenvalue 1, we conclude that $R_1\mathbf{s} = \pm\sqrt{1-\xi^2}\mathbf{e}_1$. Now the rotation matrix R_1 can easily be adjusted in such a way that

$$R_1\mathbf{s} = -\sqrt{1-\xi^2}\mathbf{e}_1 \tag{59}$$

Hence

$$P \simeq \rho(\sqrt{1-\xi^2}\mathbf{e}_1, -\sqrt{1-\xi^2}\mathbf{e}_1, -D) = Q(\xi) \quad \text{QED} \tag{60}$$

For $\xi \,\varepsilon\, [0, 1]$ we introduce the convex hull of $\mathcal{P}_\xi$:

$$S_2^\xi = conv\mathcal{P}_\xi$$

An analogous proof to the proof of Proposition 2 establishes that $\mathcal{P}_\xi$ comprises the set of extreme points of S_2^ξ.

Remark. Observe that if $\xi \in (0, 1)$, any $\rho \in \mathcal{P}_\xi$ has the form

$$\rho = \rho(\sqrt{1-\xi^2}R\mathbf{u}, \sqrt{1-\xi^2}\mathbf{u}, -R(\tfrac{1}{2}(1-\xi)\, R_\mathbf{u} + \tfrac{1}{2}(1+\xi)I)) \tag{61}$$

where $\mathbf{u} \in S^2$, $R_\mathbf{u}$ is the rotation $R_\mathbf{u} = 2E_\mathbf{u} - I$, and $R \in SO(3)$. In fact the map $\Psi_\xi : S^2 \times SO(3) \to \mathcal{P}_\xi$, defined by

$$(\mathbf{u}, R) \mapsto \rho(\sqrt{1-\xi^2}\, R\mathbf{u}, \sqrt{1-\xi^2}\mathbf{u}, -R(\tfrac{1}{2}(1-\xi)R_\mathbf{u} + \tfrac{1}{2}(1+\xi)I)) \tag{62}$$

is a diffeomorphism of $S^2 \times SO(3)$ onto $\mathcal{P}_\xi$.

Finally, combining the results of Section 3 with those of Section 2, we have the following result:

Theorem 6. The map $T \mapsto \rho(0, 0, T)$, $T \in \mathcal{C}$, is the inverse of the affine map $\rho \mapsto T_\rho$ restricted to the set S_2^1. Moreover, it maps separable correlation matrices onto separable density operators.

Proof. The affine map $\rho \to T_\rho$, $\rho \in S_2^1$, between S_2^1 and $\mathcal{C}$ extends the bijection $P = \rho(0, 0, R) \to R$, $R \in SO(3)$, between the respective sets of extreme points and therefore is itself bijective, possessing the map $T \mapsto \rho(0, 0, T)$, $T \in \mathcal{C}$, as its inverse.

To show that it maps separable correlation matrices onto separable density operators, it suffices to show that for $\mathbf{x}, \mathbf{y} \in \mathcal{R}^3$, $\rho(0, 0, T_{p(\mathbf{x})\otimes P(\mathbf{y})})$ is separable. But

$$\rho(0, 0, T_{P(\mathbf{x})\otimes P(\mathbf{y})}) = 1/2(P(\mathbf{x}) \otimes P(\mathbf{y}) + P(-\mathbf{x}) \otimes P(-\mathbf{y})) \quad \text{QED}$$

We finally consider two examples. The first was put forward by Horodecki *et al.*[1]

Example 1. Let

$$\phi_1 = \cos\alpha(e_1 \otimes e_1) + \sin\alpha(e_2 \otimes e_2)$$

and

$$\phi_2 = \cos\alpha(e_1 \otimes e_2) + \sin\alpha(e_2 \otimes e_1)$$

Then $P_{\phi_1}, P_{\phi_2}, \in \mathcal{P}_\xi$, where $\xi = |\sin 2\alpha|$.
For $p \in [0, 1]$ define

$$\rho = pP_{\phi_1} + (1 - p)P_{\phi_2}$$

Then according to a necessary and sufficient condition for separability given by Horodecki *et al.*,[1] ρ is nonseparable precisely if $p \neq 1/2$ and $\xi \neq 0$. But since

$$T_\pi = \begin{bmatrix} \sin 2\alpha & 0 & 0 \\ 0 & (1 - 2p)\sin 2\alpha & 0 \\ 0 & 0 & 2p - 1 \end{bmatrix}$$

T_ρ is separable iff

$$0 < |1 - 2p| \leq \frac{1 - \xi}{1 + \xi}$$

by Corollary 1; e.g., $\xi = 1/2$ ($\alpha = \pi/12$) and $p = 1/3$ yields an example of a nonseparable density operator ρ whose correlation matrix is separable. In fact the example shows that each S_2^ξ for $\xi \in (0, 1)$ contains density operators with this property.

Example 2 (Werner[5]). Clearly a density operator ρ is *invariant* with respect to the group $U_1 \otimes U_1$ iff ρ is of the form

$$\rho = \rho(0, 0, \lambda I)$$

By the inequalities (36), $\lambda I \in \mathcal{C}$ iff $\lambda \in [-1, 1/3]$. Furthermore, by Corollary 1 and Theorem 7, ρ is separable iff $\lambda \in [-1/3, 1/3]$.

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