Bound entangled Gaussian states

R. F. Werner* and M. M. Wolf†
Institut für Mathematische Physik, TU Braunschweig,
Mendelssohnstr.3, 38106 Braunschweig, Germany.
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I. INTRODUCTION

Many experiments in the young field of quantum information physics are not carried out on finite dimensional quantum systems, for which most of the basic theory has been developed, but in the quantum optical setting. In that setting the basic variables are quadratures of field modes, which satisfy canonical commutation relations, and hence have no finite dimensional realizations. It would seem that the theory therefore becomes burdened with all the technical difficulties of infinite dimensional spaces, while theoreticians are on the other hand still struggling to answer some simple questions about qubit systems. However, the states relevant in quantum optics are often of a special kind, and for this class the typical questions of quantum information theory are luckily of the same complexity as for the usual finite dimensional systems.

This simple class of states of “continuous variable systems” is the class of Gaussian states, i.e., those states whose Wigner function is a Gaussian on phase space. Such a state is therefore completely specified by its mean and its covariance matrix, where the mean is irrelevant for entanglement questions, because it can be shifted to zero by a local unitary (phase space translation). It turns out that the basic entanglement properties of a Gaussian density matrix (as a state on two infinite dimensional Hilbert spaces) can be translated very nicely into properties of its covariance matrix (see Section 2), so that problems involving Gaussian states are reduced to problems of finite dimensional linear algebra rather reminiscent of the problems involving finite dimensional density matrices.

For the latter it is well known [3] that the positivity of the partial transpose (“ppt”) is necessary for separability, but sufficient only for the smallest non-trivial systems, namely systems in dimensions $2 \otimes 2$ and $2 \otimes 3$. In all higher dimensions we can find “bound entangled states”, which are not separable, but nevertheless have a positive partial transpose, and are hence not distillable [4]. In the case of continuous variable systems the first nontrivial examples of this kind were obtained in [5]. In the Gaussian setting it was shown by Simon [5] that for bipartite systems with one canonical degree of freedom on each side (Alice and Bob), i.e., once again for the simplest possible systems, the equivalence of ppt and separability also holds. For this system it was also shown that non-ppt states are indeed distillable [3].

In the present paper we settle the relationship between separability and ppt for all higher dimensions, showing that the equivalence holds also for systems of $1 \times N$ oscillators, but fails for all higher dimensions. We show this by giving explicit examples for $2 \times 2$ oscillators.

The key idea for constructing bound entangled Gaussian states is the notion of “minimally ppt” covariance matrices. These are defined as the covariance matrices of ppt Gaussian states, which are not larger (in matrix ordering) than the covariance matrix of any other ppt Gaussian state. It is easy to see that a minimally ppt covariance matrix belongs to a separable state iff that state is a product state. Hence bound entangled Gaussians arise from all minimally ppt covariance matrices, which are not block diagonal. Numerically, minimally ppt covariance matrices can be obtained very efficiently by successively subtracting rank one operators from a given covariance matrix. This algorithm is reminiscent of techniques for density matrices in the context of “best separable approximation” [6]. Running this procedure for $2 \times 2$ or larger systems generically gives bound entangled Gaussian states.

Our paper is organized as follows: In Section 2 we will set up the basic notation, and the translation of separability and ppt conditions into properties of covariance matrices (for separability this appears to be new). We also describe the minimally ppt covariance matrices. In Section 3 we prove the equivalence for the $1 \times N$ case, and in Section 4 we present a five parameter family of $2 \times 2$ bound entangled states.

*Electronic Mail: r.werner@tu-bs.de
†Electronic Mail: mm.wolf@tu-bs.de
II. GAUSSIAN STATES AND ENTANGLEMENT

A system of $f$ canonical degrees of freedom is described classically in a phase space, which is a $2f$-dimensional real vector space $X$. The canonical structure is given by a $2f \times 2f$ matrix $\sigma$, known as the symplectic matrix, which is antisymmetric and non-singular. With a suitable choice of coordinates (“canonical coordinates”), it can be brought into a standard form: The $2f$ variables are then grouped into $f$ canonical pairs (e.g., position and momentum), for each of which the symplectic matrix takes the form $\sigma = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, and all other matrix elements vanish.

The symplectic matrix also governs the canonical commutation relations for the corresponding quantum system: if $R_\alpha$, $\alpha = 1, \ldots, 2f$ are canonical operators (for canonical coordinates these are naturally grouped into $f$ standard position operators and $f$ standard momentum operators), the commutation relations read

$$i[R_\alpha, R_\beta] = \sigma_{\alpha\beta}1 \, .$$

These relations may be exponentiated to the Weyl relations involving unitaries $W(\xi) = \exp(i\xi \cdot \sigma \cdot R)$, where $\xi \in X$, and $\xi \cdot \sigma \cdot R = \sum_{\alpha\beta} \xi_\alpha \sigma_{\alpha\beta} R_\beta$. These Weyl operators implement the phase space translations. We will assume that they act irreducibly on the given Hilbert space, i.e., that there are no further degrees of freedom.

Then by von Neumann’s uniqueness Theorem 8 the $R_\alpha$ are unitarily equivalent to the usual position and momentum operators in the $L^2$ space over position space.

For a general density operator $\rho$ we define the mean as the vector $m_\alpha = \text{tr}(\rho R_\alpha)$, and the covariance matrix $\gamma$ by

$$\gamma_{\alpha\beta} + i\sigma_{\alpha\beta} = 2 \text{tr}[\rho(R_\alpha - m_\alpha 1)(R_\beta - m_\beta 1)] \, ,$$

which is well-defined whenever all of the unbounded positive operators $R_\alpha^2$ have finite expectations in $\rho$. Due to the canonical commutation relations the antisymmetric part of the right hand side is indeed the symplectic matrix, independently of the state $\rho$. The state-dependent covariance matrix $\gamma$ is therefore real and symmetric. Moreover, $\gamma + i\sigma$ is obviously positive definite.

A Gaussian state is best defined in terms of its characteristic function, which for a general state is $\xi \mapsto \text{tr}(\rho W(\xi))$. This should be seen as the quantum Fourier transform of $\rho$, and is indeed the Fourier transform of the Wigner function of $\rho$. Hence we call $\rho$ Gaussian, if its characteristic function is of the form

$$\text{tr}[\rho W(\xi)] = \exp(\text{im}^T \xi - \frac{1}{4} \xi^T \gamma \xi) \, .$$

Here the coefficients were chosen such that $\gamma$ and $m$ are indeed covariance and mean of $\rho$, as is readily verified by differentiation. The necessary condition $\gamma + i\sigma \geq 0$, which is equivalent to $\gamma - i\sigma \geq 0$ by complex conjugation, is also sufficient for Equation 3 to define a positive operator $\rho$. We note for later use that a Gaussian state is pure iff $(\sigma^{-1}\gamma)^2 = -1$, which is equivalent to $\gamma + i\sigma$ having maximal number of null eigenvectors, i.e., the null space $N = \{ \Phi(\gamma + i\sigma)\Phi = 0 \}$ has dimension $(\dim X)/2$. Note that this null space must always be considered as a complex linear subspace of $\mathbb{C}^{2f}$, the complexification of $X$. For such a complex subspace we denote by $\mathbb{R}N$ the subspace of $X$ consisting of all real parts of vectors in $N$. Then a Gaussian state is pure iff $\Re N = X$.

Let us now consider bipartite systems. The phase space is then split into two phase spaces $X = X_A \oplus X_B$, where $A$ stands for Alice and $B$ for Bob. This is a “symplectic direct sum”, which means that $\gamma = \sigma_A \oplus \sigma_B$ is block diagonal with respect to this decomposition. In other words, Alice’s canonical operators $R_\alpha$ commute with all of Bob’s. The Weyl operators are naturally identified with tensor products: $W(\xi_A \otimes \xi_B) \equiv W(\xi_A) \otimes W(\xi_B)$. We call this an $f_A \times f_B$ system, if $\dim X_A = 2f_A$, and $\dim X_B = 2f_B$.

It is clear from (2) and (3) that the covariance matrix of a product state is block diagonal and, conversely, a Gaussian state with block diagonal $\gamma$ is a product state. Separability is characterized as follows:

**Proposition 1.** Let $\gamma$ be the covariance matrix of a separable state with finite second moments. Then there are covariance matrices $\gamma_A$ and $\gamma_B$ such that

$$\gamma \geq \begin{pmatrix} \gamma_A & 0 \\ 0 & \gamma_B \end{pmatrix} \, .$$

Conversely, if this condition is satisfied, the Gaussian state with covariance $\gamma$ is separable.

In order to show the first statement suppose the given state is decomposed into product states with covariance $\gamma^k$ and mean $m^k$ with convex weight $\lambda_k$. Then $m_\alpha = \sum_k \lambda_k m_\alpha^k$ and, similarly, for the second moments we have

$$\gamma_{\alpha\beta} + 2m_\alpha m_\beta = \sum_k \lambda_k (\gamma_A^k + 2m_A^k m_B^k) \, .$$

Hence the difference between $\gamma$ and the block diagonal $\sum_k \lambda_k \gamma^k$ is the matrix

$$\Delta_{\alpha\beta} = 2 \left( \sum_k \lambda_k m_A^k m_B^k - \sum_{k\ell} \lambda_k \lambda_\ell m_A^k m_B^\ell \right) \, ,$$

which is positive definite, because $\sum \xi_\alpha \xi_\beta \Delta_{\alpha\beta} = \sum_{k\ell} \lambda_k \lambda_\ell (s_k - s_\ell)^2 \geq 0$, where $s_k = \sum_\alpha \xi_\alpha m_\alpha$.

In order to show the converse, let $\sigma$ be the Gaussian product state with covariance $\gamma_A \oplus \gamma_B$, and let $\gamma' = \gamma - \gamma_A \oplus \gamma_B \geq 0$. Then $\gamma'$ is the covariance of a classical Gaussian probability distribution $P$, and the characteristic function of the given state $\rho$ is the product of the characteristic function of $\sigma$ and the Fourier transform of $P$. Hence $\rho$ is the convolution of $\sigma$ and $P$ in the sense of 9, which is the average of the phase space
translates \( W(\xi)\sigma W(\xi)^* \) over \( \xi \) with weight \( P \). Since all these states will be product states, \( \rho \) is separable.

There are different ways of characterizing the partial transpose. One simple way is to say that with respect to some set of canonical coordinates the momenta in Alice’s system are reversed, while her position coordinates and all of Bob’s canonical variables are left unchanged. In addition, the order of factors in the partial transpose of \( R_\alpha R_\beta \) is reversed when both factors belong to Alice. When we replace \( \rho \) in \ref{eq_1} by its partial transpose, we therefore find the antisymmetric part of the equation unchanged, whereas \( \gamma_{\alpha\beta} \) picks up a factor \(-1\) whenever just one of the indices corresponds to one of Alice’s momenta. Let us call the resulting covariance matrix by \( \tilde{\gamma} \). Clearly, if the partial transpose of \( \rho \) is again a density operator, we must have \( \tilde{\gamma} + i\sigma \geq 0 \). But this is equivalent to \( \gamma + i\tilde{\sigma} \geq 0 \), where in \( \tilde{\sigma} \) the corresponding components are reversed, so that \( \sigma = (-\sigma_A) \oplus \sigma_B \). This form of the condition is even valid if we do not insist on canonical variables. Combining it with the positivity condition for Gaussian states we get the following characterization:

**Proposition 2** Let \( \gamma \) be the covariance matrix of a state with finite second moments, which has positive partial transpose. Then

\[
\gamma + i\tilde{\sigma} \geq 0 \ , \text{ where } \tilde{\sigma} = \begin{pmatrix} -\sigma_A & 0 \\ 0 & \sigma_B \end{pmatrix} .
\]

Conversely, if this condition is satisfied, the Gaussian state with covariance \( \gamma \) has positive partial transpose.

When \( \rho \) is separable, Proposition \ref{2} shows the existence of a block diagonal \( \gamma' = \gamma_A \oplus \gamma_B \) with \( \gamma \geq \gamma' \). Since \( \gamma_A \) and \( \gamma_B \) are covariance matrices in their own right, we have \( \gamma_A \pm i\sigma_A \geq 0 \), and similarly for Bob’s side. But this means that \( \gamma \geq \gamma' \geq -i\sigma \) and \( \gamma \geq \gamma' \geq -i\tilde{\sigma} \), and \( \gamma \) has positive partial transpose, as a separable density operator should. We have made this explicit, because it shows that it may be interesting to see how much “space” there is between \( \gamma \) and \( -i\sigma \) and \( -i\tilde{\sigma} \). This leads to the central definition of this paper:

**Definition 1** We say that a real symmetric matrix \( \gamma \) is a ppt-covariance, if \( \gamma + i\sigma \geq 0 \) and \( \gamma + i\tilde{\sigma} \geq 0 \), and that it is minimally ppt, if it is a ppt-covariance, and any ppt-covariance \( \gamma' \) with \( \gamma \geq \gamma' \) must be equal to \( \gamma \).

Note that a minimally ppt matrix \( \gamma \) is separable if and only if it is a direct sum, i.e., if the corresponding state factorizes. There is a rather effective criterion for deciding whether a given ppt-covariance is even minimally ppt: First of all, if there were any \( \gamma' \leq \gamma \) with \( \gamma' \neq \gamma \), we can also choose \( \gamma - \gamma' = \Delta \) to be a rank one operator, i.e., a matrix of the form \( \Delta_{\alpha\beta} = \xi_{\alpha}\xi_{\beta} \). Then we have \( \gamma + i\sigma \geq \epsilon\Delta \) for sufficiently small positive \( \epsilon \) if and only if \( \xi \) is in the support of the positive operator \( \gamma + i\sigma \).

The same reasoning applies to \( \tilde{\sigma} \), so that \( \gamma \) is minimally ppt iff there is no real vector \( \xi \), which is in the support of both \( \gamma + i\sigma \) and \( \gamma + i\tilde{\sigma} \). Rephrasing this in terms of the orthogonal complements of the supports, we get the following characterization which we will use later on:

**Proposition 3** Let \( \gamma \) be a ppt-covariance, and let \( \mathcal{N} \) and \( \tilde{\mathcal{N}} \) denote the null spaces of \( \gamma + i\sigma \) and \( \gamma + i\tilde{\sigma} \), respectively. Then \( \gamma \) is minimally ppt if and only if \( \Phi, \mathcal{N} \) and \( \tilde{\Phi}, \tilde{\mathcal{N}} \) together span \( X \).

This gives an effective procedure to find a minimally ppt \( \gamma' \) below a given \( \gamma \): in each step one substracts the largest admissible multiple of a rank one operator with vector \( \xi \) orthogonal to the span of \( \Phi, \mathcal{N} \) and \( \tilde{\Phi}, \tilde{\mathcal{N}} \), which is then in the supports of \( \gamma + i\sigma \) and \( \gamma + i\tilde{\sigma} \). In every step this will either increase \( \mathcal{N} \) or \( \tilde{\mathcal{N}} \), so that a minimally ppt covariance matrix is reached after a finite number of steps.

### III. THE 1 × N CASE

This section is devoted to the proof that, for Gaussian states of \( 1 \times N \) systems, ppt implies separability. It is clear from the previous section that this is equivalent to saying that every minimally ppt covariance matrix is block diagonal, i.e., belongs to a product state. So throughout this section we assume that \( \gamma \) is a minimally ppt covariance matrix.

As a first step we get rid of irrelevant pure state factors in the following sense: Suppose that the two null spaces have a non-trivial intersection, i.e., there is a \( \Phi \neq 0 \) with \( \Phi \in \mathcal{N} \cap \tilde{\mathcal{N}} \). Then \( \langle \sigma - \tilde{\sigma} \rangle \Phi = (i\gamma - i\tilde{\gamma}) \Phi = 0 \), so \( \Phi \) has non-zero components only in Bob’s part of the system. So let \( X_C \) denote the subspace of \( X_B \) spanned by real and imaginary part of \( \Phi \). Then the restriction of the state to the subsystem \( C \) satisfies the pure state condition (its covariance matrix \( \gamma_C + i\sigma_C \) has a null vector by construction). It follows that the density matrix factorizes: \( \rho_{A,B,C} = \rho_{A,B} \otimes \rho_C \), where \( \rho_C \) is a pure state. (This conclusion can also be obtained purely on the level of covariance matrices, by introducing in \( X_B \) a basis of canonical variables containing a canonical basis of \( X_C \)). Clearly, the separability of such a state is equivalent to the separability of \( \rho \), and the covariance matrix restricted to \( X_A \oplus X_{B\setminus C} \) is again minimally ppt. Hence we have reduced the problem to the analogous one for the smaller space \( X_A \oplus X_{B\setminus C} \).

We may therefore assume without loss of generality that the null spaces \( \mathcal{N} \) and \( \tilde{\mathcal{N}} \) have trivial intersection. This means that we proceed by contradiction, since we want to prove ultimately that the state is a product of “irrelevant pure state factors”.

Now let \( 0 \neq \Phi \in \mathcal{N} \) and \( 0 \neq \tilde{\Phi} \in \tilde{\mathcal{N}} \). Then because \( \gamma \) is hermitian, we have \( \langle \tilde{\Phi}, \gamma \Phi \rangle = \langle \gamma \tilde{\Phi}, \Phi \rangle \). Using the null space conditions and the skew hermiticity of \( \gamma \), we can rewrite this as

\[
\langle \tilde{\Phi}, \gamma \Phi \rangle = \langle \gamma \tilde{\Phi}, \Phi \rangle = \sum_i \gamma_{i\alpha} \tilde{\Phi}_\alpha = 0 \ , \text{ where } \Phi = \sum_i \Phi_i \ , \text{ and } \tilde{\Phi} = \sum_i \tilde{\Phi}_i .
\]
\[ \langle \Phi, (\sigma - \sigma)\Phi \rangle = 0 . \] (8)

Now the vector \((\sigma - \sigma)\Phi \) must be non-zero, since otherwise we would have \(\Phi \in \mathcal{N} \cap \tilde{\mathcal{N}}\). This is a condition on the \(X_A\)-components \(\Phi_A\) of \(\Phi\), since \(\sigma\) and \(\tilde{\sigma}\) differ only on that two-dimensional subspace. By the same token the \(X_A\)-component \(\tilde{\Phi}_A\) of \(\tilde{\Phi}\) must be non-zero. Hence all vectors \((\sigma - \sigma)\Phi \) lie in the one dimensional subspace of \(\mathcal{C} \times X\) orthogonal to \(\tilde{\Phi}_A \neq 0\). The proportionality constant is thus a linear functional on \(\mathcal{N}\) vanishing only for \(\Phi = 0\), which means that \(\mathcal{N}\) must be one dimensional. By symmetry dim \(\tilde{\mathcal{N}} = 1\). By Proposition 3 the spaces \(\mathcal{H}_A \mathcal{N}\) and \(\mathcal{H}_A \tilde{\mathcal{N}}\) together span \(X\), and since they are two dimensional, it follows that dim \(X \leq 4\), i.e., we can have at most a \(1 \times 1\) system. For such systems our claim has been shown by Simon [3], and is hence proved.

**IV. 2 × 2 BOUND ENTANGLED STATES**

It was already mentioned in the introduction that numerical examples of minimally ppt covariances, which do not split into \(\gamma_A \oplus \gamma_B\) are easily generated by the subtraction method. In contrast, the subtraction method for \(1 \times N\) systems always ends up at a block diagonal \(\gamma\). This is rather striking, but not really conclusive, because the numerical determination of the null space of a matrix which may have small eigenvalues may depend critically on rounding errors. We have therefore prepared the following all integer \(2 \times 2\) example \(\gamma\):

\[
\gamma = \begin{pmatrix}
2 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 2 & 0 \\
0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
\end{pmatrix}
\]. (9)

The key to getting simple examples is symmetry, which in turn simplifies the verification of the basic properties. The most important symmetry in the example is the multiplication operator \(S\) with diagonal matrix elements \((1, 1, -1, -1, 1, -1, 1, 1)\). It satisfies \(S\sigma + \bar{\sigma}S = 0\), and \(S\gamma = \gamma S\). Consequently, \(\gamma + i\sigma\) and \(\gamma - i\bar{\sigma} = S(\gamma + i\sigma)S\) are unitarily equivalent, so it suffices to check the positivity and to compute the null space of \(\gamma + i\sigma\). We note in passing that this unitary equivalence is not necessary for bound entangled Gaussian states, since generically the spectra of \(\gamma + i\sigma\) and \(\gamma + i\bar{\sigma}\) are different.

Further unitaries commuting with the covariance matrix [3] are the multiplication operator \(C\) with diagonal matrix elements \((-1, -1, 1, -1, 1, -1, 1, 1)\), and the skew symmetric operator \(R\) with \(R_{13} = R_{24} = R_{75} = R_{86} = 1\), and zero remaining entries. All these operators have square \(\pm 1\), and commute with each other and the symplectic forms up to signs. Therefore, if we start with a generic vector \(\Omega_1 \in \mathcal{N}\), the application of \(R, C, S\) and products of these operators yields eight vectors \(\Omega_i\), which form a basis of \(\mathcal{C}^8\). Since these vectors lie in either \(\mathcal{N}, \tilde{\mathcal{N}}\) or their complex conjugates we know how \(\gamma\) acts on them and the covariance matrix is thus determined by \(\gamma = \Lambda\Omega^{-1}\), where \(\Lambda, \Omega\) denote the matrices consisting of column vectors \(\Lambda_k = \gamma \Omega_k\). The above \(\gamma\) is generated in this manner from

\[
\Omega_1 = (-1, i, 2, -3i, 1, -i, 1, 0) .
\] (10)

Then the condition of Proposition 3 is satisfied by construction, and we only have to verify that \(\gamma + i\sigma \geq 0\), which is again simplified by this operator commuting with \(R\). Explicitly, we get the eigenvalues \(0, 3 - \sqrt{3}, 3 + \sqrt{3}\), each with multiplicity 2.

Generalizing this example we can construct a five parameter family of bound entangled Gaussian states commuting with \(R, S\) and \(C\) in the same manner as above. We start with a generic vector

\[
\Omega_1 = (-a, ib, c, -id, e, -if, 1, 0) , \quad a, b, \ldots , f > 0.
\] (11)

Then \(\gamma\) being real and symmetric requires \(d = (bc + f)/a\) and from the characteristic function of \(\langle \Omega_k, \Lambda_i + \sigma \Omega_i \rangle\) we obtain that \(\gamma + i\sigma \geq 0\) iff \(a \leq c\), where equality is ruled out since this would be equivalent to \(\det(\Omega) = 0\).

States obtained from (11) are all of a non block diagonal form similar to (3), and are hence bound entangled.

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