

Bound Entangled Gaussian States

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(Received 4 October 2000)

We discuss the entanglement properties of bipartite states with Gaussian Wigner functions. For the separability, and the positivity of the partial transpose, we establish explicit necessary and sufficient criteria in terms of the covariance matrix of the state. It is shown that, for systems composed of a single oscillator for Alice and an arbitrary number for Bob, positivity of the partial transpose implies separability. However, this implication fails with two oscillators on each side, as we show by constructing a five parameter family of bound entangled Gaussian states.

DOI: 10.1103/PhysRevLett.86.3658

PACS numbers: 03.65.Ud, 03.67.-a

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 type, 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 II), 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 [1,2] that the positivity of the partial transpose (“ppt”) is necessary for separability, but sufficient only for the smallest nontrivial 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 [3]. In the case of continuous variable systems the first nontrivial examples of this kind were obtained in [4]. In the Gaussian setting it was shown by Simon [5] that for bipartite systems with one canonical degree of freedom on each side, i.e., once again for the simplest possible systems, the equivalence of ppt and separability also holds. For this system

another equivalent entanglement criterion was provided in [6], and it was also shown that non-ppt states are indeed distillable [7]. In this 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 2×2 oscillators.

The key idea for constructing bound entangled Gaussian states is the notion of “minimal 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 minimal ppt covariance matrix belongs to a separable state if, and only if, that state is a product state. Hence bound entangled Gaussians arise from all minimal ppt covariance matrices, which are not block diagonal. Numerically, minimal 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” [8]. Running this procedure for 2×2 or larger systems generically gives bound entangled Gaussian states.

Our paper is organized as follows: In Section II 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 minimal ppt covariance matrices. In Section III we prove the equivalence for the $1 \times N$ case, and in Section IV we present a five parameter family of 2×2 bound entangled states.

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 σ , known as the *symplectic matrix*, which is antisymmetric and nonsingular. 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_α , $\alpha = 1, \dots, 2f$ are canonical operators (for canonical coordinates these are naturally grouped into f standard position operators and f standard momentum operators), the commutation relations read

$$i[R_\alpha, R_\beta] = \sigma_{\alpha\beta} \mathbf{1}. \quad (1)$$

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 [9] the R_α are unitarily equivalent to the usual position and momentum operators in the \mathcal{L}^2 space over position space.

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

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

which is well defined whenever all of the unbounded positive operators R_α^2 have finite expectations in ρ . Because of the canonical commutation relations the antisymmetric part of the right-hand side is indeed the symplectic matrix, independently of the state ρ . The state-dependent covariance matrix γ 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 [10] of ρ , and is indeed the Fourier transform of the Wigner function of ρ . Hence we call ρ Gaussian, if its characteristic function is of the form

$$\text{tr}[\rho W(\xi)] = \exp(im^T \xi - \frac{1}{4} \xi^T \gamma \xi). \quad (3)$$

Here the coefficients were chosen such that γ and m are indeed the covariance and mean of ρ , 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 Eq. (3) to define a positive operator ρ . We note for later use that a Gaussian state is pure if, and only if, $(\sigma^{-1}\gamma)^2 = -\mathbf{1}$ [11], which is equivalent to $\gamma + i\sigma$ having the maximal number of null eigenvectors, i.e., the null space $\mathcal{N} = \{\Phi \mid (\gamma + i\sigma)\Phi = 0\}$ 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 $\text{Re}\mathcal{N}$ the subspace of X consisting of all real parts of vectors in \mathcal{N} . Then a Gaussian state is pure if, and only if, $\text{Re}\mathcal{N} = X$.

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 $\sigma = \sigma_A \oplus \sigma_B$ is block diagonal with respect to this decomposition. In other words, Alice's canonical operators R_α commute with all of Bob's. The Weyl operators are naturally identified with tensor products: $W(\xi_A \oplus \xi_B) \cong W(\xi_A) \otimes W(\xi_B)$. 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 γ is a product state. Separability is characterized as follows:

Proposition 1: *Let γ be the covariance matrix of a separable state with finite second moments. Then there are covariance matrices γ_A and γ_B such that*

$$\gamma \geq \begin{pmatrix} \gamma_A & 0 \\ 0 & \gamma_B \end{pmatrix}. \quad (4)$$

Conversely, if this condition is satisfied, the Gaussian state with covariance γ is separable.

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

$$\gamma_{\alpha\beta} + 2m_\alpha m_\beta = \sum_k \lambda_k (\gamma_{\alpha\beta}^k + 2m_\alpha^k m_\beta^k). \quad (5)$$

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

$$\Delta_{\alpha\beta} = 2 \left(\sum_k \lambda_k m_\alpha^k m_\beta^k - \sum_{k\ell} \lambda_k \lambda_\ell m_\alpha^k m_\beta^\ell \right), \quad (6)$$

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

In order to show the converse, let σ be the Gaussian product state with covariance $\gamma_A \oplus \gamma_B$, and let $\gamma' = \gamma - \gamma_A \oplus \gamma_B \geq 0$. Then γ' is the covariance of a classical Gaussian probability distribution P , and the characteristic function of the given state ρ is the product of the characteristic function of σ and the Fourier transform of P . Hence ρ is the convolution of σ , and P in the sense of [10], which is the average of the phase space translates $W(\xi)\sigma W(\xi)^*$ over ξ with weight P . Since all these states will be product states, ρ is separable. \square

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 ρ in (2) 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 ρ 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 $\tilde{\sigma} = (-\sigma_A) \oplus \sigma_B$. This form of the condition is valid even 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 γ be the covariance matrix of a state, with finite second moments, which has positive partial transpose. Then*

$$\gamma + i\tilde{\sigma} \geq 0, \quad \text{where } \tilde{\sigma} = \begin{pmatrix} -\sigma_A & 0 \\ 0 & \sigma_B \end{pmatrix}. \quad (7)$$

Conversely, if this condition is satisfied, the Gaussian state with covariance γ has positive partial transpose.

When ρ is separable, Proposition 2 shows the existence of a block diagonal $\gamma' = \gamma_A \oplus \gamma_B$ with $\gamma \geq \gamma'$. Since γ_A and γ_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 γ 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 γ and $-i\sigma$ and $-i\tilde{\sigma}$. This leads to the central definition of this paper:

Definition: *We say that a real symmetric matrix γ is a ppt covariance, if $\gamma + i\sigma \geq 0$ and $\gamma + i\tilde{\sigma} \geq 0$, and that it is minimal ppt, if it is a ppt covariance, and any ppt covariance γ' with $\gamma \geq \gamma'$ must be equal to γ .*

Note that a minimal ppt matrix γ is separable if, and only if, it is a direct sum, i.e., if the corresponding state factorizes (and is thus a product of pure states). There is a rather effective criterion for deciding whether a given ppt covariance is even minimal ppt: First, 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 $\Delta_{\alpha\beta} = \xi_\alpha \xi_\beta$. Second, we have $\gamma + i\sigma \geq \epsilon\Delta$ for sufficiently small positive ϵ if, and only if, ξ is in the support of the positive operator $\gamma + i\sigma$. The same reasoning applies to $\tilde{\sigma}$, so that γ is minimal ppt if, and only if, there is no real vector ξ , 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:

Proposition 3: *Let γ 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 γ is minimal ppt if, and only if, $\text{Re}\mathcal{N}$ and $\text{Re}\tilde{\mathcal{N}}$ span X together.*

This gives an effective procedure to find a minimal ppt γ' below a given γ : in each step one subtracts the largest admissible multiple of a rank one operator with vector ξ orthogonal to the span of $\text{Re}\mathcal{N}$ and $\text{Re}\tilde{\mathcal{N}}$, which is then in the supports of $\gamma + i\sigma$ and $\gamma + i\tilde{\sigma}$. This will

either increase \mathcal{N} or $\tilde{\mathcal{N}}$, so that a minimal ppt covariance matrix is reached after a finite number of steps.

III. The $1 \times N$ case.—This section is devoted to the proof that, for Gaussian states of $1 \times N$ systems, where N is arbitrarily large, ppt implies separability. It is clear from the previous section that this is equivalent to saying that every minimal ppt covariance matrix is block diagonal, i.e., belongs to a product state. So throughout this section we assume that γ is a minimal 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 nontrivial intersection, i.e., there is a $\Phi \neq 0$ with $\Phi \in \mathcal{N} \cap \tilde{\mathcal{N}}$. Then $(\sigma - \tilde{\sigma})\Phi = (i\gamma - i\gamma)\Phi = 0$, so Φ has nonzero components only in Bob's part of the system. So let X_C denote the subspace of X_B spanned by the real and imaginary parts of Φ . 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: $\rho_{A,B \setminus C} = \rho_{A,B \setminus C} \otimes \rho_C$, where ρ_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 ρ , and the covariance matrix restricted to $X_A \oplus X_{B \setminus C}$ is again minimal 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 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 γ 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 σ , we can rewrite this as

$$\langle \tilde{\Phi}, (\sigma - \tilde{\sigma})\Phi \rangle = 0. \quad (8)$$

Now the vector $(\sigma - \tilde{\sigma})\Phi$ must be nonzero, since otherwise we would have $\Phi \in \mathcal{N} \cap \tilde{\mathcal{N}}$. This is a condition on the X_A components Φ_A of Φ , since σ 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 nonzero. Hence all vectors $(\sigma - \tilde{\sigma})\Phi$ lie in the one-dimensional subspace of $\mathbb{C}X_A$ 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 $\text{Re}\mathcal{N}$ and $\text{Re}\tilde{\mathcal{N}}$ together span X , and, since they are two dimensional, it follows that $\dim X \leq 4$, i.e., we can have at most a 1×1 system. For such systems our claim has been shown by Simon [5], and is hence proved.

IV. 2×2 bound entangled states.—It was already mentioned in the introduction that numerical examples of

minimal 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 γ . 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 2×2 example γ :

$$\gamma = \begin{pmatrix} 2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 2 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 4 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 2 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix}. \quad (9)$$

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 $S\sigma + \tilde{\sigma}S = 0$, and $S\gamma = \gamma S$. Consequently, $\gamma + i\sigma$ and $\gamma - i\tilde{\sigma} = S(\gamma + i\sigma)S$ 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 Gaussians, since generically the spectra of $\gamma + i\sigma$ and $\gamma + i\tilde{\sigma}$ are different.

Further unitaries commuting with the covariance matrix (9) are the multiplication operator C with diagonal matrix elements $(1, -1, 1, -1, 1, -1, 1, -1)$, the skew symmetric operator R with $R_{13} = R_{24} = R_{75} = R_{86} = 1$, and zero remaining entries. All these operators have square ± 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 Ω_i , which form a basis of \mathbb{C}^8 . Since these vectors lie in either $\mathcal{N}, \tilde{\mathcal{N}}$ or their complex conjugates, we know how the covariance matrix acts on them and it is thus determined by $\gamma = \Lambda\Omega^{-1}$, where Λ and Ω denote the matrices consisting of column vectors $\Lambda_k = \gamma\Omega_k$ (expressed in terms of $\sigma, \tilde{\sigma}$). The above γ is generated in this manner from

$$\Omega_1 = (-1, i, 2, -3i, 1, -i, 1, 0). \quad (10)$$

Then the condition of Proposition 1 is satisfied by construction, and we have only to verify that $\gamma + i\sigma \geq 0$, which is again simplified by this operator commuting with R . Explicitly, we get the eigenvalues $0, 3 - \sqrt{3}, 3, 3 + \sqrt{3}$, each with multiplicity 2.

By 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

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

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

States obtained from (11) are all of a nonblock diagonal form similar to (9), and are hence bound entangled.

Funding by the European Union Project EQUIP (Contract No. IST-1999-11053) and financial support from the DFG (Bonn) are gratefully acknowledged.

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