Covariance matrices and the separability problem

O. Gühne,1 P. Hyllus,2,3 O. Gittsovich,4,1 and J. Eisert3

1Institut für Quantenoptik und Quanteninformation,
Österreichische Akademie der Wissenschaften, 6020 Innsbruck, Austria,
2Institut für Theoretische Physik, Universität Hannover, Appelstraße 2, 30167 Hannover, Germany,
3QLS, Blackett Laboratory, Imperial College London, Prince Consort Road, London SW7 2BW, UK
and Institute for Mathematical Sciences, Imperial College London, Prince’s Gate, London SW7 2PE, UK
4Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria

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We propose a unifying approach to the separability problem using covariance matrices of locally measurable observables. From a practical point of view, our approach leads to strong entanglement criteria that allow to detect the entanglement of many bound entangled states in higher dimensions and which are at the same time necessary and sufficient for two qubits. From a fundamental perspective, our approach leads to insights into the relations between several known entanglement criteria – such as the computable cross norm and local uncertainty criteria – as well as their limitations.

Entanglement plays a central role in applications of quantum information science as well as in the foundations of quantum theory. Quite naturally, one of the problems that have received a significant amount of attention is the question to decide whether a given state is entangled or separable. In fact, the development of separability criteria [1,2,3,4,5,6] has been one of the key activities in quantum information theory: On top of certifying a given state is separable. In fact, the development of separability criteria and which are at the same time necessary and sufficient for two qubits. From a fundamental perspective, our approach leads to insights into the relations between several known entanglement criteria – such as the computable cross norm and local uncertainty criteria – as well as their limitations.

The main idea. – Let us start by defining CMs. Let be a given quantum state and let \( \{ M_k : k = 1, \ldots, N \} \) be some observables. Then the \( N \times N \) CM \( \gamma \) – dependent on the state \( \varrho \) and the choice for \( \{ M_k \} \) – is given by

\[
\gamma_{i,j} = \frac{\langle M_i M_j \rangle + \langle M_j M_i \rangle}{2} - \langle M_i \rangle \langle M_j \rangle.
\]

This is a real, positive definite matrix \([14]\) and its diagonal entries are just the familiar variances, \( \gamma_{i,i} = \delta^2(M_i)_{\varrho} \). The CM has a useful concavity property: if \( \varrho = \sum_k p_k \varrho_k \) is a convex combination of arbitrary states, then

\[
\gamma(\varrho) \geq \sum_k p_k \gamma(\varrho_k).
\]

This can be shown to emerge from the generating function of the moments \([8,11]\), reflecting the fact that the variance of an observable increases under mixing.

Now, let \( \varrho \) be a bipartite state on \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \), where \( d_A \) (\( d_B \)) is the dimension of \( \mathcal{H}_A \) (\( \mathcal{H}_B \)). We can choose \( d_A \) observables \( \{ A_k \} \) on \( \mathcal{H}_A \) such that they form a Hilbert-Schmidt orthonormal basis of the observable space, that is, they obey \( \text{Tr}[A_k A_l] = \delta_{k,l} \). E.g. for a qubit, we may choose normalized Pauli matrices including the identity. Similarly, we may take \( \{ B_k \} \) as a basis of observables in \( \mathcal{H}_B \), and consider the total set \( \{ M_k \} = \{ A_k \otimes 1, 1 \otimes B_k \} \).

The CM then has the block structure

\[
\gamma(\varrho, \{ M_k \}) = \begin{bmatrix} A & C \\ C^T & B \end{bmatrix},
\]

where \( A = \gamma(\varrho_A, \{ A_k \}) \) and \( B = \gamma(\varrho_B, \{ B_k \}) \) are CMs of the reduced states, and \( C \) has the entries \( C_{i,j} = \langle A_i \otimes B_j \rangle - \langle A_i \rangle \langle B_j \rangle \). This matrix will form the starting point to characterize the separability properties of \( \varrho \).

To formulate the separability criterion, recall that a state is separable iff is a convex combination of product states, i.e., \( \varrho = \sum_k p_k |a_k b_k \rangle \langle a_k b_k | \). We then use Eq. (2) and the fact that for a product state the block \( C \) in Eq. (3) vanishes, to arrive at the following observation:

**Observation 1 (CM criterion).** Let \( \gamma(\varrho) \) be a CM as in Eq. (3). If \( \varrho \) is separable, then there exist states...
\([a_k](a_k)\) on \(\mathcal{H}_A\), \([b_k](b_k)\) on \(\mathcal{H}_B\), and convex weights \(p_k\) such that for \(\kappa_A = \sum_k p_k \gamma([a_k](a_k))\) and \(\kappa_B = \sum_k p_k \gamma([b_k](b_k))\) we have \(12\).

\[\gamma(\rho, \{M_k\}) \geq \kappa_A \oplus \kappa_B. \quad (4)\]

If no such \(\kappa_{A/B}\) exist, \(\rho\) must be entangled.

We refer to this criterion as covariance matrix criterion (CMC) \([16]\). Subsequently, we will show that this condition can be made an efficient and physically plausible test. We will see that as such the condition is independent of the choice of the observables \(\{A_k\}, \{B_k\}\), but that a certification of a violation of the criteria is simplified by choosing the Schmidt-basis in operator space or by first using an appropriate local filtering.

Let us first note some facts concerning the CM \(\gamma\) and the \(\kappa_{A/B}\), a detailed presentation will be given elsewhere \([14]\). A general change of the observables \(\{\hat{M}_k\} \rightarrow \{\hat{M}_k\}\) with \(\hat{M}_k = \sum_\lambda \mu_k, \hat{M}_\lambda\) gives rise to a map \(\gamma(\hat{M}_k) = \gamma(\hat{M}_\lambda)\mu^T\). From this it is easy to see that the CMC is, in principle, independent of the choice of the orthonormal \(\{A_k\}, \{B_k\}\), however, a suitable choice of them simplifies the falsification of Eq. 4. A unital transformation \(\rho \rightarrow U \rho U^\dagger\) induces a transformation \(\hat{M}_k \rightarrow \hat{M}_k = U \hat{M}_\lambda U^\dagger = \sum_\lambda \mu_k, \hat{M}_\lambda\) where \(O\) is orthogonal. The orthogonality of \(O\) is equivalent to the statement that the \(\{\hat{M}_k\}\) are also orthogonal \([3]\). So the eigenvalues of \(\gamma(\hat{M}_k)\) are invariant under unitary transformations of the state. This also means, notably, that by a suitable choice of the observables, the matrix \(C\) in Eq. 6 can be made diagonal by a singular value decomposition. If \(\rho\) is a \(d\)-dimensional pure state and the \(\{\hat{M}_k\}\) are orthogonal, then \(\gamma = \rho/2\) is a projector onto a \(2(d-1)\)-dim subspace of the total \(d^2\)-dim space. This can be directly calculated for a specific state and some \(\{\hat{M}_k\}\) \([18]\). Then, the general statement follows from the second property. This also implies for Eq. 4 that \(\text{Tr}[\kappa_A] = d_A - 1\) and \(\text{Tr}[\kappa_B] = d_B - 1\).

**Evaluation for two qubits.** As a first example, we take as observables the normalized Pauli matrices, i.e., \(\{A_k\} = \{B_k\} = \{1, \sigma_x, \sigma_y, \sigma_z, 2\}\). Then, in the definition of \(\gamma\) in Eq. 4 two rows and columns (corresponding to the \(A_1, B_1 = 1/\sqrt{2}\)) equal zero, thus it suffices to consider \(\gamma\) as a \(6 \times 6\) matrix, originating only from \(\{A_k\}\) and \(\{B_k\}\) for \(k = 2, 3, 4\). To characterize the \(\kappa_A\), note that for a pure state on \(\mathcal{H}_A\) the \(3 \times 3\) matrix \(\gamma(a)(a)\) is a two-dimensional projector, i.e., \(\gamma = \rho/2 = (I_3 - |\phi\rangle\langle\phi|)/2\), where \(|\phi\rangle\in R^3\). In turn, each matrix of the form \((I_3 - |\phi\rangle\langle\phi|)/2\) is a valid CM, since any such matrix can be obtained from a special \((I_3 - |\phi\rangle\langle\phi|)/2\) by an orthogonal transformation (in \(R^3\)), and for the special case of a qubit there is a one to one correspondence between such orthogonal transformations and unitary transformations of the state \([19]\). From this, it is easy to see that \(\kappa_A = (I_3 - \rho_A)/2\) where \(\rho_A\) is a real density matrix on \(R^3\), and we can summarize:

**Proposition 2 (Qubit criterion).** Let \(\rho\) be a state of two qubits, and \(\gamma\) be the \(6 \times 6\) CM as in Eq. 6 with \(\{A_k\} = \{B_k\} = \{\sigma_x, \sigma_y, \sigma_z, 2\}\). \(\rho\) fulfills the CMC iff there exist \(3 \times 3\) density matrices \(\rho_A, \rho_B\) with

\[\gamma - 1/6 + \rho_A + \rho_B \geq 0. \quad (5)\]

If we find complex \(\rho_A, \rho_B\), their real part saturates Eq. 5 as well. Finding the \(\rho_{A/B}\) is a simply solvable semidefinite feasibility problem \([4]\). Eq. 5 will become important later in the context of LURs. But let us discuss the general case first.

**Evaluation of the CMC for the general case.** Let us first assume that \(d_A = d_B = d\).

**Proposition 3 (General criterion).** Let \(\rho\) be a state with \(d_A = d_B = d\) and \(A, B, C\) be as in Eq. 6. If \(\rho\) is separable, then

\[2 \sum_{i=1}^d |C_{i,i}| \leq (\text{Tr}[A] - d + 1) + (\text{Tr}[B] - d + 1)\]

\[= (1 - \text{Tr}[\rho^2_A]) + (1 - \text{Tr}[\rho^2_B]). \quad (6)\]

**Proof.** First note that a necessary condition for a \(2 \times 2\) matrix \(X = \begin{pmatrix} a & c \\ c & b \end{pmatrix}\) to be positive is that \(2|c| \leq a + b\). If \(\rho\) were separable, then by the CMC we have \(Y = \gamma - \kappa_A \oplus \kappa_B \geq 0\). This implies that all \(2 \times 2\) minor submatrices of \(Y\) have to be positive. Hence, for all \(i, j\) \(2|C_{i,j}| \leq A_{i,i} + B_{j,j} - (\kappa_A)_{i,i} - (\kappa_B)_{j,j}\). Summing over all \(i, j\) proves the claim. Using \(\text{Tr}[A] = \text{Tr}[B] = d - 1\), Eq. 6 always holds since \(\sum_k A_k^2 = d_1\) \([21]\), hence \(\sum_i A_{i,i} = \sum_k \delta(A_k)^2 = d - \text{Tr}[\rho^2_A]\).

As explained before, one may choose \(C\) diagonal, so considering the diagonal only is no restriction of generality \([20]\). One may further try to improve Proposition 3 by taking \(4 \times 4\) submatrices into account \([17]\). Physically, Proposition 3 states that if the correlations \(C_{i,i}\) are large, then \(\rho\) is entangled. The question remains how to find those observables for which the \(C_{i,i}\) are large. This problem can be overcome by making use of the Schmidt decomposition in operator space \([21]\). Recall that we can express any state as \(\rho = \sum_k \lambda_k (G_k^A \otimes G_k^B)\). Here, \(\lambda_k \geq 0\) for all \(k\), and the \(\{G_k\}\) form an orthonormal basis of the operator space. Denoting \(g_{k}^{A/B} = \text{Tr}[G_{k}^{A/B}]\) we can now use the set \(\{G_{k}^{A/B}\}\) in Proposition 3:

**Proposition 4 (CMC for Schmidt form states).** If \(\rho\) is separable, then

\[2 \sum_k |\lambda_k - \lambda_k^2 g_{k}^{A} g_{k}^{B}| \leq 2 - 2 \sum_k |\lambda_k^2 (g_{k}^{A})^2 + (g_{k}^{B})^2|.
\]

This is a direct application of Proposition 3 to the diagonal of \(C\). One can find examples of states, which are detected by the CMC via Proposition 2, but not by Proposition 4 \([22]\). However, Proposition 4 connects now the CMC to the CCNR criterion \([2, 21]\):
Corollary 5 (Connection to the CCNR criterion). If \( \varrho \) is separable, then \( \sum_k \lambda_k \leq 1 \).

This follows from Proposition 4 and the general relation \( a^2 + b^2 \geq 2ab \). Since the condition \( \sum_k \lambda_k \leq 1 \) is just the CCNR criterion, this implies that the well-known CCNR criterion is a direct corollary of our theory \([23]\).

Enhancing the criterion via local filtering. A general strategy strengthening the presented test is the joint use of the CMC with local filtering operations. Such operations are maps of the form \( \varrho \rightarrow \tilde{\varrho} = (F_A \otimes F_B) \varrho (F_A \otimes F_B)^\dagger \) where the \( F_A, F_B \) are arbitrary invertible matrices. They preserve the entanglement or separability of a given state. Local filtering transforms a generic (full rank) \( \varrho \) into

\[
\tilde{\varrho} = \frac{1}{d_A d_B} \left( 1 + \sum_{i=1}^{d^2_A - 1} \xi_i (\tilde{G}_i^A \otimes \tilde{G}_i^B) \right)
\]

where \( \xi_i \geq 0 \) for all \( i \) and the \( \{\tilde{G}_i^A/B\} \) are traceless and orthogonal observables \([24, 25, 26]\). The matrices \( F_A, F_B \) can be found constructively \([27]\). We will refer to this form as the filter normal form (FNF). The extraordinarily helpful property is that for a state in the FNF with the \( \{\tilde{G}_i^A/B\} \) as observables the blocks in the CM are diagonal. We have then in Eq. \( \text{[5]} \)

\[
A = \text{diag}(0, 1, 1, \ldots, 1)/d_A, \quad B = \text{diag}(0, 1, 1, \ldots, 1)/d_B, \quad \text{and} \quad C = \text{diag}(0, \xi_1, \xi_2, \ldots, \xi_{d^2_A - 1})/(d_A d_B), \quad \text{and obtain:}
\]

Proposition 6 (CMC under filtering). If a generic state \( \varrho \) is separable and \( d_A = d_B = d \) we have in its FNF

\[
\sum_{i=1}^{d^2 - 1} \xi_i \leq d^2 - d.
\]

This is a very strong criterion for separability, as some examples will show. Interestingly, it is also necessary and sufficient for two qubits \([23]\). For them, it is easy to see that the \( \{\tilde{G}_i^{A/B}\} \) in Eq. \( \text{[7]} \) are effectively the Pauli matrices, and the separable states of this form are known to be an octahedron inside some tetrahedron \([19]\), the borders of which are described by Proposition 6. Alternatively, this can be seen from the results in Ref. \([22]\).

Let us consider the asymmetric case, when \( d_A < d_B \). The CM \( \gamma \) in the FNF is then similar as before, however \( A \) and \( B \) are not of the same dimension. Two observations are now helpful: First, we do not sum over all \( B_{i,i} \). On the other hand, we cannot subtract all of the \( (\kappa_{B})_{i,i} \) anymore, since \( d_B^2 - d_A^2 \) diagonal elements of \( \kappa_B \) do not occur in the sum. Moreover, \( \gamma \) consists of a linear part \( \gamma^L_{i,j} = \langle M_i M_j + M_j M_i \rangle/2 \) and a nonlinear part \( \gamma^N_{i,j} = \langle M_i \rangle \langle M_j \rangle \). Since the linear part is compatible with convex combinations, the linear part on the right hand side of Eqs. \( \text{[23]} \) has to coincide with the linear part on the left hand side. The non-vanishing elements of \( \gamma \) origin from the linear part only, so the missing \( \kappa_{B} \) are \((\kappa_{B})_{i,i} = 1/d_B - \sum_k p_k \langle G_i \rangle^2_{[k]} \langle b_i \rangle^2_{[k]} \) hence \((\kappa_{B})_{i,i} \leq 1/d_B \). So, if \( \varrho \) in the FNF is separable, then

\[
\sum_i \xi_i \leq d_A d_B \left( 1 - 1/d_A + (d_A^2 - 1)/d_B \right) + \min\{0; -(d_B - 1) + (d_B^2 - d_A^2)/d_B\} / 2.
\]

The possibility of taking zero in the minimization comes from the fact that one may also omit the summation over \((\kappa_{B})_{i,i} \). Especially if \( d_A \ll d_B \) this yields better bounds.

It is instructive to compare this with the CCNR criterion which requires for separable states in the FNF

\[
\sum_i \xi_i \leq d_A d_B - (d_A d_B)^{1/2}, \quad \text{and the} \quad \text{dV-criterion \([12]\), requiring} \quad \sum_i \xi_i \leq (d_A d_B(d_A - 1)(d_B - 1))^{1/2}.
\]

For \( d_A = d_B \) all three criteria coincide. One can directly see that for \( d_A < d_B \) Eq. \( \text{[8]} \) is stronger than the CCNR criterion, but the dV-criterion is also stronger than CCNCR. If \( d_B - d_A \) is small, the dV-criterion is slightly better than Eq. \( \text{[8]} \), for \( d_A \ll d_B \), however, Eq. \( \text{[8]} \) is drastically better than the CCNR and dV-criterion.

Connection with the LURs. LURs allow detection of entanglement in the following way \([13]\): One takes observables \( \{\hat{A}_k\} \) and \( \{\hat{B}_k\} \) on Alice’s (resp. Bob’s) space and computes two bounds \( U_A, U_B \) such that \( \sum_k \delta^2(\hat{A}_k) \geq U_A, \quad \sum_k \delta^2(\hat{B}_k) \geq U_B \). Then for separable states \( \sum_k \delta^2(\hat{A}_k \otimes 1 + 1 \otimes \hat{B}_k) \geq U_A + U_B \) holds. Physically, LURs show that separable states inherit the uncertainty relations from their reduced states, which is not the case for entangled states. For a given state \( \varrho \), however, it is usually not clear which \( \{\hat{A}_k\} \) and \( \{\hat{B}_k\} \) are suitable to detect its entanglement. We can formulate:

Proposition 7 (Connection to LURs). A state \( \varrho \) violates the CMC if it can be detected by a LUR.

Proof. The proof is given in the Appendix.

This equivalence has two consequences: Results concerning LURs can be transferred to the CMC. E.g., Ref. \([21]\) gives now an alternative proof that the CMC is stronger than the CCNR criterion. Also, our results concerning the CMC allow to gain new insights in LURs:

Corollary 8 (LURs for two qubits). There exist entangled two-qubit states which can not be detected by a LUR.

Examples of such states can be found numerically \([22]\), showing that the filtering indeed improves the CMC.

Examples and extensions. Firstly, we take the \( 3 \times 3 \) bound entangled states arising from an unextendible product basis, mixed with white noise \([24]\). These states \( \varrho_UBP(p) \) are detected by Proposition 6 for \( p \geq 0.8723 \) while the best known positive map detects them only for \( p > 0.8744 \) \([21]\). Secondly, we checked randomly generated \( 3 \times 3 \) chessboard states \([31]\). The CCNR criterion detected 18.1% of them, Proposition 4 detected 19.1% and Proposition 6 detected 97.8%.

Finally, let us note that the theory developed in this paper may be complemented by considering non-symmetric CMs \([17]\). That is, one may define \( \gamma^A_{i,j} = \langle M_i M_j \rangle - \langle M_i \rangle \langle M_j \rangle \). For such matrices (which are now
hermitian, but still positive) one can directly derive a statement corresponding to Proposition 1. This criterion implies then the CMC as given for a symmetric $\gamma$.

**Conclusion.** – We have proposed to investigate the separability of finite dimensional quantum states using the CM for certain observables. We have demonstrated that this approach reveals the entanglement of many states and can lead to new insights into already existing criteria. It hence provides a further systematic framework of studying entanglement for composite quantum systems.

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**Appendix.** – Here, we prove Proposition 7. Note that the CM can be used to compute variances: if $N = \sum_k \nu_k M_k$ is a linear combination of the $M_k$ then

$$\delta^2(N) = \sum_{i,j} \nu_i \nu_j \langle M_k | i\rangle | j\rangle = \langle \nu | (M_k \nu) | \nu \rangle.$$  

If $\rho$ violates the LURs we can find $A_k$ and $B_k$ as above. We write $A_k = \sum_l \alpha_l \hat{A}_l$ and $B_k = \sum_i \beta_i \hat{B}_i$ with $A_k$ and $B_k$ as in the definition of $\gamma$ in Eq. (3), leading to

$$\delta^2(A_k \otimes \mathbb{1} \otimes \mathbb{1} \otimes B_k) = \langle (\alpha(k) \otimes \beta(k)) | (\alpha(k) \otimes \beta(k)) \rangle.$$

For the $\alpha \otimes \beta$ we have $\alpha \otimes \beta = \sum_k p_k \gamma(\{a_k\} \otimes \{b_k\}) \langle \gamma(\{b_k\}) | \langle \gamma(\{b_k\}) |$ hence $\langle (\alpha \otimes \beta) | \alpha \otimes \beta \rangle = \sum_{i,j} p_i \langle \delta^2(A_k) | a_i \rangle | a_j \rangle + \delta^2(B_k) | b_i \rangle | b_j \rangle \rangle$ if the CMC were fulfilled, summing up over $k$ would yield $\sum_k \delta^2(A_k \otimes \mathbb{1} \otimes \mathbb{1} \otimes B_k) \geq \sum_k \delta^2(B_k) | b_i \rangle | b_j \rangle \rangle \geq U_A + U_B$, which contradicts the violation of the LURs.

Conversely, let us define $X$ as the set of all matrices which can be written as $\alpha \otimes \beta + P$ with some $\alpha$ and $\beta$ as in Observation 1 and a positive $P$. In other words, the CMC states that for separable states $\gamma \in X$. Geometrically, $X$ is a closed convex cone. According to a Corollary of the Hahn-Banach Theorem for each $\gamma \notin X$ there must be a symmetric matrix $W$ and a number $C$ such that $Tr[W | X | X ] < C$ while $Tr[W | X | X ] > C$ for all $X \in X$. Since $Tr[W | P ] \geq 0$ for all $P \geq 0$, we have $W \geq 0$. Now we use the spectral decomposition and write $W = \sum_k \lambda_k | \psi_k \rangle \langle \psi_k | = \sum_k \lambda_k | \alpha(k) \otimes \beta(k) \rangle | \alpha(k) \otimes \beta(k) \rangle$. Defining $A_k = \sqrt{\lambda_k} \sum_l \alpha_l | \hat{A}_l \rangle$ and $B_k = \sqrt{\lambda_k} \sum_i \beta_i | \hat{B}_i \rangle$, we have for $\gamma$ that $Tr[W | \gamma ] = \sum_k \delta^2(A_k \otimes B_k) \otimes B_k) < C$.

Furthermore, we have that all $\gamma \otimes \beta \otimes B \in X$ and even more, we have that all $\gamma \alpha \otimes B \in X$. Hence, for a product state $\gamma = \alpha \otimes \beta$ we have $C < Tr[W | \gamma | \gamma ] = (\sum_k \delta^2(A_k) | \alpha \rangle \langle \alpha |) + (\sum_k \delta^2(B_k) \otimes \beta \rangle \langle \beta |) \rangle$ which implies that $C < \min_{\alpha \beta} \left( \sum_k \delta^2(A_k) \otimes \beta \rangle \langle \beta |) \right) + \min_{\alpha \beta} \left( \sum_k \delta^2(B_k) \otimes \beta \rangle \langle \beta |) \right) =: U_A + U_B$ leading to a violation of the LURs. □

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[27] For that, one minimizes the function $f(\rho_A, \rho_B) = Tr[\rho_A \otimes \rho_B] / (det(\rho_A)^{1/d_A} det(\rho_B)^{1/d_B})$, takes the optimal $\rho_A, \rho_B$ and defines $F_A F_B = \rho_A$ and $F_B F_A = \rho_B$.
[28] For the two-qubit case, one uses a filtering as in Ref. [24]. In some cases, one will not directly arrive at the FNF, then one can use a further filter which brings $\gamma$ arbitrarily close to a maximally entangled state.
[29] These states are defined by $| \psi_0 \rangle = |0\rangle (|0\rangle - |1\rangle) / \sqrt{2}$, $| \psi_1 \rangle = (|0\rangle - |1\rangle) / \sqrt{2}$, $| \psi_2 \rangle = |2\rangle (|1\rangle - |2\rangle) / \sqrt{2}$, $| \psi_3 \rangle = (|1\rangle - |2\rangle) (|0\rangle / \sqrt{2} - |2\rangle)$, /3.
then $g_{BE} = (1 - \sum_{i=0}^{4} |\psi_i)(\psi_i|)/4$ and finally $g_{UPB}(p) = p g_{BE} + (1-p)I/9$. See C.H. Bennett et al., Phys. Rev. Lett. 82, 5385 (1999).

[30] D. Bruß and A. Peres, Phys. Rev. A 61, 030301(R) (2000). We used the five parameter (equally distributed in $[-1;1]$) family with $g = g^n$. The result is similar for other distributions.