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Modular construction of special mixed quantum states

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Abstract. For a homogeneous quantum network of N subsystems with n levels each we consider separable generalized Werner states. A generalized Werner state is defined as a mixture of the totally mixed state and an arbitrary pure state $|\psi\rangle$: $\hat{\rho}_{\text{Werner}} = (1-\epsilon)\hat{1} + \epsilon|\psi\rangle\langle\psi|$ with a mixture coefficient ϵ. For this density operator $\hat{\rho}_{\text{Werner}}$ to be separable, ϵ will have an upper bound $\epsilon_{\text{sep}} \leq 1$. Below this bound one should alternatively be able to reproduce $\hat{\rho}_{\text{Werner}}$ by a mixture of entirely separable input-states. For this purpose we introduce a set of modules, each contributing elementary coherence properties with respect to a generalized coherence vector. Based on these there exists a general step-by-step mixing process for any $\epsilon_{\text{mix}} \leq \epsilon_{\text{max}}$. For $|\psi\rangle$ being a cat-state it is possible to define an optimal process, which produces states right up to the separability boundary ($\epsilon_{\text{max}} = \epsilon_{\text{sep}}$).

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1 Introduction

In the last couple of years our understanding of the quantum mechanical world has considerably been improved. Concepts like "teleportation" [1,2] "quantum cryptography" [1,3,4] and "quantum computation" [1,5] are well-known, not only in professional circles. One of the most astonishing features of quantum mechanics is entanglement or inseparability originally mentioned by Schrödinger (*cf.* [6,7]). Multipartite entanglement (*cf.* [8,9]) is a property of quantum networks, *i.e.* systems consisting of several subsystems μ with n_μ energy levels each ($\mu = 1, ..., N$). Measurements on entangled subsystems lead to correlations, which cannot be described by a classical local realistic theory [7,10]. It has been shown recently that speed-up in pure state quantum computation requires multi-partite entanglement [11]. Quantum networks could be found either in an entangled or a separable ("classical") state, but the boundary between these states is far from being understood completely.

To discriminate between separable and entangled states it would be desirable to have universally valid separability criteria. For pure states such a criterion is available: a pure network state is separable if all subsystems are locally in pure states, too, or if it does not violate a Bell inequality [12,13]. Up to now there is no generally valid operational criterion for the separability in case of mixed states, but a large variety of either necessary or sufficient conditions. A very important necessary condition is the Peres criterion (positive-partial-transpose-criterion) [14]. This criterion is sufficient, too, for a network consisting of two 2-level systems or a 2- and a 3-level-system [15]. Pittenger and Rubin [16] have shown that the Peres criterion is also sufficient for larger networks and a special state class, the so-called Werner states [17]. In the neighborhood of the totally mixed state, all states should be separable [18,19]. For such mixed states it is possible to use the sufficient criterion by Braunstein *et al.* [20]. Another interesting sufficient criterion valid for a larger part of the separable region is the recursive demixing procedure by Otte [21], which is not only able to proof separability of a mixed state but even to produce the decomposition into a convex combination of product states. (For further information concerning separability see [22–26].)

Recently some doubts have been raised about the significance of entanglement, mainly in relation with NMR quantum computation [20,27], where often highly mixed quantum states are used, for example the Werner states [17] with small ϵ. Here we want to consider a generalization of the already mentioned Werner states. These states are mixtures out of the "totally mixed state" and an arbitrary pure state weighted by a mixture coefficient ϵ (in the original Werner state the pure state is the EPR state). If the pure state was entangled, the corresponding generalized Werner state can be entangled or not, depending on the mixture coefficient ϵ. Special ensemble experiments (for example EPR measurements) based on such a separable Werner state would lead to the same

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interference pattern as an experiment with the entangled pure EPR state, though scaled down by ϵ.

A separable generalized Werner state should alternatively be producible by mixing separable states only (*i.e.* convex combination of product states). Such a decomposition into a convex combination of separable states is neither unique nor easily generated. To produce such a decomposition, we introduce a set of separable states, so-called modules, with a very special type of "classical" correlation (minimum number of elementary correlations). With this set of states it is then possible to mix every generalized Werner state, with a rather small ϵ. While an optimal algorithm would produce a separable generalized Werner state right up to the separability boundary, this will not be the case here, in general. To approach the boundary, specially adapted building blocks are needed, as will be shown for the original Werner states.

One may say that this mixture simulates in a "classical" way all the down-scaled correlations of the respective pure state, including its entanglement. "Classical", because mixing processes are not able to produce "real" entanglement, thus all these states definitely remain separable. There have been other concepts of classical entanglement simulation: one version aims at the simulation of individual measurement sequences on N entangled spins [28,29] by means of additional classical resources (*e.g.* shared random bits). It turns out that number of bits of communication needed grows exponentially with N. A second version deals with classical wave simulation [30], again with exponential scaling. Thus, classical simulation of quantum mechanical behavior is often costly [31]: also we find this cost to increase exponentially with the number of subsystems N.

2 Operator representations

As is well-known, any density-operator can be expanded in terms of a set of orthonormal basis-operators for the Liouville space. For a quantum mechanical system with n levels there are various possible sets of basis-operators for its n^2-dimensional Liouville space $\mathcal{L}$. Here we use an unitary operator basis [32,33] as defined by the set

$$\hat{U}_{a,b} := \sum_{p=0}^{n-1} \omega^{bp} |\underline{p+a}\rangle\langle p| \quad \text{with} \quad \omega = \mathrm{e}^{\frac{2\pi \mathrm{i}}{n}}, \tag{1}$$

where underlining a term indicates the modulo function $\underline{x} = (x \mod n)$ and with indices $a, b = 0, ..., n-1$. The identity operator is included as $\hat{U}_{0,0}$. One can merge the two indices a and b into one single index c by the relation:

$$c = na + b \quad \text{with} \quad c = 0, ..., n^2 - 1. \tag{2}$$

Note that for n not being prime some of the unitary operators $\hat{U}_{a,b}$ can additionally be Hermitian. For $n = 2$ all the unitary operators are directly related to the well-known Hermitian Pauli-operators $\hat{\sigma}_i$, $i = 0, x, y, z$:

$$\hat{U}_{0,0} = \hat{\sigma}_0,\ \hat{U}_{0,1} = \hat{\sigma}_z,\ \hat{U}_{1,0} = \hat{\sigma}_x,\ \hat{U}_{1,1} = \mathrm{i}\,\hat{\sigma}_y. \tag{3}$$

Forming a complete orthogonal basis in Liouville space with $\mathrm{Tr}\left\{\hat{U}_{a,b}\,\hat{U}^{\dagger}_{a',b'}\right\} = n\,\delta_{aa'}\delta_{bb'}$, any operator $\hat{A}$ acting on the system can be expanded as

$$\hat{A} = \frac{1}{n} \sum_{c=0}^{n^2-1} u_c(\hat{A})\,\hat{U}_c, \tag{4}$$

where $u_c = \mathrm{Tr}\left\{\hat{U}_c^{\dagger}\,\hat{A}\right\}$. Applying this expansion to the density operator $\hat{\rho}$ and leaving aside the term $u_0 = 1$ the $(n^2 - 1)$, in general, complex values u_c form the so-called *coherence vector*, which describes all state properties of the system under investigation.

Consider now a (N, n) homogeneous quantum network, *i.e.* a set of N subsystems, n levels each. As a basis in the n^{2N}-dimensional Liouville space one can use now the *product operators*

$$\hat{C}_{\{\mathbf{a},\mathbf{b}\}} = \bigotimes_{\mu=1}^{N} \hat{U}_{a_\mu, b_\mu}, \tag{5}$$

$\mathbf{a}$ and $\mathbf{b}$ are index vectors of N components each, containing all subsystem indices a_μ and b_μ. $\hat{C}_{\{0,0\}}$ is the identity operator of the complete Liouville space $\hat{1}^{(n^N)}$. As mentioned above it is again possible to form a new index vector $\mathbf{c}$ to represent a pair of vectors $\{\mathbf{a}, \mathbf{b}\}$. Every component c_μ of the vector $\mathbf{c}$ can be evaluated by equation (2). All adjoint operators $\hat{C}^{\dagger}_{\{\mathbf{a},\mathbf{b}\}}$ are members of the complete orthogonal set, *via*:

$$\hat{C}^{\dagger}_{\{\mathbf{a},\mathbf{b}\}} = \omega^{\mathbf{a}\cdot\mathbf{b}} \hat{C}_{\{\mathbf{n}-\mathbf{a},\mathbf{n}-\mathbf{b}\}} \quad \text{with} \quad \mathbf{n} = \{n, ..., n\}. \tag{6}$$

For some special index vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{n}$ the unitary product operator will also be Hermitian, in particular, if all its local operators have this property. All product operators $\hat{C}_{\{\mathbf{a},\mathbf{b}\}}$ are trace free (for $\mathbf{c} \neq \mathbf{0}$) and fulfill the orthogonality relation

$$\mathrm{Tr}\left\{\hat{C}_{\{\mathbf{a},\mathbf{b}\}}\hat{C}^{\dagger}_{\{\mathbf{a}',\mathbf{b}'\}}\right\} = n^N \delta_{\mathbf{a},\mathbf{a}'}\delta_{\mathbf{b},\mathbf{b}'}. \tag{7}$$

Therefore the set of operators $\hat{C}_{\mathbf{c}}$ form a complete orthogonal set in the Liouville space of the (N, n) network. Any operator can be expanded in terms of these, in particular

$$\hat{\rho} = \frac{1}{n^N}\left(\hat{1} + \sum_{\mathbf{c}\neq\mathbf{0}} u_{\mathbf{c}}(\hat{\rho})\,\hat{C}_{\mathbf{c}}\right). \tag{8}$$

All elements $u_{\mathbf{c}}$ ($\mathbf{c} \neq \mathbf{0}$) obey $|u_{\mathbf{c}}(\rho)| \leq 1$; they form again the *coherence vector* of the whole system,

$$u_{\mathbf{c}}(\hat{\rho}) = \mathrm{Tr}\left\{\hat{C}^{\dagger}_{\mathbf{c}}\,\hat{\rho}\right\}. \tag{9}$$

In general, the vector components are complex; however, hermiticity of $\hat{\rho}$ implies

$$u^{*}_{\{\mathbf{a},\mathbf{b}\}} = \omega^{-\mathbf{a}\cdot\mathbf{b}} u_{\{\mathbf{n}-\mathbf{a},\mathbf{n}-\mathbf{b}\}} \tag{10}$$

leaving only $n^{2N}-1$ independent real parameters. The vector $u_{\mathbf{c}}$ contains not only local information about the individual subsystems but also correlations between any number of different subsystems (see [32]). The coherence vector length is given by

$$L^2=\sum_{\mathbf{c}\neq\mathbf{0}}|u_{\mathbf{c}}(\rho)|^2=n^N\,\mathrm{Tr}\left\{\rho^2\right\}-1\geq 0. \tag{11}$$

For a mixed state, $L^2<n^N-1$.

Now, let $\hat{\rho}(j)$ be a set of, in general, non-pure but separable density operators. Then, the non-orthogonal decomposition of a mixed state into states $\hat{\rho}(j)$,

$$\hat{\rho}=\frac{1}{\sum_j K(j)}\sum_j K(j)\;\hat{\rho}(j) \tag{12}$$

with $u_{\mathbf{c}}(\hat{\rho})=\sum_j K(j)u_{\mathbf{c}}(\hat{\rho}(j))$ is also separable. For a given set, however, it is not guaranteed that all separable states can be represented in this way. The decomposition (12) has to be seen in contrast to the orthogonal decomposition into unitary operators (8). We are looking for basis operators $\hat{\rho}(j)$, which, in addition of being separable, have a coherence vector with the minimum number of non-zero entries. This is desirable, as each mixing coefficient will then control very few different vector components only, allowing a modular construction of almost arbitrary mixed-state coherence vectors of small length.

3 Separable state modules

In a (N,n) network a possible basis of non-orthogonal separable basis operators $\hat{\rho}(j)$ are the modules defined by the following expansion in terms of product operators ($\mathbf{c}\neq\mathbf{0}$)

$$\hat{\rho}^{(N)}_{\mathrm{mod}}(\mathbf{c},u_{\mathbf{c}})=\frac{1}{n^N}\left(\hat{1}+u_{\mathbf{c}}\hat{C}_{\mathbf{c}}+u^*_{\mathbf{c}}\hat{C}^\dagger_{\mathbf{c}}\right). \tag{13}$$

All these operators represent quantum mechanical states for $\Xi=|u_{\mathbf{c}}|\leq 1/2$ (otherwise the modules may violate positivity), but with arbitrary argument or phase ϕ. As the product operators are trace-less, the trace of these modules is one. These modules contain the minimal number of non-zero coherence vector entries: one, if the respective product operators are Hermitian, two otherwise. In particular for $n=2$ the coherence vectors of all the modules have only one non-zero entry. The purity P_{mod} is according to equation (11) given by

$$P_{\mathrm{mod}}=\left\{\hat{\rho}^{(N)}_{\mathrm{mod}}(\mathbf{c},u_{\mathbf{c}})^2\right\}=\frac{1}{n^N}\left(2\Xi^2+1\right). \tag{14}$$

The modules are thus mixed, $P_{\mathrm{mod}}<1$. For a maximal distance to the totally mixed state it is vital to choose Ξ maximal, as will be assumed to have been done in the following unless specified otherwise ($\hat{\rho}_{\mathrm{mod}}(\mathbf{c},u_{\mathbf{c}})=\hat{\rho}_{\mathrm{mod}}(\mathbf{c},\phi)$).

It is remarkable that all these modules are separable; this can be shown by complete induction: consider a module for N subsystems with n levels each and a special phase $\phi+(2\pi/n)k$ (with k integer),

$$\hat{\rho}^{(N)}_{\mathrm{mod}}\left(\mathbf{c},\phi+\frac{2\pi}{n}k\right). \tag{15}$$

Suppose that this module is separable. For networks with only one subsystem ($N=1$), modules $\hat{\rho}^{(1)}_{\mathrm{mod}}(c,\phi-(2\pi/n)k)$ are trivially separable. We then prove that the following separable state

$$\hat{\rho}=\frac{1}{n}\sum_{k=0}^{n-1}\hat{\rho}^{(N)}_{\mathrm{mod}}\left(\mathbf{c},\phi+\frac{2\pi}{n}k\right)\otimes\hat{\rho}^{(1)}_{\mathrm{mod}}\left(c_{N+1},\phi-\frac{2\pi}{n}k\right) \tag{16}$$

is equivalent to the module $\hat{\rho}^{(N+1)}_{\mathrm{mod}}(\{\mathbf{c},c_{N+1}\},2\phi)$ in a system of $N+1$ subsystems. The state represented by the density operator (16) is separable, because it consists of a convex combination of, by induction hypothesis, separable states. To show the equivalence we put equation (13) into equation (16) and collect terms with phases $\mathrm{e}^{\frac{2\pi\mathrm{i}}{n}k}$. Sums over these phases from $k=0,\ldots\,n-1$ are zero. Only two terms remain, which can be identified with those of the respective module $\hat{\rho}^{(N+1)}_{\mathrm{mod}}(\{\mathbf{c},c_{N+1}\},2\phi)$. This completes the proof from step N to $N+1$.

The modules as separable states can be generated by a mixture of product states. To describe this mixing here in detail, however, would go beyond the scope of this article.

In general, it is very hard to decide whether an *ad hoc* coherence vector (for a (N,n) network) corresponds to an allowed state in Hilbert space. To the best of our knowledge the geometrical shape generated by the set of all pure-state coherence vectors is unknown; it is anything but a simple hyper sphere (the Bloch-sphere, applicable to the 2-dimensional Hilbert space, is an exception).

However, restrictions on the vector components fade away as we decrease the coherence-vector length. With mixtures based on the separable modules it is possible to construct any coherence vector $u_{\mathbf{c}}$ of down scaled length L^2. So, for N and n finite any direction of this vector is allowed, if only its length is taken to be small enough (though finite). The set of accessible states is given by

$$\hat{\rho}_{\mathrm{mix}}=\frac{1}{N_{\mathrm{mod}}}\sum_{\mathbf{c}\neq\mathbf{0}}K(\mathbf{c})\;\hat{\rho}^{(N)}_{\mathrm{mod}}(\mathbf{c},\phi_{\mathbf{c}}) \tag{17}$$

with the mixture coefficients $K(\mathbf{c})\geq 0$ constrained by

$$\sum_{\mathbf{c}\neq\mathbf{0}}K(\mathbf{c})=N_{\mathrm{mod}} \tag{18}$$

and some fixed phase $\phi_{\mathbf{c}}$ for each module. By construction all these states $\hat{\rho}_{\mathrm{mix}}$ are separable.

4 Special mixed states

We will focus now on special 1-parameter classes of mixed quantum states, the generalized Werner states. These states are mixtures out of the totally mixed state $(1/n^N)\hat{1}$

(with $L^2 = 0$) and an arbitrary pure state $\hat{\rho}_{\text{pure}} = |\psi\rangle\langle\psi|$ weighted by a mixture coefficient $0 \leq \epsilon \leq 1$:

$$\hat{\rho}_{\text{Werner}} = \frac{1}{n^N}(1-\epsilon)\hat{1} + \epsilon\hat{\rho}_{\text{pure}}. \tag{19}$$

It is possible to expand the generalized Werner state in terms of product operators (Eq. (5)). Applying the expansion (8) to the pure state in the definition of the generalized Werner state (19) one finds

$$\hat{\rho}_{\text{Werner}} = \frac{1}{n^N}\left(\hat{1} + \epsilon\sum_{\mathbf{c}\neq\mathbf{0}} u_{\mathbf{c}}(\hat{\rho}_{\text{pure}})\,\hat{C}_{\mathbf{c}}\right). \tag{20}$$

Compared with the product operator expansion of the pure state $\hat{\rho}_{\text{pure}}$, the generalized Werner state has the coherence vector of the pure state scaled down by ϵ; one may say that all properties have become "pale". For this density operator $\hat{\rho}_{\text{Werner}}$ to be separable, ϵ will have an upper bound $\epsilon_{\text{sep}} \leq 1$, depending on the pure state considered.

If the pure state $\hat{\rho}_{\text{pure}}$ is taken to be the cat state

$$|\psi\rangle = |\text{cat}\rangle = \frac{1}{\sqrt{n}}\sum_{i=0}^{n-1}|i,...,i\rangle, \tag{21}$$

one gets the original (cat-) Werner state [17]. For cat states the coherence vector is easily evaluated with the aid of equation (9). We find

$$u_{\{\mathbf{a},\mathbf{b}\}} = \begin{cases} 1 & \mathbf{a} = \{a,...,a\}, \quad \underline{\sum_{\mu=1}^{N} b_\mu} = 0 \\ 0 & \text{else} \end{cases} \tag{22}$$

where the underlining, again, indicates the modulo function. A short-hand notation of equation (22) is

$$u_{\{\{a,...,a\},\mathbf{b}\}} = \delta(\underline{\textstyle\sum_{\mu=1}^{N} b_\mu} = 0), \tag{23}$$

where it is understood that the element of the vector is one if the index condition in brackets is fulfilled, else zero. Note that $\underline{\sum_{\mu=1}^{N} b_\mu} = 0$ is fulfilled for exactly $n^N - 1$ different vectors $\mathbf{b}$.

5 Mixing generalized Werner states

In the following we develop a mixing process which is able to reproduce an arbitrary generalized Werner state for $\epsilon_{\text{mix}} \leq \epsilon_{\text{max}}$.

To carry out a mixing process with the aid of the modules we have to analyze the coherence vector of the state of interest. Because we want to produce a generalized Werner state it is sufficient to investigate the coherence vector of the pure state $\hat{\rho}_{\text{pure}}$ (see Eq. (20)). The coherence vector entry $u_{\mathbf{c}}(\hat{\rho}_{\text{pure}})$ is a complex number and hence we set

$$u_{\mathbf{c}}(\hat{\rho}_{\text{pure}}) = K(\mathbf{c})\,\mathrm{e}^{\mathrm{i}\phi(\mathbf{c})} \quad \text{with} \quad 1 > K(\mathbf{c}) \geq 0. \tag{24}$$

The phase $\phi(\mathbf{c})$ of this coherence vector entry $u_{\mathbf{c}}(\hat{\rho}_{\text{pure}})$ tells us, which module phase we should use. Therefore we must provide the modules

$$\hat{\rho}_{\text{mod}}^{(N)}(\mathbf{c}, \phi(\mathbf{c}))\,. \tag{25}$$

The modulus $K(\mathbf{c})$ of the coherence vector entry $u_{\mathbf{c}}(\hat{\rho}_{\text{pure}})$ corresponds to these mixing coefficients.

Now it is possible to mix all modules with correctly adjusted phases and proper mixing coefficients,

$$\hat{\rho}_{\text{mix}} = \frac{1}{N_{\text{mod}}}\sum_{\mathbf{c}\neq\mathbf{0}} K(\mathbf{c})\,\hat{\rho}_{\text{mod}}^{(N)}(\mathbf{c}, \phi(\mathbf{c})) \tag{26}$$

with the real normalization N_{mod} (see Eq. (18)). If we put our definition of modules (13) into the mixture (Eq. (26)), we get:

$$\hat{\rho}_{\text{mix}} = \frac{1}{n^N}\left(\hat{1} + \frac{\Xi}{N_{\text{mod}}}\sum_{\mathbf{c}\neq\mathbf{0}}\left(K(\mathbf{c})\mathrm{e}^{\mathrm{i}\phi(\mathbf{c})}\hat{C}_{\mathbf{c}} + K(\mathbf{c})\mathrm{e}^{-\mathrm{i}\phi(\mathbf{c})}\hat{C}_{\mathbf{c}}^{\dagger}\right)\right). \tag{27}$$

Based on equation (24) this can be recast into

$$\hat{\rho}_{\text{mix}} = \frac{1}{n^N}\left(\hat{1} + \frac{\Xi}{N_{\text{mod}}}\sum_{\mathbf{c}\neq\mathbf{0}}\left(u_{\mathbf{c}}(\hat{\rho}_{\text{pure}})\hat{C}_{\mathbf{c}} + u_{\mathbf{c}}^{*}(\hat{\rho}_{\text{pure}})\hat{C}_{\mathbf{c}}^{\dagger}\right)\right). \tag{28}$$

Obviously the sum over $u_{\mathbf{c}}(\hat{\rho}_{\text{pure}})\hat{C}_{\mathbf{c}}$ is the product operator expansion of our pure state. With equations (6, 10), we are able to transform the second sum of the mixture (28) into a sum over product operators instead of a sum over adjoint product operators. This sum is equivalent to the first sum because it runs over all indices $\mathbf{c}$. Therefore we get the expansion:

$$\hat{\rho}_{\text{mix}} = \frac{1}{n^N}\left(\hat{1} + \frac{2\Xi}{N_{\text{mod}}}\sum_{\mathbf{c}\neq\mathbf{0}} u_{\mathbf{c}}(\hat{\rho}_{\text{pure}})\hat{C}_{\mathbf{c}}\right). \tag{29}$$

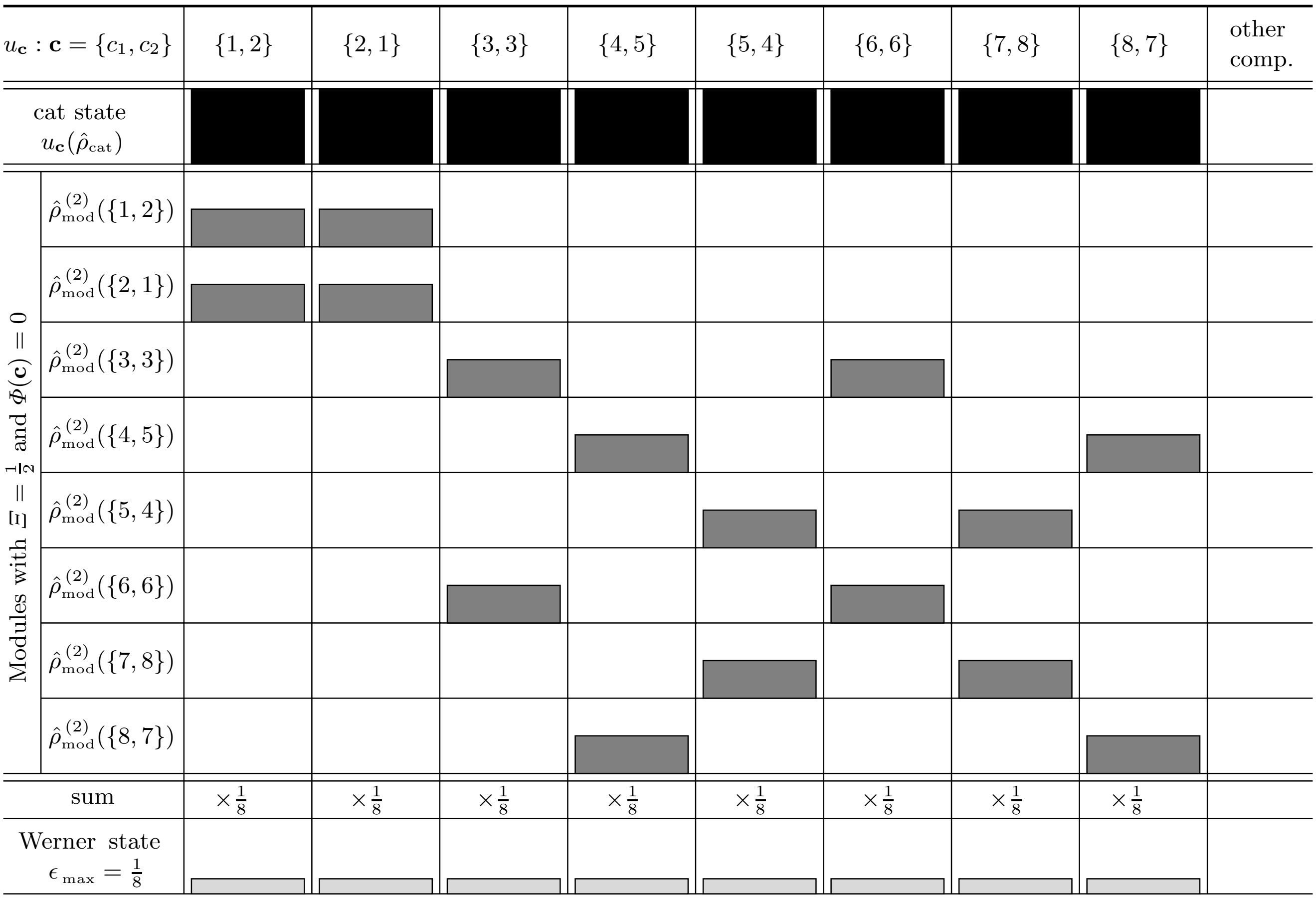
This mixed state is separable, because it is constructed by a convex combination of separable quantum states, the modules. For an example see Appendix A or Figure 1.

We finally compare the mixed state (29) with the generalized Werner state (see Eq. (20)) to extract the mixture coefficient

$$\epsilon_{\text{mix}} = \frac{2\Xi}{N_{\text{mod}}} \leq \epsilon_{\text{max}}. \tag{30}$$

If we are able to provide modules with the maximal possible $\Xi = 1/2$, we get $\epsilon_{\text{max}} = 1/N_{\text{mod}}$. Obviously, it is possible to reach now every generalized Werner state with $\epsilon \leq \epsilon_{\text{max}}$ by mixing. Because the mixed state is known to be separable one may say that this mixing process is a *sufficient criterion for separability* of generalized Werner states.

Note, that for all systems with n prime we may sort the basis operators $\hat{C}_{\mathbf{c}}$ into pairs of operators and their adjuncts. Then it is possible to halve the number of modules needed (see Fig. 1) and thus improve ϵ_{max} by a factor of two. Also in other cases it may be possible to improve the present mixing process, but not in general.



$u_{\mathbf{c}} : \mathbf{c} = \{c_1, c_2\}$		$\{1,2\}$	$\{2,1\}$	$\{3,3\}$	$\{4,5\}$	$\{5,4\}$	$\{6,6\}$	$\{7,8\}$	$\{8,7\}$	other comp.
cat state $u_{\mathbf{c}}(\hat{\rho}_{\text{cat}})$		■	■	■	■	■	■	■	■	
Modules with $\Xi = \frac{1}{2}$ and $\Phi(\mathbf{c}) = 0$	$\hat{\rho}^{(2)}_{\text{mod}}(\{1,2\})$	▨	▨							
	$\hat{\rho}^{(2)}_{\text{mod}}(\{2,1\})$	▨	▨							
	$\hat{\rho}^{(2)}_{\text{mod}}(\{3,3\})$			▨			▨			
	$\hat{\rho}^{(2)}_{\text{mod}}(\{4,5\})$				▨				▨	
	$\hat{\rho}^{(2)}_{\text{mod}}(\{5,4\})$					▨		▨		
	$\hat{\rho}^{(2)}_{\text{mod}}(\{6,6\})$			▨			▨			
	$\hat{\rho}^{(2)}_{\text{mod}}(\{7,8\})$					▨		▨		
	$\hat{\rho}^{(2)}_{\text{mod}}(\{8,7\})$				▨				▨	
sum		$\times\frac{1}{8}$	$\times\frac{1}{8}$	$\times\frac{1}{8}$	$\times\frac{1}{8}$	$\times\frac{1}{8}$	$\times\frac{1}{8}$	$\times\frac{1}{8}$	$\times\frac{1}{8}$	
Werner state $\epsilon_{\max} = \frac{1}{8}$		░	░	░	░	░	░	░	░	

Fig. 1. Mixing as a pattern composition: the non-zero components of the target vector $u_{\mathbf{c}}$ for an original Werner state ($N = 2, n = 3$) are shown in the first line. This vector can be reconstructed using 8 modules ($\Xi = 1/2$), leading to $\epsilon_{\max} = 1/8$. Note that in the present case the module pattern are pairwise identical, so that 4 modules suffice, allowing to improve $\epsilon_{\max} = \epsilon_{\text{sep}} = 1/4$.

6 Separability boundary

For the original Werner state Pittenger and Rubin have found a criterion for full separability [16]: a Werner states is separable if and only if

$$\epsilon \leq \epsilon^{(\text{cat})}_{\text{sep}} = \frac{1}{n^{N-1}+1}. \tag{31}$$

Note that this is only valid if the pure state corresponds to the cat state. For the generalized Werner states such a separability criterion has not been found yet. There are some special cases, *e.g.* if the pure state is a product state, where the generalized Werner state is separable for arbitrary ϵ. In the special case of original Werner states we have $n^N - 1$ mixture coefficients $K = 1$ (see Eqs. (22, 24) and thus, according to equation (18), $N_{\text{mod}} = n^N - 1$. Equation (30) then implies

$$\epsilon_{\max} = \frac{1}{n^N - 1} < \epsilon^{(\text{cat})}_{\text{sep}}. \tag{32}$$

It is obvious that this $\epsilon_{\max}$ is usually far below the separability boundary $\epsilon^{(\text{cat})}_{\text{sep}}$ of equation (31). But for the special case of original Werner states and n prime, we have been able to produce states directly at the Pittenger boundary. For this purpose we need a different type of basis states, which are better adapted to this special case, which we will call *packages*. Packages are defined here, for n prime, by the product operator expansion:

$$\hat{\rho}^{(N)}_{\text{pack}}(\mathbf{c}) = \frac{1}{n^N}\left(\hat{1} + \sum_{\sigma=1}^{n-1} \hat{C}^{\sigma}_{\mathbf{c}}\right). \tag{33}$$

Here, we have introduced the power of a product operator $\hat{C}^{\sigma}_{\{\mathbf{a},\mathbf{b}\}}$, which is another operator out of the set proportional to $\hat{C}_{\{\underline{\sigma\mathbf{a}},\underline{\sigma\mathbf{b}}\}}$. All these operators commute and their common eigenstates are product states; (33) can thus be written as a mixture of product states and is therefore separable. The purity is $P_{\text{pack}} = 1/n^{N-1}$.

Which package one needs for the mixture, can be extracted again from the coherence vector, here given by equation (22). To reach states directly at the separability boundary we need only packages whose index vectors fulfill the conditions $\mathbf{a} = \{1, ..., 1\}$ and $\underline{\sum_{\mu=1}^{N} b_\mu} = 0$. We mix these N_{pack} packages with mixture coefficients $K(\mathbf{c}) = 1$:

$$\hat{\rho}^{(N)}_{a=1} = \frac{1}{N_{\text{pack}}} \sum_{\mathbf{b}} \hat{\rho}^{(N)}_{\text{pack}}(\{\mathbf{a},\mathbf{b}\})\, \delta(\underline{\textstyle\sum_{\mu=1}^{N} b_\mu} = 0) \tag{34}$$

where $\mathbf{a} = \{1, ..., 1\}$ and with the δ-function from equation (23). Furthermore, we need another special separable state:

$$\hat{\rho}^{(N)}_{\text{spec}} = \frac{1}{n}\sum_{i=0}^{n-1} |i, ..., i\rangle\langle i, ..., i|. \tag{35}$$

Mixture of all selected states with equal weights and correct normalization leads to the density operator:

$$\hat{\rho}_{\text{mix}} = \frac{1}{N_{\text{pack}} + 1}\left(N_{\text{pack}}\, \hat{\rho}^{(N)}_{a=1} + \hat{\rho}^{(N)}_{\text{spec}}\right). \tag{36}$$

Because here all mixture coefficients are equal to one $N_{\text{pack}} = n^{N-1}$ is the number of used packages. If the packages (33) are inserted into equation (36) and $\hat{\rho}^{(N)}_{\text{spec}}$ is expanded in terms of product operators, one can get finally the expansion in terms of product operators:

$$\hat{\rho}_{\text{mix}} = \frac{1}{n^N}\left(\hat{1} + \frac{1}{n^{N-1} + 1}\sum_{a=0}^{n-1}\sum_{\mathbf{b}} \hat{C}_{\{\mathbf{a},\mathbf{b}\}}\,\delta(\underline{\textstyle\sum_{\mu=1}^{N} b_\mu} = 0)\right), \tag{37}$$

which is equivalent to the product operator expansion of the original Werner state, with

$$\epsilon_{\max} = \epsilon^{(\text{cat})}_{\text{sep}} = \frac{1}{n^{N-1} + 1}\cdot \tag{38}$$

Note that this process only works for n prime. This follows from the special operator basis in this case and underlines the peculiarities of finite groups of prime order (*cf.* [34]).

7 Conclusions

We have based our considerations on the (in general complex) coherence-vector description applicable to any quantum state of a finite composite system. The vector components comprise the various coherence properties of the state; their real and imaginary parts may be said to define a one-dimensional discrete pattern. This pattern uniquely specifies the respective state.

Mixed states are characterized by a vector length L smaller than the maximum reached for pure states. We have introduced a concrete mixing procedure, in which the target coherence vector is reconstructed step-by-step *via* the combination of elementary pattern provided by our modules.

This concept has been applied to the original and generalized Werner states (1-parameter-families of mixed states). The geometrical interpretation of mixing in terms of pattern combinations allows for an intuitive and simple explanation of the "classical simulation of entanglement": as any vector component is available based on separable module states, one can compose any pattern one likes, including those of truly entangled states, though with reduced vector length. As might have been expected, these classical simulations are exponentially costly, taking as a measure of cost the number of different modules needed for the mixture: there are $n^{2N} - 1$ different product operators and thus the same number of different modules. If we additionally account for the hermiticity of all density operators, it is necessary to mix $(n^{2N} - 1)/2$ modules, in the worst case. This number grows exponentially with the number of subsystems.

However, this mixture process is not optimal, *i.e.* it is, in general, not possible to reach mixed states directly at the boundary of separability. This is basically due to the fact that too many modules are needed (which already have low purity), implying a too short coherence vector length. Specially adapted modules have been shown to be needed to reach this goal for the original Werner states. To find such optimized modules for other state classes (coherence vectors with other target patterns) will be quite challenging. One should note that having found the set of optimum modules valid for any mixed target state would be equivalent to a complete solution of the general separability problem!

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Appendix A: Example of a modular mixture for a $(\mathbf{N = 2, n = 3})$ network

Based on the cat state $|\psi\rangle = (|00\rangle + |11\rangle + |22\rangle)/\sqrt{3}$, we consider the Werner state

$$\hat{\rho}_{\text{Werner}} = \frac{1}{9}(1 - \epsilon)\hat{1} + \epsilon|\psi\rangle\langle\psi|. \tag{A.1}$$

From its expansion in terms of product operators ($\mathbf{c} = \{c_1, c_2\}$):

$$\hat{\rho}_{\text{Werner}} = \frac{1}{9}\Bigg(\hat{1} + \epsilon\Bigg(\hat{C}_{\{1,2\}} + \hat{C}_{\{2,1\}} + \hat{C}_{\{3,3\}} + \hat{C}_{\{4,5\}} + \hat{C}_{\{5,4\}} + \hat{C}_{\{6,6\}} + \hat{C}_{\{7,8\}} + \hat{C}_{\{8,7\}}\Bigg)\Bigg), \tag{A.2}$$

we read off the non-zero coherence vector entries (*cf.* Eq. (8)):

$$\begin{aligned} &u_{\{1,2\}} = \epsilon, \quad u_{\{2,1\}} = \epsilon, \quad u_{\{3,3\}} = \epsilon, \quad u_{\{4,5\}} = \epsilon,\\ &u_{\{5,4\}} = \epsilon, \quad u_{\{6,6\}} = \epsilon, \quad u_{\{7,8\}} = \epsilon, \quad u_{\{8,7\}} = \epsilon. \end{aligned} \tag{A.3}$$

This coherence vector can now be reproduced using our modules or packages.

The phases and mixing coefficients for the mixing of the general modules are (note that $\mathbf{c} = \{c_1, c_2\} \equiv \{\mathbf{a}, \mathbf{b}\} = \{\{a_1, a_2\}, \{b_1, b_2\}\}$) *cf.* equation (22):

$$\Phi(\mathbf{c}) = 0,\; K(\mathbf{c}) = \begin{cases} 1 & \mathbf{a} = \{a, a\},\; \underline{b_1 + b_2} = 0\\ 0 & \text{else.} \end{cases} \tag{A.4}$$

The number of modules needed is: $N_{\text{mod}} = 3^2 - 1 = 8$ (see Eq. (18)). The resulting mixtures reads:

$$\hat{\rho}_{\text{mix}} = \frac{1}{N_{\text{mod}}} \sum_{\mathbf{c}\neq\mathbf{0}} K(\mathbf{c}) \hat{\rho}^{(2)}_{\text{mod}}(\mathbf{c}, 0)$$

$$\hat{\rho}_{\text{mix}} = \frac{1}{9}\left(\hat{1} + \frac{2\Xi}{8}\left(\hat{C}_{\{1,2\}} + \hat{C}_{\{2,1\}} + \hat{C}_{\{3,3\}} + \hat{C}_{\{4,5\}} + \hat{C}_{\{5,4\}} + \hat{C}_{\{6,6\}} + \hat{C}_{\{7,8\}} + \hat{C}_{\{8,7\}}\right)\right) \qquad \text{(A.5)}$$

with $\epsilon_{\text{mix}} = \frac{\Xi}{4}$. This mixing process of general modules for reaching the original Werner state for a $(2, 3)$ network is illustrated in Figure 1.

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