Concurrence of quasi pure quantum states

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(Dated: April 1, 2022)

We derive an analytic approximation for the concurrence of weakly mixed bipartite quantum states - typical objects in state of the art experiments. This approximation is shown to be a lower bound of the concurrence of arbitrary states.

PACS numbers: 03.67.-a, 03.67.Mn, 03.65.Ud

Entangled states constitute one of the most fundamental differences between quantum and classical mechanics. The objects of prime interest in most experiments are pure entangled states. Therefore, experimental setups are designed such that unavoidable environment coupling is minimised, in order to keep the system state as pure as possible. On the theoretical side, most efforts are concerned with arbitrary mixed states - so far with limited success. Hardly any entanglement measure can be calculated for systems larger than bipartite two-level systems - the smallest ones of interest.

It is astonishing that theory did not proceed more closely along the lines indicated by experiments, although approximations inspired by experimental facts are frequently - and successfully - used in other branches of physics. In this letter we present an estimate for the entanglement of almost pure states - an approach naturally emerging from experimental reality, where the evolution into a mixed state - due to non-unitary dynamics - occurs on a time scale much larger than any other relevant experimental time scale [1, 2, 3]. Therefore, notwithstanding the unavoidable evolution of an initially pure state into a mixed one, the system state remains quasi pure during the period of interest, i.e. its density matrix has one single eigenvalue \( \mu_1 \) that is much larger than all the other ones. Under this condition, all terms proportional to integer powers of \( \mu_i \), \( i > 1 \), are small, and higher order terms can be safely neglected in our subsequent treatment of concurrence, which is one of the generally accepted entanglement indicators.

The concurrence \( c \) of a pure, bipartite quantum state \( |\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \) can be defined [3] as

\[
c(\Psi) = \sqrt{\text{Tr}(|\Psi\rangle\langle\Psi|^2) - \text{Tr}_1 \varrho_1^2 - \text{Tr}_2 \varrho_2^2 + (\text{Tr}(|\Psi\rangle\langle\Psi|)^2)},
\]

with the reduced density matrices \( \varrho_1 = \text{Tr}_2 |\Psi\rangle\langle\Psi| \) and \( \varrho_2 = \text{Tr}_1 |\Psi\rangle\langle\Psi| \); the trace over both subsystems is denoted by \( \text{Tr} \). An equivalent and widely used expression reads \( c(\Psi) = \sqrt{2(\text{Tr}(|\Psi\rangle\langle\Psi|^2)^2 - \text{Tr} \varrho_c^2)} \), where \( \varrho_c \) is either one of the reduced density matrices. Though, as we will see in the sequel, the former definition will turn out to be advantageous in our following generalisation for mixed states \( \varrho \), where concurrence is defined through the convex roof

\[
c(\varrho) = \inf_{\{p_i, |\Psi_i\rangle\}} \sum_i p_i c(\Psi_i), \quad \varrho = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|, \quad p_i > 0.
\]

Here, the infimum is to be found among all ensembles \( \{p_i, |\Psi_i\rangle\} \) representing \( \varrho \). If we start from a given decomposition (e.g., the eigensystem of \( \varrho \), \( \varrho |\Psi_i\rangle = \mu_i |\Psi_i\rangle \), \( i = 1, \ldots, n \)), all ensembles can be parametrised through a left-unitary transformation \( V \in \mathbb{C}^{N \times n} \), where possibly \( N \geq n \):

\[
\sqrt{\mu_i} |\Psi_i\rangle = \sum_{j=1}^N V_{ij} \sqrt{\mu_j} |\Phi_j\rangle, \quad \sum_{i=1}^N V_{ki}^\dagger V_{ij} = \delta_{j,k}.
\]

The concurrence of a mixed state \( \varrho \) can therefore be expressed as [4, 5]

\[
c(\varrho) = \inf_V \sum_i \left( [V \otimes V \mathcal{A} \otimes V^\dagger]_{ii} \right)^{\frac{1}{2}},
\]

where the tensor \( \mathcal{A} \) is defined as

\[
\mathcal{A}_{jk}^{lm} = \sqrt{\mu_j \mu_k \mu_l \mu_m} \times \left[ \text{Tr} (|\Phi_j\rangle\langle\Phi_l| |\Phi_k\rangle\langle\Phi_m|) - \text{Tr}_1 (\text{Tr}_2 (|\Phi_j\rangle\langle\Phi_l| |\Phi_k\rangle\langle\Phi_m|)) - \text{Tr}_2 (\text{Tr}_1 (|\Phi_j\rangle\langle\Phi_l| |\Phi_k\rangle\langle\Phi_m|)) + \text{Tr} (|\Phi_j\rangle\langle\Phi_l| |\Phi_k\rangle\langle\Phi_m|) \right].
\]

\( \mathcal{A} \) is a positive, hermitian operator satisfying \( \mathcal{A}_{jk}^{lm} = \mathcal{A}_{kj}^{lm} = \mathcal{A}_{kj}^{mk} \). The latter symmetry is inherited from the symmetric definition of concurrence in eq. [1], and is crucial for our further analysis. In particular, it implies that \( \mathcal{A} \) can always be expressed in terms of complex symmetric matrices \( T^a \) as \( \mathcal{A}_{jk}^{lm} = \sum_a T_{jk}^a (T_{lm}^a)^* \) [6]. Whereas the concurrence of a pure state is characterized by a single matrix \( \tau := T^1 \), with only one non-vanishing element, a mixed state in general requires more than one matrix. The crucial idea underlying our approximation is now that the concurrence of a quasi pure state can still be well described by a single matrix \( \tau \), though with more than just one non-vanishing element.

This becomes clear when we remind ourselves of the obvious proportionality \( \mathcal{A}_{jk}^{lm} \sim \sqrt{\mu_j \mu_k \mu_l \mu_m} \). For quasi
pure states with \( \mu_1 \gg \mu_i, \ i > 1 \), this relation induces a natural order in terms of the small eigenvalues \( \mu_i, \ i > 1 \).

The leading term \( A_{kl}^{11} \sim \mu_1^2 \) (lowest order in the \( \mu_i \)) is sufficient to characterize the concurrence of the pure state \( \ket{\Phi_1} \). For mixed states, however, there are also terms of first order, alike \( A_{jk}^{11} \sim \sqrt{\mu_j \mu_k}, \ j, k > 1 \), of second order, such as \( A_{jk}^{11} \sim \sqrt{\mu_j \mu_k}, \ j, k > 1 \), and of third and fourth order. The approximation

\[
A_{jk}^{11} \approx \tau_{jk} \tau^{*}_{lm}, \quad \text{with} \quad \tau_{jk} = \frac{A_{jk}^{11}}{A_{11}^{11}}, \quad (6)
\]
is exact up to first order, and even correctly represents second order elements of type \( A_{11}^{11} \). Importantly, this quasi pure approximation (qpa) simplifies eq. (4) significantly:

\[
c(\rho) \approx c_{qp}(\rho) = \inf_{\gamma} \sum_{i} \left| [V \tau V^{T}]_{ii} \right| , \quad (7)
\]

and a closed expression for the right hand side of this equation is known \( \Phi_1 \). It can be given in terms of the singular values \( \lambda_i \) of \( T \), this is the square roots of the eigenvalues of the positive hermitian matrix \( \tau^{T} \tau \),

\[
c_{qp}(\rho) = \max(\lambda_1 - \sum_{i>1} \lambda_i, \ 0) , \quad (8)
\]

with the \( \lambda_i \) labeled in decreasing order.

Note that, in eq. (6), we implicitly assumed that \( A_{11}^{11} \) does not vanish, or, equivalently, that \( \ket{\Phi_1} \) is not separable. This does not limit, however, the range of applicability of our approximation. If the dominant contribution \( \ket{\Phi_1} \) to a given mixed state \( \rho \) is separable, \( \rho \) will typically be separable anyway.

A major advantage of our present estimate is that – with respect to other methods \( \Phi_1 \) – it even further reduces the computational resources for the evaluation of the degree of entanglement of a given state: In \( \Phi_1 \), it was necessary to diagonalize a matrix quadratically larger than \( \rho \), eventually followed by an optimization procedure. Here, we need not optimize, and only have to diagonalize a matrix of the size of the given statistical operator. Consequently, significant speed-up can be achieved when a large number of mixed states has to be assessed, such as, e.g., monitoring the time evolution of entanglement under environment coupling \( \Phi_2 \), without significant loss of the quality of the estimation. To illustrate that, let us consider a bipartite system of dimension \( 3 \times 5 \), coupled to an environment. The total Hamiltonian acting on system and bath reads \( H = \alpha_s H_s \otimes \mathbb{1}_b + \alpha_{sb} H_{sb} \), where \( H_s \) acts on the system alone, \( H_{sb} \) represents the system-bath interaction, and \( \alpha_s \) and \( \alpha_{sb} \) determine the strength of system dynamics and environment coupling, respectively. In our following example, the matrix elements of \( H_s \) and \( H_{sb} \) are random numbers, and the coupling constants are fixed at \( \alpha_s = 0.2 \) and \( \alpha_{sb} = 0.02 \). The total state of system and bath, initially prepared in a pure system state tensored with the maximally mixed bath state, evolves under the unitary time evolution operator \( U = \exp(iHt) \), and the dynamics of the system state alone is obtained upon tracing over the environmental degrees of freedom, what induces decoherence, i.e., mixing. In fig. (a), the time evolution of concurrence is plotted in qpa for the above parameter values, over three different time intervals. Also optimized lower \( \Phi_1 \) and upper \( \Phi_1 \) bounds of concurrence are shown. The degree of mixing of \( \rho(t) \) is characterized by its von Neumann entropy. While the degree of mixing is rather small in fig. (a), it steadily increases in figs. (b) and (c). Nonetheless, our qpa captures the actual value of the concurrence rather precisely over the entire time interval, even for already significantly mixed states – i.e., beyond its initially anticipated range of validity.

Finally, let us note that the quasi pure approximation
FIG. 2: Concurrence in qpa for the class of $3 \times 3$ states defined in eq. (9). Although $\rho_a$ exhibits rather large mixing (with von Neumann entropy approx. equal to $1.3 \ldots 1.8$, for $a > 0.1$) and positive partial transpose, the qpa (solid line) detects $\rho_a$ as entangled, and provides a rather good approximation of the actual value of concurrence, which is confined by upper \footnote{\cite{13}} (dots) and lower \footnote{\cite{7,8}} (dashed line) bounds.

also provides a lower bound on concurrence, and, in particular, can distinguish entangled states from separable ones: We have shown in \footnote{\cite{7}} that any symmetric matrix $\sum_k z_k T_k$, with $\sum_k |z_k|^2 = 1$ and $A_{jk} = \sum_k T_{jk} (T_{ka})^*$, defines a lower bound of concurrence. One easily verifies that $\tau$ defined in eq. (6) indeed is precisely of this form, with $z_\alpha = (T_{11})^*/\sqrt{\sum_{\beta} |T_{11}|^2}$. Even entangled states with positive partial transpose can be characterised with the qpa: Consider, for example, the class of states

$$
\rho_a = \frac{1}{1+8a} \begin{bmatrix}
a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\
0 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 \\
0 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & a & 0 & 0 & 0 & 0 \\
a & 0 & 0 & a & 0 & 0 & 0 & \gamma & \beta \\
a & 0 & 0 & a & 0 & 0 & \beta & \gamma & \alpha \\
a & 0 & 0 & a & 0 & 0 & \gamma & \alpha & \beta 
\end{bmatrix}, \ a \in [0,1], \quad (9)
$$

of a $3 \times 3$-system, with $\beta = (1+a)/2$ and $\gamma = \sqrt{1-a^2}/2$, which were introduced in \footnote{\cite{13}}. Fig. 2 compares the qpa to upper and lower bounds \footnote{\cite{7,8}} of concurrence, as a function of the parameter $a$. The qpa is indeed positive in the entire interval, i.e. the non-separability of $\rho_a$ is detected by purely algebraic means.

Thus, our qpa does not only provide tools for an efficient estimation of concurrence of states with moderate mixing, but it is even applicable to general states. We reckon that the concept of quasi purity which we have exploited here may be a remedy also for various other, so far virtually uncomputable entanglement measures, and it appears promising to check whether such approximations have an equally large range of applicability.

We are indebted to André Ricardo Ribeiro de Carvalho and Marek Kuś for fruitful discussions, comments and remarks. Financial support by VolkswagenStiftung is gratefully acknowledged.

\footnotesize

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