Estimation of purity in terms of correlation functions

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We prove a rigorous inequality that estimates the purity of a reduced density matrix of a composite quantum system in terms of cross correlation of the same state and an arbitrary product state. Various immediate applications of our result are proposed, in particular, concerning Gaussian wave-packet propagation under classically regular dynamics.

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The autocorrelation function of time evolution, also known as *survival probability* or as *fidelity* in the context of echo dynamics [1], is an important tool in the discussion of quantum systems. Indeed, the autocorrelation function contains a large amount of information, but analysis in terms of the more general concept of cross-correlation functions can bring additional insight. This has been recently demonstrated for spectral statistics [2]. In this paper, we shall seek a better understanding of the evolution of entanglement in terms of cross-correlation functions. This is particularly interesting, because entanglement is at the very root of quantum mechanics, and we shall therefore test the usefulness of cross-correlation functions in this context. Note that the first experimental test on the value of cross correlations for the analysis of spectral statistics was carried out in a microwave experiment with classical fields [3] rather than in the context of quantum mechanics.

Entanglement indicates that to what extent the state under consideration can be written as a product of states in two subsystems selected due to their interest in the physical context. For pure states, entanglement is reflected in the properties of the reduced density matrix for any of the two subsystems. It is tempting to use some form of entropy to describe this property, but this makes analytic work very difficult. We shall therefore use the purity of a subsystem [4] as a measure of entanglement. Purity is defined as the trace of the square of the reduced density matrix. The fact that we use an analytic function allows us to obtain the basic inequalities with cross correlations, which give the main result of this paper. To explore that to what extent these inequalities can be exhausted, we shall turn to two examples, which first called for our attention to this problem.

First, considering the time evolution under an integrable Jaynes-Cummings Hamiltonian of a wave packet forming a product state, Nemes and co-workers [5] observed a strong maximum in the purity after half the period of the classical orbit around which the packet was constructed [5]. It is intuitively clear that the autocorrelation function will show a revival only after a full period, and thus cannot contribute an explanation for this phenomenon. Note that the Jaynes-Cummings Hamiltonian

$$H=\hbar\omega a^\dagger a+\hbar\epsilon J_z+\frac{\hbar G}{\sqrt{2J}}(aJ_+ + a^\dagger J_-), \tag{1}$$

describing an oscillator with the standard annihilation operator a and SU(2) spin $\vec{J}$, has a mirror symmetry given by

$$a\to -a,\quad J_\pm\to -J_\pm,\quad J_z\to J_z, \tag{2}$$

which is also evident in Figs. 1 and 2 of Ref. [5]. We may then conjecture that the oscillations seen in the linear entropy, defined as one minus purity, are due to maxima in the autocorrelation functions for full periods and maxima in the cross-correlation functions with the mirror image of the initial state for the half period.

Second, following the time evolution of a similar packet under echo dynamics with the same Hamiltonian and a slight detuning as perturbation, we found that coherent states conserved purity to a higher order in $\hbar$ than other states, e.g., random states [6]. Here the conjecture is that the cross-correlation function with the classically transported image of the original packet will yield an explanation.

These examples serve to illustrate our analytic results in the framework of a model, whose use is widespread in atomic physics and quantum optics, in particular, for Rydberg atoms in cavities and for atoms in Paul traps with externally driven fields. The first case will become rather obvious once the inequalities are derived, and for the second case we shall derive the result within the linear-response approximation.

Consider a composite system with a Hilbert space

$$\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2, \tag{3}$$

consisting of two factor spaces $\mathcal{H}_{1,2}$ which may have either finite or infinite dimensions.

Let $|\psi\rangle$ be an arbitrary pure state of a composite system which, after tracing over the subsystem 2, defines a reduced density operator over the subsystem 1:

$$\rho_1=\mathrm{tr}_2|\psi\rangle\langle\psi|. \tag{4}$$

We can prove the following general inequality for estimating the purity:

$$I[\rho_1]=\mathrm{tr}_1\rho_1^2 \tag{5}$$

of a reduced state ρ_1.

Theorem. The following inequality holds

$$|\langle\phi|\psi\rangle|^4 \leqslant I[\rho_1] \tag{6}$$

for any product state $|\phi\rangle = |\phi_1\rangle\otimes|\phi_2\rangle$.

Proof. Uhlmann's theorem [7] states for pure states $\rho = |\psi\rangle\langle\psi|$ and $\sigma = |\phi\rangle\langle\phi|$ that

$$|\langle\phi|\psi\rangle|^2 = \mathrm{tr}\,\rho\sigma \leqslant \mathrm{tr}_1[\mathrm{tr}_2\rho\,\mathrm{tr}_2\sigma] = \langle\phi_1|\rho_1|\phi_1\rangle. \tag{7}$$

Then, applying the Cauchy-Schwartz inequality for operators $|\mathrm{tr}(A^\dagger B)|^2 \leqslant \mathrm{tr}(AA^\dagger)\mathrm{tr}(BB^\dagger)$, we get

$$|\mathrm{tr}_1[\mathrm{tr}_2\rho\,\mathrm{tr}_2\sigma]|^2 \leqslant \mathrm{tr}_1[\mathrm{tr}_2\rho]^2\mathrm{tr}_1[\mathrm{tr}_2\sigma]^2 = I[\rho_1]. \tag{8}$$

Combining inequalities (7) and (8), we get result (6).

Corollary 1. An interesting special case of the above result is obtained if $|\phi\rangle = |\psi(0)\rangle$ is an initial disentangled state of a unitary quantum *time evolution* $|\psi\rangle = |\psi(t)\rangle$. Then our result says that the entanglement growth, as measured by purity, is bounded from below by the autocorrelation function $|\langle\psi(0)|\psi(t)\rangle|^4$.

Corollary 2. A more general situation arises if $|\phi\rangle$ is any factorizable state as required by the theorem. Then, we obtain that the growth of entanglement, as measured by the purity is bounded from below by all cross-correlation functions of the type $|\langle\phi|\psi(t)\rangle|^4$.

The second corollary includes the first as a special case and is the general result that we need in order to apply cross-correlation functions to understand oscillations or slow growth of the entanglement.

To explore the possibility of approaching equality in the second corollary (and the main theorem), we have to look at the eigenvalues of the reduced density matrix (which are identical for both subspaces [8]). Since the purity is the trace of an analytic function of the reduced density matrix, the optimal function ϕ, with which we can establish a cross-correlation, is a product of the eigenfunctions corresponding to the largest eigenvalue. Note that the eigenvalues are the same for the reduced density matrix in both subspaces. If we denote this eigenvalue by $1-\delta$, the cross-correlation function will take the value $|\langle\phi|\psi(t)\rangle|^4 = (1-\delta)^2$. Actually, purity I will obey the slightly sharper inequality

$$(1-\delta)^2+\delta^2 \geqslant I \geqslant (1-\delta)^2 + \frac{\delta^2}{\min(\dim(\mathcal{H}_1),\dim(\mathcal{H}_2))-1}, \tag{9}$$

where dim indicates the dimension of the corresponding Hilbert space. We obtain this inequality by assuming the two extreme cases: either the missing intensity δ^2 is concentrated to a single product state or it is evenly distributed among all such states. The former provides the upper bound and the latter the lower bound. As the lower limit is larger than the value $(1-\delta)^2$, we obtain from Corollary 2 that equality in Eq. (6) can only be reached for $I=1$. Note that inequality (6) provides a fairly sharp lower bound if the purity is close to 1 because then $1-I\sim\delta$ while $I-|\langle\phi|\psi(t)\rangle|^4\sim\delta^2$, i.e., the error of the lower bound is quadratic in the deviation of the purity from unity.

We can now hope to find sets of functions ϕ_i such that the cross correlation with these will explain the behavior of the purity as long as the latter is near to 1. Yet, to elucidate we must be able to construct such a set without diagonalizing the density matrix. If we have a symmetry group that acts separately on the two subspaces, this set is trivially generated by applying the symmetry operations to the initial function $\psi(0)$. For the example discussed earlier, a cross correlation with the function, obtained by applying reflection (2) to $\psi(0)$, will have maxima at 1/2,3/2, ... of the full period. We shall now turn to the other example we mentioned, namely, the slow decay of purity for coherent states in an integrable system. This question was discussed in Ref. [6] for arbitrary Gaussian packets in the context of echo dynamics, and illustrated again in the Jaynes-Cummings model.

We can follow the line of considering cross correlations a little further in this context if we consider the quantity $\mathrm{tr}_1[\mathrm{tr}_2\rho\,\mathrm{tr}_2\sigma] = R(\rho_1,\sigma_1)$ considered in Eq. (7). For $\rho = \rho(t)$ and $\sigma = \rho(0)$, this quantity was introduced as reduced fidelity in Ref. [9] implying a reduced autocorrelation function if we do not treat an echo situation. With this notation, we have $I(\rho_1) \geqslant R^2(\rho_1,\sigma_1) \geqslant |\langle\phi|\psi\rangle|^4$, but, in addition, the second identity is fulfilled if ϕ is chosen as the eigenfunction of the largest eigenvalue of ρ_1. By choosing $\rho_1 = \rho(t)$ and σ arbitrary, we have an additional cross correlation that we may use. The basic advantage of this quantity is that it is, just like purity, defined on the subspace alone, and may therefore be useful in some situations. As far as approaching the identity with purity is concerned, this quantity has no advantages.

We shall next follow the same line of reasoning to find an optimized factorizable function ϕ to understand the behavior of the purity when it is near identity for a general Gaussian wave packet:

$$\langle\vec{x}|\psi\rangle = C\exp\left(\frac{i}{\hbar}[(\vec{x}-\vec{X})\cdot A(\vec{x}-\vec{X}) + \vec{P}\cdot\vec{x}]\right), \tag{10}$$

centered at $(\vec{X},\vec{P})$ and having the shape described by the (generally complex) matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \tag{11}$$

corresponding to a division of a $d = d_1 + d_2$ dimensional configuration space into d_1- and d_2-dimensional parts $\vec{x} = (x_1,x_2)$. The purity of a reduced wave-packet $\rho(x_1,x_1') = \int dx_2\langle x_1,x_2|\psi\rangle\langle\psi|x_1',x_2\rangle$ is $I = \int dx_1 dx_1' |\rho(x_1,x_1')|^2$ which can be evaluated in terms of a $2d$-dimensional Gaussian integral [6]

$$I = (\det \mathrm{Im}\,A) \times \begin{vmatrix} \mathrm{Im}\,A_{11} & \frac{\mathrm{i}}{2}A_{12}^* & 0 & -\frac{\mathrm{i}}{2}A_{12} \\ \frac{\mathrm{i}}{2}A_{21}^* & \mathrm{Im}\,A_{22} & -\frac{\mathrm{i}}{2}A_{21} & 0 \\ 0 & -\frac{\mathrm{i}}{2}A_{12} & \mathrm{Im}\,A_{11} & \frac{\mathrm{i}}{2}A_{12}^* \\ -\frac{\mathrm{i}}{2}A_{21} & 0 & \frac{\mathrm{i}}{2}A_{21}^* & \mathrm{Im}\,A_{22} \end{vmatrix}^{-1/2}, \tag{12}$$

where the vertical lines indicate the determinant of a matrix. According to our result, this expression should be bounded from below by cross correlation with any disentangled state which we again choose to be a Gaussian packet centered at the same point in phase space

$$\langle\vec{x}|\phi\rangle = D\exp\left(\frac{i}{\hbar}[(\vec{x}-\vec{X})\cdot B(\vec{x}-\vec{X})+\vec{P}\cdot\vec{x}]\right), \qquad (13)$$

with

$$B=\begin{pmatrix} B_{11} & 0 \\ 0 & B_{22}\end{pmatrix}. \qquad (14)$$

A straightforward evaluation of the Gaussian integral yields for the cross correlation

$$|\langle\phi|\psi\rangle|^4 = \frac{(\det \mathrm{Im}\,A)(\det \mathrm{Im} B)}{|\det(A-B^*)|^2} \qquad (15)$$

which, as we have shown, is strictly smaller than Eq. (12) for any B of form (14).

One may now ask the following question: Which packet (13) optimizes inequality (6)? In general, this is a complex optimization problem, however we may solve it asymptotically when purity is close to 1. In this case, off-diagonal elements of the shape matrix are small, so we may write $A_{12}=\epsilon Z_{12}, A_{21}=\epsilon Z_{21}$, where ϵ is small. It turns out that the inequality is optimized to the leading order in ϵ if we take $B_{11}=A_{11}, B_{22}=A_{22}$, namely, in this case $|\langle\phi|\psi\rangle|^4=1-c_1\epsilon^2+O(\epsilon^4)$, $I=1-c_2\epsilon^2+O(\epsilon^4)$, where $c_1=c_2$.

We note that the cross correlation (15) is manifestly $\hbar$ independent. It may be used to compute the dynamical, time-dependent, cross-correlation function of a propagating Gaussian packet $|\psi(t)\rangle$ (as long as linearized dynamics is a good approximation), since we know that the time dependence of the shape matrix $A=A(t)$ is given by the ratio of two pieces of the classical monodromy matrix [10]. We have thus shown that to the lowest order we can easily optimize the reference wave function $|\phi\rangle$, though it will clearly have to vary with time. We could first simply use the transported original (and factorizable) state $|\psi(0)\rangle$ centered around the new position, i.e., $B=A(0)$, where $\langle\phi|\psi(t)\rangle$ may be called the transported autocorrelation function. This would not optimize the lower bound, but for short times it might be quite good, and it would certainly make the bound $\hbar$ independent. Furthermore, one could apply bound (15) to the case of echo dynamics where the linear-response approximation is valid even for long times if the perturbation is sufficiently small (see Ref. [6]).

We may summarize our results by stating that we found a general inequality between the fourth power of the cross (and auto) -correlation functions and the purity. Furthermore, we were able to assert that the lower limit is almost identical to the value if the purity is near to one. Thus, any such value of purity can be explained by the fact that the evolving state acquires a large overlap with a factorizable state, and the difference between purity and our lower bound is of second order in the deviation of purity from identity. The knowledge of this factorizable state may contribute to the understanding of the slow decay or renewed maxima (also known as recoherence) for the purity. Particular examples of such situations are given in the case of a symmetry group whose representation factorizes in the variables in which we wish to split the spaces, and in the case of coherent states.

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