Thermal and magnetic quantum discord in Heisenberg models

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(Received 19 November 2009; published 1 April 2010)

We investigate how quantum correlations [quantum discord (QD)] of a two-qubit one-dimensional XYZ Heisenberg chain in thermal equilibrium depend on the temperature T of the bath and also on an external magnetic field B. We show that the behavior of thermal QD differs in many unexpected ways from thermal entanglement. For example, we show situations where QD increases with T when entanglement decreases, cases where QD increases with T even in regions with zero entanglement, and that QD signals a quantum phase transition even at finite T. We also show that by properly tuning B or the interaction between the qubits we get nonzero QD for any T and we present an effect not seen for entanglement, the "regrowth" of thermal QD.

DOI: 10.1103/PhysRevA.81.044101 PACS number(s): 03.65.Ud, 75.10.Pq, 05.30.−d

Introduction. Since the seminal work of John S. Bell [1], who brought to the realm of experimental physics the ideas of Einstein, Podolsky, and Rosen [2] concerning the nonlocal aspects of quantum mechanics, it became clear that the constituents of some quantum composite systems possessed correlations among themselves that were unachievable in the classical world. Those states belong to the class of entangled states, although not all entangled states possess stronger-than-classical correlations in the sense of violating Bell inequalities [3]. However, given a composite quantum state whose constituents are correlated, how can one determine the origin of the correlations? In other words, how can one divide the total correlation into a classical part and a purely quantum one? This is particularly important for mixed states, since their quantum correlations are many times hidden by their classical correlations. An answer to these questions is given by quantum discord (QD), a measure of the quantumness of correlations introduced in Ref. [4]. QD is built on the fact that two classical equivalent ways of defining the mutual information turn out to be inequivalent in the quantum domain. In addition to its conceptual role, some recent results [5] suggest that QD and not entanglement may be responsible for the efficiency of a mixed-state-based quantum computer.

Due to its fundamental and practical significance, we wish to investigate the amount of QD in a concrete system, such as a pair of qubits (spin-1/2) within a solid at finite temperature whose interaction is given by the Heisenberg model (XYZ model in general). Such Heisenberg models can describe fairly well the magnetic properties of real solids [6] and are well adapted to the study of the interplay of disorder and entanglement, as well as of entanglement and quantum phase transitions [7]. We characterize the dependence of QD on temperature and also on external magnetic fields applied to the qubits. We also compare the behavior of QD against the entanglement of formation (EoF) between the two qubits [8–10]. We obtain several interesting results for the behavior of QD *at nonzero T*, many of them in contrast to the behavior of EoF. First, we show that QD can *increase* with temperature in the *absence* of external fields applied to the qubits. This is in sharp contrast to the behavior of EoF, since one can show [10] that this effect never occurs without the presence of an external magnetic field. We also show that there exist regions where QD is different from zero while EoF is always zero, confirming a generic feature of QD [11]. In particular, we show that for the isotropic XXX model, both the ferromagnetic and anti-ferromagnetic Hamiltonians possess relatively high values of QD while EoF is absent for the ferromagnetic model [8]. These properties of QD can have important practical consequences for the realization of a quantum computer at finite temperatures. Indeed, we show that, once it is established that what is at stake for the correct functioning of a quantum computer is the existence of a certain level of QD (just having non-null QD might not be enough since almost all states have QD > 0 [11]), Heisenberg solids are better than previously thought as good candidates for the construction of a quantum computer at $T > 0$: For some parameter sets they have high values of QD while having no EoF at all. We also show that by properly adjusting the coupling constants [9] one can achieve any desired level of QD for any T. Finally, we show that for finite T we observe the sudden change of QD [12] as we change the coupling constant of the Hamiltonian and we show the "regrowth" of the thermal QD with increasing T.

The thermalized Heisenberg system. The Hamiltonian of the XYZ model with an external magnetic field acting on both qubits is

$$H = B\left(S_z^1 + S_z^2\right) + J_x S_x^1 S_x^2 + J_y S_y^1 S_y^2 + J_z S_z^1 S_z^2, \qquad (1)$$

with J_x, J_y, and J_z the coupling constants, $S^j_{x,y,z} = \sigma^j_{x,y,z}/2$, σ_x^j, σ_y^j, and σ_z^j the usual Pauli matrices acting on qubit j, and B the external magnetic field. We have assumed $\hbar = 1$. The density matrix describing a system in equilibrium with a thermal reservoir at temperature T (canonical ensemble) is $\rho = \exp(-H/kT)/Z$, where $Z = \mathrm{Tr}\{\exp(-H/kT)\}$ is the partition function and k is Boltzmann's constant. Therefore, Eq. (1) leads to the following thermal state in the standard basis:

$$\rho = \frac{1}{Z}\begin{pmatrix} A_{11} & 0 & 0 & A_{12} \\ 0 & B_{11} & B_{12} & 0 \\ 0 & B_{12} & B_{11} & 0 \\ A_{12} & 0 & 0 & A_{22} \end{pmatrix}. \qquad (2)$$

Here $A_{11} = e^{-\alpha}[\cosh(\beta) - 4B\sinh(\beta)/\eta]$, $A_{12} = -\Delta e^{-\alpha}\sinh(\beta)/\eta$, $A_{22} = e^{-\alpha}[\cosh(\beta) + 4B\sinh(\beta)/\eta]$, $B_{11} = e^{\alpha}\cosh(\gamma)$, $B_{12} = -e^{\alpha}\sinh(\gamma)$, and $Z = 2[\exp(-\alpha)\cosh(\beta) + \exp(\alpha)\cosh(\gamma)]$, where $\Delta = J_x - J_y$,

$\Sigma = J_x + J_y$, $\eta = \sqrt{\Delta^2 + 16B^2}$, $\alpha = J_z/(4kT)$, $\beta = \eta/(4kT)$, and $\gamma = \Sigma/(4kT)$.

Entanglement. For a pair of qubits there exists an analytical expression, called EoF, to quantify its amount of entanglement [13]. Given the density matrix ρ describing thermalized two qubits, EoF is the average entanglement of the pure-state decomposition of ρ, minimized over all possible decompositions, $\mathrm{EoF}(\rho) = \min \sum_k p_k E(\phi_k)$, where $\sum_k p_k = 1$, $0 < p_k \leqslant 1$, and $\rho = \sum_k p_k |\phi_k><\phi_k|$. $E(\phi_k)$ is the entanglement of the pure state $|\phi_k\rangle$ [14]. For a pair of qubits, Wootters [15] has shown that EoF is a monotonically increasing function of the concurrence C (an entanglement monotone), $\mathrm{EoF} = -f(C)\log_2 f(C) - [1 - f(C)]\log_2[1 - f(C)]$, where $f(C) = (1 + \sqrt{1 - C^2})/2$. The concurrence is simply [15] $C = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$, where λ_1, λ_2, λ_3, and λ_4 are the square roots of the eigenvalues, in decreasing order, of the matrix $R = \rho\tilde{\rho}$. Here $\tilde{\rho}$ is the time-reversed matrix $\tilde{\rho} = (\sigma_y^1 \otimes \sigma_y^2)\rho^*(\sigma_y^1 \otimes \sigma_y^2)$. The symbol ρ^* means complex conjugation of the matrix ρ in the standard basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. For a density matrix in the X form given previously, $C = 2\max\{0, \Lambda_1, \Lambda_2\}/Z$, with $\Lambda_1 = |B_{12}| - \sqrt{A_{11}A_{22}}$ and $\Lambda_2 = |A_{12}| - B_{11}$.

Quantum discord. In classical information theory (CIT), the total correlation between two systems (two sets of random variables) $\mathcal{A}$ and $\mathcal{B}$ described by a joint distribution probability $p(\mathcal{A}, \mathcal{B})$ is given by the mutual information (MI),

$$\mathcal{I}(\mathcal{A}, \mathcal{B}) = H(\mathcal{A}) + H(\mathcal{B}) - H(\mathcal{A}, \mathcal{B}), \quad (3)$$

with the Shannon entropy $H(\cdot) = -\sum_j p_j \log_2 p_j$. Here p_j represents the probability of an event j associated to system $\mathcal{A}$ or $\mathcal{B}$ or the joint system $\mathcal{AB}$. Using Bayes's rule we may write MI as

$$\mathcal{I}(\mathcal{A}, \mathcal{B}) = H(\mathcal{A}) - H(\mathcal{A}|\mathcal{B}), \quad (4)$$

where $H(\mathcal{A}|\mathcal{B})$ is the classical conditional entropy. In CIT these two expressions are equivalent but in the quantum domain this is no longer true [4]. The first quantum extension of MI, denoted by $\mathcal{I}(\rho)$, is obtained directly replacing the Shannon entropy in (3) with the von Neumann entropy, $S(\rho) = -\mathrm{Tr}(\rho \log_2 \rho)$, with ρ, a density matrix, replacing probability distributions. To obtain a quantum version of (4), it is necessary to generalize the classical conditional entropy. This is done by recognizing $H(\mathcal{A}|\mathcal{B})$ as a measure of our ignorance about system $\mathcal{A}$ after we make a set of measurements on $\mathcal{B}$. When $\mathcal{B}$ is a quantum system, the choice of measurements determines the amount of information we can extract from it. We restrict ourselves to von Neumann measurements on $\mathcal{B}$ described by a complete set of orthogonal projectors, $\{\Pi_j\}$, corresponding to outcomes j. After a measurement, the quantum state ρ changes to $\rho_j = [(\mathbb{I} \otimes \Pi_j)\rho(\mathbb{I} \otimes \Pi_j)]/p_j$, with $\mathbb{I}$ the identity operator for system $\mathcal{A}$ and $p_j = \mathrm{Tr}[(\mathbb{I} \otimes \Pi_j)\rho(\mathbb{I} \otimes \Pi_j)]$. Thus, one defines the quantum analog of the conditional entropy as $S(\rho \mid \{\Pi_j\}) = \sum_j p_j S(\rho_j)$ and, consequently, the second quantum extension of the classical MI as [4] $\mathcal{J}(\rho \mid \{\Pi_j\}) = S(\rho^{\mathcal{A}}) - S(\rho \mid \{\Pi_j\})$. The value of $\mathcal{J}(\rho \mid \{\Pi_j\})$ depends on the choice of $\{\Pi_j\}$. Henderson and Vedral [16] have shown that the maximum of $\mathcal{J}(\rho \mid \{\Pi_j\})$ with respect to $\{\Pi_j\}$ can be interpreted as a measure of classical correlations. Therefore, the difference between the total correlations $\mathcal{I}(\rho)$ and the classical correlations $\mathcal{Q}(\rho) = \sup_{\{\Pi_j\}} \mathcal{J}(\rho \mid \{\Pi_j\})$ is defined as

$$D(\rho) = \mathcal{I}(\rho) - \mathcal{Q}(\rho), \quad (5)$$

giving, finally, a measure of quantum correlations [4] called QD. For pure states, QD reduces to entropy of entanglement [14], highlighting that in this case all correlations come from entanglement. However, it is possible to find separable (not entangled) mixed states with nonzero QD [4], meaning that entanglement does not cause all nonclassical correlations contained in a composite quantum system. Also, QD can be operationally seen as the difference between work that can be extracted from a heat bath using a bipartite system acting either globally and that extracted using a bipartite system acting only locally [17]. For more insights into QD, the reader is referred to [18]. In this work, when $B = 0$, the density operator (2) is such that QD is given by an analytical expression obtained in [19]. When $B \neq 0$, we computed QD numerically [20].

Results. Let us start presenting the important result that QD increases with temperature without an external field acting on the qubits ($B = 0$). This effect can be clearly seen when we deal with the XXZ model ($J_x = J_y = J$ and $J_z \neq 0$). Looking at Figs. 1(a) and 1(b), we see that this effect happens for several configurations of coupling constants being, thus, dense around this region. We should note that such behavior can be found for models other than the XXZ as well. As we mentioned before, in the absence of external fields [10], such increase with T occurs only for QD and not for EoF. Note also that QD starts at zero and then increases with T. In particular, for the set of coupling constants shown in

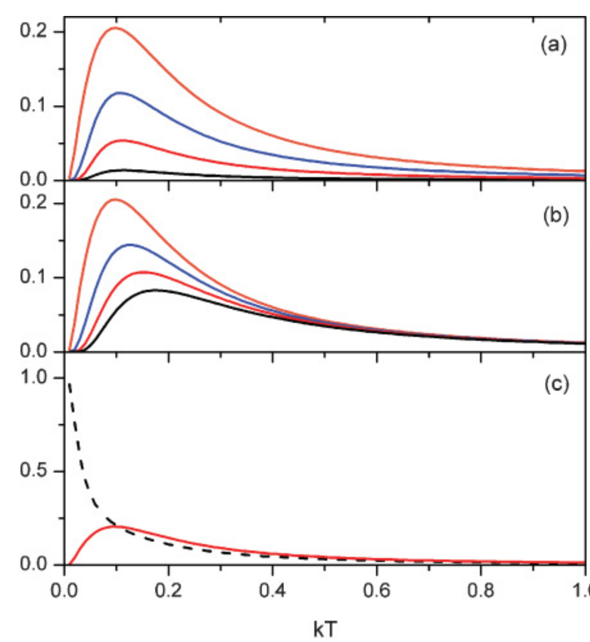

FIG. 1. (Color online) (a, b) QD as a function of the absolute temperature kT for the XXZ model with $B = 0$. (a) Here $J_z = -0.5$ and from bottom to top $J = 0.1, 0.2, 0.3, 0.4$. (b) We fix $J = 0.4$ and from bottom to top $J_z = -0.8, -0.7, -0.6, -0.5$. (c) QD [solid (red) line] and classical correlations, $\mathcal{Q}(\rho)$ [dashed (black) line], as functions of kT for $J = 0.4$ and $J_z = -0.5$. Here and in the following graphics the quantities plotted are dimensionless.

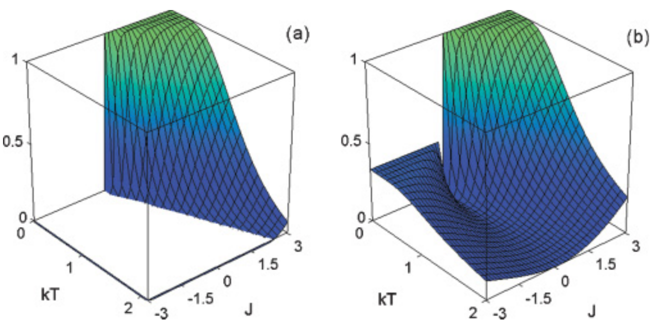

FIG. 2. (Color online) EoF (a) and QD (b) as a function of the absolute temperature kT and the coupling J. Both plots for the XXX model with $B = 0$.

Fig. 1, the EoF is always zero [10]. Furthermore, one can show that the classical correlation decreases when QD increases [see Fig. 1(c)]. We have, therefore, a genuine increase in quantum correlations with decreasing classical correlation. This nontrivial and unexpected effect indicates the robustness of quantum correlations against classical correlations as we increase the temperature.

We now move to the XXX model ($J_x = J_y = J_z = J$) with no field. Looking at Fig. 2 we see that although EoF is zero in the ferromagnetic region ($J < 0$), we have nonzero values for QD. Also, in both the ferromagnetic and the antiferromagnetic regions QD increases if we increase the absolute value of J. Actually, for any finite T we can find a J big enough such that QD $\neq 0$. This point is justified observing that for any finite value of T, the density operator (2) when $J \to \infty$ is given by the Bell state $\rho = |\psi\rangle\langle\psi|$ with $|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$. Besides, the density operator in the limit $J \to -\infty$ for a finite T is a mixed state $\rho = \frac{1}{3}(|00\rangle\langle 00| + |11\rangle\langle 11| + |\phi\rangle\langle\phi|)$ with $|\phi\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$. The value of QD in this case is 1/3 and, as expected, the EoF is zero. We should also mention that QD behaves qualitatively differently for $T \geqslant 0$ whether $J < 0$ or $J > 0$, achieving the value zero at the critical point $J = 0$. This suggests that QD can signal the quantum phase transition (QPT) taking place at $T = 0$ (when we tune J driving the system from its antiferromagnetic to its ferromagnetic phase), even at finite T. Note that EoF does not signal this QPT at finite T: EoF goes to zero *before* the critical point for $T > 0$ while QD $= 0$ exactly at the critical point, and only there. However, just as was done for $T = 0$ [21], a detailed study of the behavior of QD and QPT for $T > 0$ is needed.

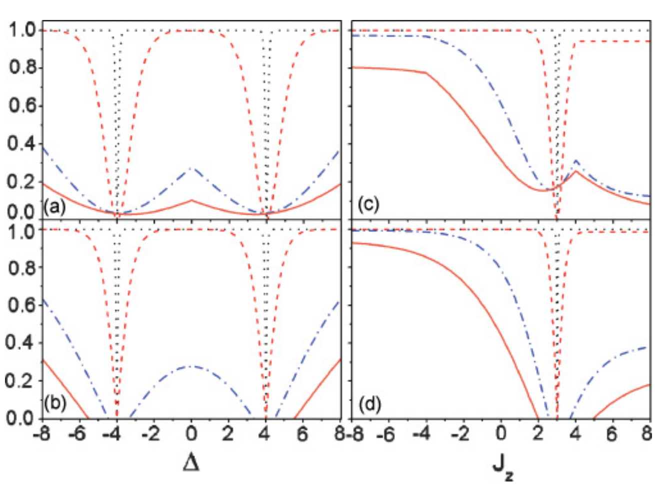

FIG. 3. (Color online) QD (a) and EoF (b) as a function of $\Delta = J_x - J_y$ for $J_x + J_y = 2$, $J_z = 1$, and various values of kT. QD (c) and EoF (d) as a function of J_z for $J_x + J_y = 1$, $\Delta = 7$, and various values of kT. For the dotted (black) line, $kT = 0.01$; dashed (red) line, $kT = 0.1$; dash-dotted (blue) line, $kT = 0.6$; and solid (orange) line $kT = 1$.

Focusing now on the XYZ model we investigate how QD behaves while we change the coupling constants for a fixed temperature T. In the left panels of Fig. 3 we plot how QD and EoF depend on the anisotropy of the J_x and J_y coupling constants for fixed J_z. We note that after a certain T the derivatives of QD with respect to $\Delta = J_x - J_y$ are undefined at $\Delta = 0$. This does not happen to EoF. The discontinuity of the derivative shown here is similar to what was observed to the dynamical decay rate of QD under decoherence in Ref. [12], where the authors coined the term "sudden change" for this behavior [22]. In the right panels of Fig. 3 we see the sudden change of QD keeping all parameters fixed but J_z. As before, we do not see sudden change for the EoF. The sudden change of QD with the coupling constants here and the one with time in [12] suggest that this behavior may be related to a technicality of QD rather than to a change in a physical property of the system. However, no proof of this point is given and further investigation is needed.

When the magnetic field B is not zero, we first analyze what happens to the Ising model ($J_x = J$ and $J_y = J_z = 0$). Looking at Fig. 4 we see that for the regions where EoF is zero QD is negligible. However, as well as with EoF [9], QD initially increases as we increase the value of B, going to zero with increasing field. This is true since the density operator (2) is $|11\rangle\langle 11|$ (separable state) when $B \to \infty$. On the other hand, as we will shortly see, this is not a general result. The behavior of QD and EoF can be quite different from each other if we work with another model.

For the XY model ($J_x, J_y \neq 0$, and $J_z = 0$) with a transverse magnetic field ($B \neq 0$), for example, QD behaves in ways quite different (and interesting) from what we have seen for the Ising model. Also, for the XY model we see a distinctive effect, the *regrowth* of QD. Contrary to the behavior of EoF, where we see its sudden death and then a revival [9], for QD there is

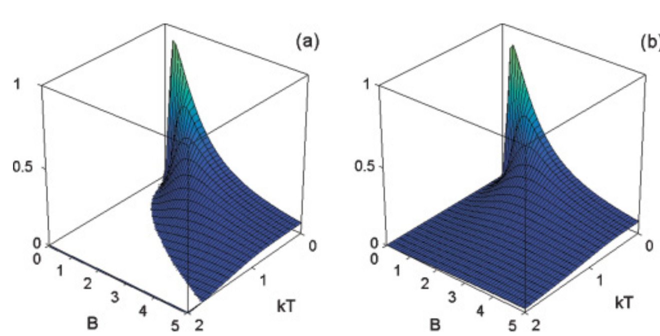

FIG. 4. (Color online) EoF (a) and QD (b) as a function of the magnetic field B and the absolute temperature kT for the Ising model when $J = 1$.

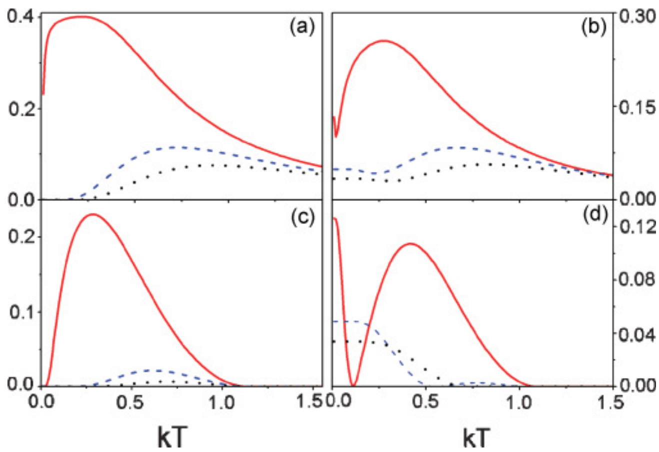

FIG. 5. (Color online) QD (a, b) and EoF (c and d) as functions of the absolute temperature kT for the XY model with transverse magnetic field B. (a, c) $J_x = J_y = 1$; (b, d) $J_x = 1.3$ and $J_y = 0.7$. The values for B are 1.1 [solid (red) line], 2.0 [dashed (blue) line], and 2.5 [dotted (black) line].

no sudden death (see Fig. 5). QD decreases with T, retaining appreciable values and then after a critical temperature T_c it starts increasing again. This is what we call regrowth. Note that in the behavior of EoF we never see a regrowth. Indeed, EoF increases after decreasing with T only after reaching the value zero (sudden death).

Moreover, looking at Figs. 5(a) and 5(c) we see that QD becomes non-null before the appearance of EoF. Also, QD continues to be non-null after EoF disappears. If we now analyze Figs. 5(b) and 5(d) we notice that we have for all three curves regimes in which QD increases while EoF decreases. This is a quite remarkable behavior since the decrease of a certain quantum aspect (entanglement) is simultaneous to the increase of another quantum aspect (quantum correlations), illustrating clearly the distinctive aspects of these two concepts.

Conclusions. We examined the behavior of the QD for a pair of qubits described by the Heisenberg model in thermal equilibrium with a reservoir at temperature T. By changing the temperature and also by applying an external magnetic field, we observed several remarkable effects for QD, many of them in sharp contrast to the behavior observed for the EoF between the two qubits. We found that for the XXX model QD signals a QPT for finite T while EoF does not. Also, we observed regimes where QD increases while EoF decreases with T. Moreover, and surprisingly, we showed that for the XXZ model there exist regions in the parameter space in which EoF is zero while the classical correlation decreases and only QD increases with T. Finally, we also observed a distinctive effect for QD which we called *regrowth*: QD decreases with T and starts increasing again after reaching a minimum different from zero.

T.W. thanks CNPq for partially funding this research.

[1] J. S. Bell, Physics **1**, 195 (1964).
[2] A. Einstein, B. Podolsky, and N. Rosen, Phys. Rev. **47**, 777 (1935).
[3] R. F. Werner, Phys. Rev. A **40**, 4277 (1989).
[4] H. Ollivier and W. H. Zurek, Phys. Rev. Lett. **88**, 017901 (2001); B. P. Lanyon, M. Barbieri, M. P. Almeida, and A. G. White, *ibid.* **101**, 200501 (2008).
[5] A. Datta, A. Shaji, and C. M. Caves, Phys. Rev. Lett. **100**, 050502 (2008).
[6] P. R. Hammar *et al.*, Phys. Rev. B **59**, 1008 (1999).
[7] J. A. Hoyos and G. Rigolin, Phys. Rev. A **74**, 062324 (2006); L. F. Santos and G. Rigolin, *ibid.* **71**, 032321 (2005); T. R. de Oliveira, G. Rigolin, M. C. deOliveira, and E. Miranda, *ibid.* **77**, 032325 (2008).
[8] M. C. Arnesen, S. Bose, and V. Vedral, Phys. Rev. Lett. **87**, 017901 (2001).
[9] G. L. Kamta and A. F. Starace, Phys. Rev. Lett. **88**, 107901 (2002).
[10] G. Rigolin, Int. J. Quantum. Inform. **2**, 393 (2004).
[11] A. Ferraro *et al.*, e-print arXiv:0908.3157.
[12] J. Maziero, L. C. Celeri, R. M. Serra, and V. Vedral, Phys. Rev. A **80**, 044102 (2009).
[13] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, and W. K. Wootters, Phys. Rev. A **54**, 3824 (1996).
[14] C. H. Bennett, H. J. Bernstein, S. Popescu, and B. Schumacher, Phys. Rev. A **53**, 2046 (1996).
[15] W. K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).
[16] L. Henderson and V. Vedral, J. Phys. A **34**, 6899 (2001).
[17] W. H. Zurek, Phys. Rev. A **67**, 012320 (2003); R. Dillenschneider, Europhys. Lett. **88**, 50003 (2009).
[18] M. Horodecki *et al.*, Phys. Rev. A **71**, 062307 (2005); K. Modi, T. Paterek, W. Son, V. Vedral, and M. Williamson, Phys. Rev. Lett. **104**, 080501 (2010).
[19] S. Luo, Phys. Rev. A **77**, 042303 (2008).
[20] T. Werlang, S. Souza, F. F. Fanchini, and C. J. VillasBoas, Phys. Rev. A **80**, 024103 (2009).
[21] R. Dillenschneider, Phys. Rev. B **78**, 224413 (2008); M. S. Sarandy, Phys. Rev. A **80**, 022108 (2009).
[22] The sudden change of QD under decoherence was experimentally seen in J.-S. Xu *et al.*, e-print arXiv:0911.2848.