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Environment-Induced Sudden Transition in Quantum Discord Dynamics

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Nonclassical correlations play a crucial role in the development of quantum information science. The recent discovery that nonclassical correlations can be present even in separable (nonentangled) states has broadened this scenario. This generalized quantum correlation has been increasing in relevance in several fields, among them quantum communication, quantum computation, quantum phase transitions, and biological systems. We demonstrate here the occurrence of the *sudden-change* phenomenon and immunity against some sources of noise for the quantum discord and its classical counterpart, in a room temperature nuclear magnetic resonance setup. The experiment is performed in a decohering environment causing loss of phase relations among the energy eigenstates and exchange of energy between system and environment, resulting in relaxation to the Gibbs ensemble.

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The quantum mechanical superposition principle, when applied to composite systems, foresees the appearance of correlations that cannot be explained in a classical context [1]. Initially, the quantum character of a correlated system was attributed to the nonlocal aspect of quantum mechanics and further associated with the violation of Bell's inequalities. The discovery of nonseparable (entangled) states that do not violate Bell's theorem led eventually to the identification of the quantumness of correlations with the separability problem; nonclassicality was attributed to entanglement. Through the development of quantum information science (QIS), an operational characterization of entanglement was introduced, as those correlations that cannot be generated by local operations and classical communication [2]. The development of these ideas led to the so-called theory of entanglement, which turned out to be a fruitful branch of research [3]. Entanglement is recognized as an important resource for several tasks in QIS [4]. Besides this strong correlation exhibited by entangled states, there is another kind of nonclassical correlation. A composite quantum system in a mixed state may exhibit some nonclassical nature in its correlations even if it is separable (nonentangled) [5]. Such quantum correlation can be measured as a "gap" between the quantum and classical versions of mutual information, which is the information-theoretic measure of the total correlation contained in a bipartite system [6].

Several approaches have been proposed to quantify this generalized quantum correlation present in a bipartite mixed quantum state [5,7–9], one of which, quantum discord [5], has received special attention [10–16]. Beyond the importance of nonclassical correlations (other than entanglement) for the foundations of quantum mechanics, the relevance of such an issue is increasing in several fields as well as in QIS applications. Concerning biological systems, it has been suggested that such correlations could play an important role in photosynthesis [10]. In condensed matter physics, quantum correlations of separable states characterize, even at finite temperature, a quantum phase transition [16]. In the context of quantum field theory, it has been shown that the Unruh effect may also lead to an abrupt change in the behavior of correlations [17]. For applications in QIS, it is interesting to know that states with nonzero quantum discord cannot be locally broadcast [18], and this kind of nonclassicality is also related to a condition for a complete positive map [12]. Quantum discord was proposed as a figure of merit for the quantum advantage in some computational models without or with little entanglement [13,14]. It also has a relevant role in mixed-state quantum metrology [19].

In particular, quantum discord has been predicted to show peculiar dynamics under decoherence [20]. Considering two noninteracting qubits (quantum bits) under the action of Pauli maps, it was shown that, under certain conditions, the decay rate of the correlations suffers an abrupt modification, a phenomenon denominated *sudden change* [20]. Moreover, either the classical or the quantum part of correlation may be unaffected by decoherence [20,21], giving rise to two distinct decoherence regimes, the classical and the quantum. In the present experiment we demonstrate that the aforementioned phenomena [20,21] are still present in a *real* thermal environment at room temperature, indicating that such peculiar behavior is quite general. We performed such experimental demonstration in a nuclear magnetic resonance (NMR) setup.

NMR systems have been extensively used as test benches for QIS ideas [22]. Most of these experiments were performed in scenarios where the existence of entanglement was ruled out. The quantum nature of NMR systems at room temperature may be ascribed to quantum correlations of separable states [23]. The main feature of the technique for QIS is the excellent control of unitary transformations over the qubit provided by the use of radio-frequency pulses, which result in unique methods for quantum state generation and manipulation [22]. In general, for room temperature liquid state NMR, the Markovian environment in which the qubit is immersed can be described by two decoherence channels, the amplitude-damping and the phase-damping, acting locally on each qubit. Our experiment is performed on a liquid state carbon-13 enriched chloroform sample at room temperature, this sample exhibits two qubits, encoded in the ^{1}H and ^{13}C spin-1/2 nuclei. The two-qubit state is represented by a density matrix in the high temperature expansion, which takes the form $\rho_{AB} = \mathbb{1}_{AB}/4 + \varepsilon\Delta\rho_{AB}$, where $\varepsilon = \hbar\omega_L/4k_BT \sim 10^{-5}$ is the ratio between the magnetic and thermal energies and $\Delta\rho_{AB}$ is the deviation matrix [22,24].

The nonclassical aspect of correlation may be revealed by the so-called quantum discord. This quantity arises from a departure between the classical and the quantum versions of information theory [9]. The quantum mutual information can be written as $\mathcal{I}(\rho_{A:B}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$, or alternatively, as $\mathcal{J}(\rho_{A:B}) = S(\rho_A) - S_{\{\Pi_j^B\}}(\rho_{A|B})$, where $S(\rho) = -\mathrm{tr}(\rho\log_2\rho)$ is the von Neumann entropy, $\rho_{A(B)} = \mathrm{tr}_{B(A)}(\rho_{AB})$ is the reduced-density operator of partition $A(B)$, $S_{\{\Pi_j^B\}}(\rho_{A|B}) = \sum_j q_j S(\rho_{A|\Pi_j^B})$ is a quantum extension of the classical conditional entropy, and $\rho_{A|\Pi_j^B}$ is the reduced state of partition A after the measurement Π_j^B performed on partition B, with outcome j [5,9]. Both expressions for mutual information, $\mathcal{I}$ and $\mathcal{J}$, are classically equivalent while in quantum mechanics they are not equivalent, in general. This nonequivalence relies on the distinct nature of the quantum measurement. The quantum discord was defined as a measure of such a nonequivalence, i.e., $\mathcal{D}(\rho_{AB}) \equiv \mathcal{I}(\rho_{A:B}) - \max_{\{\Pi_j^B\}}\mathcal{J}(\rho_{A:B})$ [5,9]. In the NMR context a suitable measure of nonclassicality is obtained from the symmetric version of quantum discord expanded to the leading order in ε [23,25], this quantifier may be written as [23]

$$\mathcal{D}^s(\rho_{AB}) = \mathcal{I}(\rho_{AB}) - \max_{\{\Pi_i^A,\Pi_j^B\}}\mathcal{K}(\chi_{AB}), \tag{1}$$

where the quantum mutual information is now given by

$$\mathcal{I}(\rho_{AB}) \approx \frac{\varepsilon^2}{\ln 2}\{2\mathrm{tr}(\Delta\rho_{AB}^2) - \mathrm{tr}[(\Delta\rho_A)^2] - \mathrm{tr}[(\Delta\rho_B)^2]\},$$

and the measurement-induced mutual information is $\mathcal{K}(\chi_{AB}) \approx \frac{\varepsilon^2}{\ln 2}\{2\mathrm{tr}[(\Delta\chi_{AB})^2] - \mathrm{tr}[(\Delta\chi_A)^2] - \mathrm{tr}[(\Delta\chi_B)^2]\}$, with $\chi_{AB} = \mathbb{1}_{AB}/4 + \varepsilon\Delta\chi_{AB}$ as the state obtained from ρ_{AB} through a complete projective measurement map ($\Delta\chi_{AB} = \sum_{i,j}\Pi_i^A \otimes \Pi_j^B(\Delta\rho_{AB})\Pi_i^A \otimes \Pi_j^B$). $\Delta\rho_{A(B)} = \mathrm{tr}_{B(A)}\{\Delta\rho_{AB}\}$ is the reduced deviation matrix while $\Delta\chi_{A(B)}$ stands for the reduced measured deviation matrix in the subspace $A(B)$. The classical counterpart of Eq. (1) is $C(\rho_{AB}) = \max_{\{\Pi_i^A,\Pi_j^B\}}\mathcal{I}(\chi_{AB})$, since the mutual information of the post-measurement system captures only classical correlations [9]. It is worth mentioning that $\mathcal{D}^s(\rho_{AB}) = 0$ if and only if ρ_{AB} can be cast in terms of the local orthogonal basis ($\{|\alpha_i\rangle\}$ and $\{|\beta_j\rangle\}$ for the subsystems state spaces $\mathcal{H}^a$ and $\mathcal{H}^b$), such as $\sum_{i=1}^{\dim\mathcal{H}_a}\sum_{j=1}^{\dim\mathcal{H}_b} p_{i,j}|\alpha_i\rangle\langle\alpha_i| \otimes |\beta_j\rangle\langle\beta_j|$, where $\{p_{i,j}\}$ is a probability distribution [25]. In other words, the symmetric quantum discord is zero if and only if ρ_{AB} has only classical correlations or no correlations at all. The aforementioned symmetric correlation quantifiers can be computed directly from the experimentally reconstructed deviation matrix.

Let us consider the class of states with maximally mixed marginals ($\rho_{A(B)} = \mathbb{1}_{A(B)}/2$), also known as Bell-diagonal states:

$$\rho_{AB} = \frac{1}{4}\Big(\mathbb{1}_{AB} + \sum_{i=x,y,z} c_i\sigma_i^A \otimes \sigma_i^B\Big), \tag{2}$$

where $\sigma_i^{A(B)}$ is the ith component of the standard Pauli operator acting on the A (B) subspace, $c_i = \mathrm{tr}[\rho_{AB}\sigma_i^A \otimes \sigma_i^B]$, and $\mathbb{1}_{AB}$ is the identity operator. It was theoretically predicted [20] that, depending on the geometry (encoded in the relations between the parameters c_i) of the state (2), the evolution of the state correlations under the action of Pauli channels presents a peculiar behavior [20]. Considering the phase-damping channel, if the state components are related as follows: $|c_x| \geq |c_y|$, $|c_z|$ or $|c_y| \geq |c_x|$, $|c_z|$, and $|c_z| \neq 0$, the correlations exhibit the so-called *sudden change* in behavior [20]. The classical correlation decays exponentially until a specific moment in time, thereafter remaining constant, while the quantum correlation suddenly changes its decay rate at that moment. On the other hand, if $|c_z| \geq |c_x|$, $|c_y|$, it was shown that the classical correlation is not affected by decoherence, while the quantum correlation decays exponentially. For the other two Pauli channels, we can see the same behavior, except that the relations between the three components of state (2) are exchanged [20].

In order to demonstrate such nontrivial dynamics we prepare two initial Bell-diagonal states with specific relations between its components. This involves the experimental mapping of the second term of the right-hand side of Eq. (2) onto $\Delta\rho_{AB}$. Starting from the thermal equilibrium state, the mapping consists of three main steps, in which the following are applied to the sample: (i) a strongly modulated pulse, (ii) a magnetic field gradient, and (iii) a pseudo Einstein-Podolsky-Rosen gate implemented by radio-frequency pulses [22,24]. After the preparation of the state, it is left to evolve freely under decoherence and the dynamics of the system is followed by quantum state tomography [26]. The symmetric quantum discord, $\mathcal{D}^s$, and its classical counterpart, $\mathcal{C}$, are computed through the above definitions from the experimentally measured deviation matrix following the methods introduced in [23]. Figure 1 illustrates the pulse sequence in the experimental procedure [27].

The relaxation process that causes phase decoherence and energy dissipation is due, mainly, to internal molecular or atomic motions that cause random fluctuations in the electromagnetic field in which the qubits are immersed. These fluctuations are characterized by the spectral densities that encode features of the motion, such as geometry and correlation times. The environment can be modeled by two independent quantum channels, described as the generalized amplitude-damping and the phase-damping channels. In previous investigations of sudden-change dynamics [20,21,28], the energy exchange channel was not take into account; however, in the present experiment this relaxation source is unavoidable. It is remarkable that the sudden-change dynamics still happens even in the presence of a thermal environment, as can be seen in Fig. 2. The small decay rate of the classical correlation, in Figs. 2 and 3 (where it should be constant under a phase damping), is due to the presence of the thermal noise source. This thermal noise source can be described by a generalized amplitude-damping channel [27]. The theoretical predictions presented in Fig. 2 are in good agreement with the experimental data [27]. We observe a sudden transition between two decoherence regimes [20], i.e., classical and quantum decoherence [21]. During the first regime ($t \lesssim 0.027$ s) the decoherence affects more strongly the classical aspects of correlation, leaving the quantum aspects with a small decay. After the sudden-change point ($t \gtrsim 0.027$ s) the classical correlation becomes more robust against decoherence and the noise degrades more effectively the quantumness of correlations. We note that the sudden change of correlations is solely due to the action of the phase-damping channel. Our results confirm that the phenomena predicted in [20,21] for phase environments take place even in the presence of an additional thermal noise.

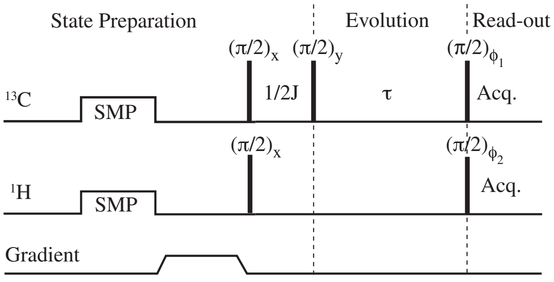

FIG. 1. Sketch of the pulse sequence used experimentally to follow the dynamics of quantum and classical correlations under decoherence. The sequence consists of three blocks: the initial state preparation, relaxation delay, and readout by quantum state tomography.

Figure 3 also confirms the theoretical prediction [20] that, in some states (depending on their geometry), the classical correlation may be robust against phase noise. The small decay rate of this correlation plotted in Fig. 3 comes entirely from the thermal source. Once more, the theoretical curves present very good agreement with the experimental data.

In both of the Figs. 2(c) and 3(c), the theoretical data analysis guarantees that the small decay rate presented by the classical correlation, where it should vanish, comes exclusively from the action of the thermal channel on the system. It is worth mentioning that the oscillations shown

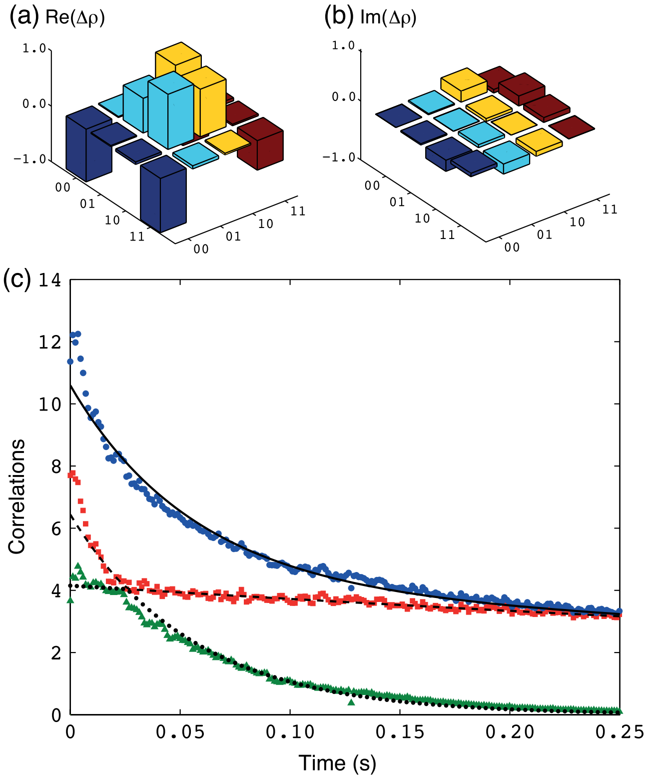

FIG. 2 (color online). Sudden change in behavior of correlations. (a) Bar representation of the real and, (b) imaginary parts of the initial deviation matrix for the sudden-change experiment, reconstructed by quantum state tomography. We adopted the usual computational basis, where $|0\rangle$ and $|1\rangle$ represent the eigenstates of σ_z for each qubit. (c) displays the predicted sudden change in behavior of the correlations during their dynamic evolution to thermal equilibrium. The blue circles are the experimental data for the quantum mutual information, while the red squares and green triangles represent the classical and quantum correlations, respectively. The black lines are the theoretical predictions. The initial state is analogous to the state in Eq. (2) with $|c_x|, |c_y| > |c_z|$. The correlations are displayed in units of $(\varepsilon^2/\ln 2)$bit.

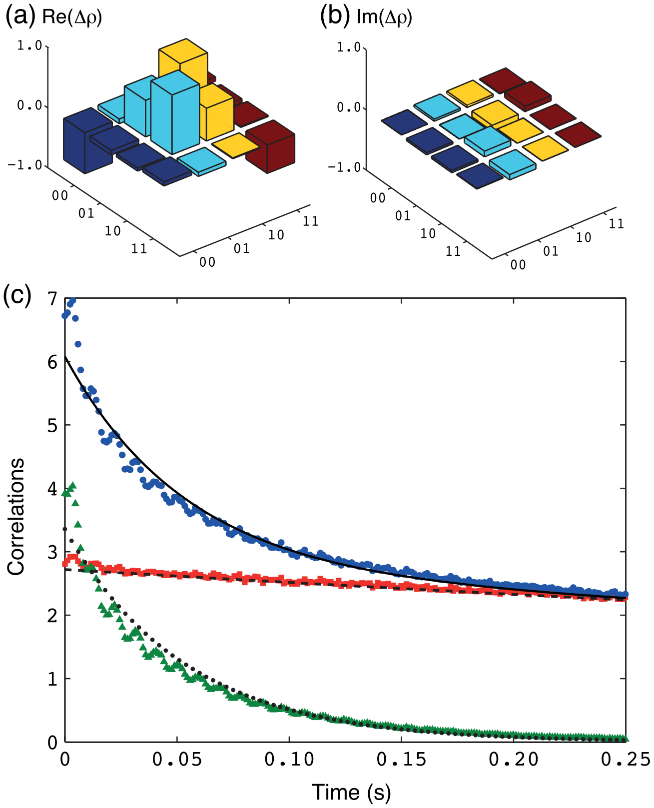

FIG. 3 (color online). Immunity against decoherence. (a) Bar representation of the real and, (b) imaginary parts of the initial deviation matrix, reconstructed by quantum state tomography. (c) shows that the classical correlation is not affected by the action of the phase-damping channel. The small decay rate is entirely due to the amplitude-damping channel. The displayed pattern is the same as in Fig. 2. For this experiment, the initial state is analogous to the state in Eq. (2) with $|c_z| > |c_x|, |c_y|$. The correlations are computed in units of $(\varepsilon^2/\ln 2)$bit.

by the experimental curves in both figures are due to experimental details (discussed in [27]).

Correlations are ubiquitous in nature. The discovery that separable quantum states can exhibit a nonclassical correlation other than entanglement has led to a new understanding of the quantum aspects of a physical system. Despite the relatively great number of theoretical articles concerning decoherence effects, up to date, only few experimental investigations of the correlation dynamics have been reported previously in literature [23,28–30]. The predictions of Refs. [20,21] were tested in a *simulated* phase noise environment [28]. This experiment was performed in an optical setup, in which the action of a phase-damping channel was *simulated* in a *controllable* way by a birefringent medium and the qubits were encoded in photon polarizations [28]. Under the action of a real global environment, the dynamics of correlations was investigated in a NMR quadrupolar system [23].

In the present experiment we observed the environment-induced sudden-change phenomenon in a *real* (uncontrollable) thermal noise environment at room temperature. The environment-induced sudden change takes place in the course of the relaxation of two nuclear spins to the Gibbs state. This demonstrates that this phenomenon may occur in a general context when a nonequilibrium system relax to a thermal equilibrium state. The methods employed in our experiment to follow the dynamics of quantum discord and its classical counterpart may be applied to other molecules (including biological ones) and also to other experimental contexts where high mixed states are present. The two decoherence regimes observed may have important consequences for applications in QIS, since the nature of correlations in a given mixed-state system is somehow related to the quantum advantage for performing a given task (as, for example, in quantum metrology [19]) or preventing local broadcasting of information [18].

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