Emergence of a metastable pointer-state basis in non-Markovian quantum dynamics

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We investigate the dynamics of classical and quantum correlations between two qubits. Each qubit is implemented by a pair of phosphorous impurities embedded in a silicon substrate. The main decoherence mechanism affecting these types of qubits is provided by the coupling of the phosphorous impurities to the acoustical vibrations of the silicon lattice. We find that depending on the temperature of the substrate and the initial state, three different dynamics can be found. These are characterized by the number of abrupt changes in both classical and quantum correlations. We also show that the correlations do not disappear. Moreover, before the classical correlations reach a constant value, they may experience successive abrupt changes associated with the apparition of a metastable pointer-states basis. Then a constant value for the classical correlations is reached when the preferred basis is established.

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Recently the study of classical and quantum correlations has become a central subject of investigation. The study of quantum correlations between quantum systems is a problem as old as quantum theory. For many years it was widely believed that quantum entanglement would be the only relevant type of correlation for quantum information protocols. However, it has been proved that efficient quantum protocols can be performed in the absence of entanglement [1]. A bipartite quantum system A-B can feature both quantum and classical correlations between its constituent parts A and B, respectively. All these correlations can be characterized by the quantum mutual information [2,3]

$$I(\hat{\rho}_{AB}) = S(\hat{\rho}_A) + S(\hat{\rho}_B) - S(\hat{\rho}_{AB}), \qquad (1)$$

where $S(\hat{\rho}) = -\mathrm{Tr}[\hat{\rho}\log_2(\hat{\rho})]$ is the von Neumann entropy [4]. Based on this expression it is commonly believed that the correlations can be separated according to their classical and quantum nature, respectively [2]. In this way the quantum discord can be introduced as [2,3] and [5–8],

$$D(\hat{\rho}_{AB}) = I(\hat{\rho}_{AB}) - C(\hat{\rho}_{AB}), \qquad (2)$$

where $C(\hat{\rho}_{AB})$ are the classical correlations [2,6] defined by the following maximization procedure: A complete set of projector operators $\{\hat{\Pi}_k\}$ must be constructed for the subsystem B. Then the quantity

$$C(\hat{\rho}_{AB}) = \max_{\{\hat{\Pi}_k\}}[S(\hat{\rho}_A) - S(\hat{\rho}_{AB} \mid \{\hat{\Pi}_k\})] \qquad (3)$$

must be maximized with respect to variation of the set of $\{\hat{\Pi}_k\}$ where $S(\hat{\rho}_{AB} \mid \{\hat{\Pi}_k\}) = \sum_k p_k S(\hat{\rho}_k)$, $p_k = \mathrm{Tr}(\hat{\rho}_{AB}\hat{\Pi}_k)$, and $\hat{\rho}_k = \mathrm{Tr}_B(\hat{\Pi}_k \hat{\rho}_{AB} \hat{\Pi}_k)/p_k$.

The competition between classical and quantum correlations parts of a quantum system has attracted increasing attention in recent years. It is widely believed that for decoherence, caused by contact with an external reservoir, both types of correlations of a system are continuously depleted and transferred to the reservoir degrees of freedom. This depletion happens on a characteristic time scale that defines the decoherence time of the system, which is the effective feature of the system's coupling to the reservoir. An alternative way to characterize the decoherence can be obtained from the dynamical raise of the system's entropy.

However, it has been pointed out that the former case is not the general one, as dynamical transitions from quantum to classical correlations may also be discontinuous [9,10]. This has been demonstrated for a system experiencing decoherence by a dephasing channel. Furthermore, it has been shown experimentally [11–13] that classical correlations may change abruptly to a nonvanishing stationary value. This feature has been proposed to determine whether a quantum system has reached its classical regime or not [12]. The appearance of a stationary classical correlation is associated by the emergence of a basis of pointer states in one of the two subsystems [12], denoted also as "preferred basis for the apparatus," where the apparatus may be understood as one of the two subsystems [14].

In this paper we show analytically that not only the quantum-to-classical transition may be discontinuous, but that these abrupt changes may also occur various times during the dynamical evolution of the system. Therefore, there may exist intermediate stages with constant classical correlation. Each stage defines a distinct and metastable basis of pointer states. Only after passing through these stages—after a sufficiently long time—the final basis of pointer states is asymptotically established.

Our system is composed of two charge quantum bits (qubits), implemented by electrons localized at donor impurities, i.e., P, that are embedded in a semiconductor host, i.e., Si [15]. Each qubit consists of a pair of impurities sharing a single electron. The quantum information is encoded as the position of the electron within the pair of impurities. At or below room temperature the dominant source of decoherence of this implementation of qubits is off-resonant scattering of acoustical phonons in the substrate. This decoherence mechanism has been shown, both numerically [16] and in analytically closed form [17,18], to provide a non-Markovian
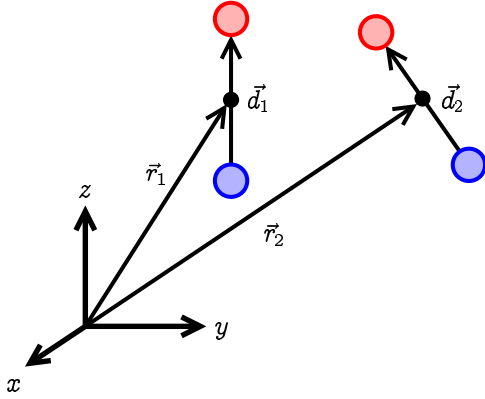
FIG. 1. (Color online) Schematic outline of the two donor-based charge qubits ($b = 1,2$) formed by four donor sites in a semiconductor material. Blue and red donor sites correspond to qubit states $m_b = -\frac{1}{2}$ and $m_b = +\frac{1}{2}$, respectively. Each qubit b is located at position $\mathbf{r}_b$ and has an intersite distance vector $\mathbf{d}_b$ pointing from site $m_b = -\frac{1}{2}$ to site $m_b = +\frac{1}{2}$.

dephasing of the qubits. It also induces a disentanglement of pairs of qubits with subsequent partial recovering of the initial entanglement [19].

At sufficiently large distances between the qubits, Coulomb repulsion and cross tunneling of electrons can be neglected. Then the dynamics is generated by off-resonant scattering of acoustical phonons at the donor-based charge qubits, which is described by the spin-boson Hamiltonian,

$$
H = \hbar \sum_b (\omega_b \hat{S}_{b,z} + \Delta_b \hat{S}_{b,x}) + \sum_{\mathbf{k}} \hbar \nu_k \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}
$$
$$
+ \hbar \sum_b \sum_{\mathbf{k}} \hat{S}_{b,z}(g_{b,\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger + g_{b,\mathbf{k}}^* \hat{a}_{\mathbf{k}}). \qquad (4)
$$

Here the spin-$\frac{1}{2}$ operators $\hat{S}_b$ act on the states $|m_b\rangle$ of the bth qubit, where $m_b = \pm \frac{1}{2}$ denotes the localization of the qubit's electron at one of the two impurity sites. Furthermore, $\hat{a}_{\mathbf{k}}$ are the bosonic annihilation operators of longitudinal acoustical phonons of wave vector $\mathbf{k}$ and linear dispersion relation $\nu_k = sk$ with s being the speed of sound in the substrate. The qubits have transition frequencies ω_b and tunneling rates Δ_b, and are interacting with the phonons via the coupling rate

$$
g_{b,\mathbf{k}} = \frac{D}{\hbar s} \sqrt{\frac{2\hbar \nu_k}{M_o}} \sum_{m_b = \pm \frac{1}{2}} \frac{m_b e^{-i\mathbf{k} \cdot (\mathbf{r}_b + m_b \mathbf{d}_b)}}{\left[1 + \left(\frac{k a_{\mathrm{B}}}{2}\right)^2\right]^2},
$$

where D is the deformation constant of the substrate, M_0 is the unit cell mass, and a_{B} is the corresponding Bohr radius in the substrate.

The geometrical configuration of the N-qubit setup is characterized by a vector $\hat{r}_b$ with $b = 1,2,3,\dots$ which labels the position of the center of each qubit, $\hat{d}_b$ is the interdonor distance, for the sake of simplicity, this parameter as well as Bohr radius are taken to be the same for each qubit, see Fig. 1. Here also, we assume the distance between two adjacent qubit is larger than the interdonor distance, this provides a condition for preventing interqubit tunneling.

Applying electric potentials via suitably positioned electrodes, the qubit's transition frequencies can be raised to surpass the tunneling rates $\omega_b \gg \Delta_b$, and tunneling can be neglected so that fully analytic solutions of the spin-boson dynamics can be found. Assuming then that the thermal excitation of substrate phonons is sufficiently low to not excite the qubit transitions $k_{\mathrm{B}} T \ll \hbar \omega_b$, each qubit can be individually manipulated to prepare a general initial state of the qubits factorized with respect to the phonon state,

$$
\hat{\rho}_{\mathrm{ph+qubits}}(0) = \sum_{\{m_b\},\{s_b\}} \rho_{\{m_b\},\{s_b\}}(0) |\{m_b\}\rangle\langle\{s_b\}| \otimes \hat{\rho}_{\mathrm{ph,th}}, \quad (5)
$$

where $|\{m_b\}\rangle = |m_1\rangle \otimes |m_2\rangle$ are the bipartite qubit states and $\hat{\rho}_{\mathrm{ph,th}}$ is the thermal state of the phonons. The reduced density matrix of the qubits can then be shown to evolve in time as [17–19]

$$
\rho_{\{m_b\},\{s_b\}}(t) = \rho_{\{m_b\},\{s_b\}}(0) f_{\{m_b\},\{s_b\}}(t), \qquad (6)
$$

where the time dependence is given by the functions [19]

$$
f_{\{m_b\},\{s_b\}}(t) = \exp\left[-\int_0^t dt' \Gamma_{\{m_b\},\{s_b\}}(t')\right]. \qquad (7)
$$

Here the decoherence rate of the bipartite qubit state results as

$$
\Gamma_{\{m_b\},\{s_b\}}(t) = \sum_{b,b'} (m_b - s_b)(m_{b'} - s_{b'}) \gamma_{b,b'}(t), \qquad (8)
$$

where the interqubit decorrelation rate is given by

$$
\gamma_{b,b'}(t) = 4 \sum_{m_b} \sum_{s_{b'}} m_b s_{b'} \gamma[t; |(\mathbf{r}_b + m_b \mathbf{d}_b) - (\mathbf{r}_{b'} + s_{b'} \mathbf{d}_{b'})|].
$$
$$
(9)
$$

The interdonor decoherence rate is defined as

$$
\gamma(t;l) = \frac{2\pi s}{l} \frac{T}{T_{\mathrm{s}}} \sum_{\sigma = \pm 1} \sigma \left(\frac{x^3}{6} + \frac{x^2}{2} + \frac{5x}{8} + \frac{5}{16}\right) e^{-2x},
$$

with $x = |l - \sigma st|/a$. This decoherence rate is proportional to the substrate temperature T, where the temperature scale is defined in terms of parameters of the substrate as $T_{\mathrm{s}} = a\rho_{\mathrm{s}} s^4 h^2 / (k_{\mathrm{B}} D^2)$, with ρ_{s} being the substrate mass density.

As the initial qubit state we consider a statistical mixture of two Bell states ($p \in [0,1]$),

$$
\hat{\rho}_{\mathrm{qubits}}(0) = p |\Psi_+\rangle\langle\Psi_+| + (1-p) |\Phi_+\rangle\langle\Phi_+|. \qquad (10)
$$

Thus, the initial state can be expressed in the basis $\{|\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle, |-\frac{1}{2}, \frac{1}{2}\rangle, |-\frac{1}{2}, -\frac{1}{2}\rangle\}$ as an X state and remains in this form throughout the nondissipative time evolution, as

$$
\rho_{\mathrm{qubits}}(t) = \frac{1}{2} \begin{bmatrix} p & 0 & 0 & b(t) \\ 0 & 1-p & c(t) & 0 \\ 0 & c(t) & 1-p & 0 \\ b(t) & 0 & 0 & p \end{bmatrix},
$$

where we defined $b(t) = p f_{\frac{1}{2},\frac{1}{2};-\frac{1}{2},-\frac{1}{2}}(t)$ and $c(t) = (1 - p) f_{\frac{1}{2},-\frac{1}{2};-\frac{1}{2},\frac{1}{2}}(t)$. This density matrix reaches a stationary state for $t \gg d/s$, where d is the characteristic distance between donor sites, and $b(t)$ and $c(t)$ attain constant values that depend on the geometric configuration of the qubit pair. In general analytical solutions for the correlations of a two-qubit state are yet unknown. However, for the X state present here, analytical
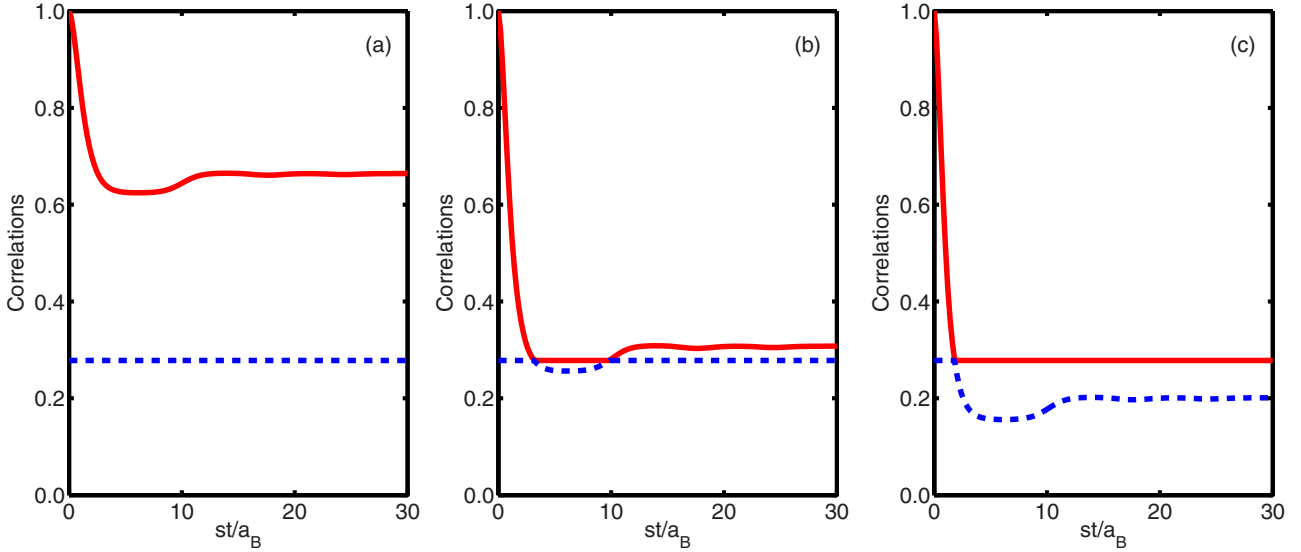
FIG. 2. (Color online) Evolution of the classical correlation (red solid line), the quantum discord (blue dotted line) for an initial state characterized by $p = 0.8$ and different temperatures, (a) $T/T_B = 0.01$, (b) $T/T_B = 0.035$, and (c) $T/T_B = 0.05$. Geometrical parameters are $|\boldsymbol{d}_1| = |\boldsymbol{d}_2| = 10a_B$, $|\boldsymbol{r}_1 - \boldsymbol{r}_2| = 20a_B$, $\angle(\boldsymbol{d}_1, \boldsymbol{d}_2) = 45°$.

solutions for the correlations can be found following the lines of Ref. [20]. The result for the classical correlations is

$$C(t) = 1 - K(w(t)), \qquad (11)$$

where

$$w(t) = \max[|a|, b + c], \qquad (12)$$

with $a = 2p - 1$ and the function K reads

$$K(x) = -\frac{1+x}{2} \log_2\left(\frac{1+x}{2}\right) - \frac{1-x}{2} \log_2\left(\frac{1-x}{2}\right).$$

Furthermore, the quantum discord is obtained as

$$\begin{aligned} D(t) = {} & 1 + p \log_2(p) + (1-p) \log_2(1-p) + K(w(t)) \\ & - pK\left(\frac{b(t)}{p}\right) - (1-p)K\left(\frac{c(t)}{1-p}\right). \end{aligned} \qquad (13)$$

The classical correlation (11) and the quantum discord (13) of the state (10) are shown in Fig. 2 as functions of time. It can be seen that three cases exist depending on the temperature. For very low temperature the classical correlation is well above the quantum discord, the latter being constant, see Fig. 2(a). Increasing slightly temperature, the minimum of the classical correlation merges with quantum discord, so that the latter now shows a minimum, as seen in Fig. 2(b). Further increasing the temperature leads to a third case where the classical correlation becomes constant after an initial decay, see Fig. 2(c). The latter case has been observed previously for dephasing qubits [9–12].

Whereas the above results have been obtained in a general way, we may also derive these results by explicitly performing the variation over the set of projectors in Eq. (3). In this way a basis of two orthogonal states is obtained that maximizes the classical information at a certain instant of time. Whenever the classical information is constant as a function of time, this basis is the basis of pointer states. Here the system is identified as the two qubits, whereas the measurement apparatus is given by the decohering environment. The latter represents a measurement apparatus that continuously measures without recording the

outcomes. To study these features in more detail, we may analytically determine the basis of pointer states, when it exists. Without loss of generality, the subsystem B is considered as an apparatus that performs measurements on subsystem A. Defining for subsystem B the arbitrary basis of two orthonormal states, $|\psi_1\rangle_B = \cos(\theta/2)|-\frac{1}{2}\rangle_B + e^{i\phi} \sin(\theta/2)|\frac{1}{2}\rangle_B$ and $|\psi_2\rangle_B = \cos(\theta/2)|\frac{1}{2}\rangle_B - e^{-i\phi} \sin(\theta/2)|-\frac{1}{2}\rangle_B$, the measurement projectors can be constructed as $\hat{\Pi}_k = |\psi_k\rangle_{BB}\langle\psi_k|$ ($k = 1,2$).

The classical information is of the form

$$C(t) = \max_{\{\theta,\phi\}}[G(\theta,\phi,t)],$$

where

$$G(\theta,\phi,t) = 1 + \tfrac{1}{2}[(1+g) \log_2(1+g) + (1-g) \log_2(1-g)],$$

with

$$g(\theta,\phi,t) = \sqrt{a^2 \cos^2\theta + \sin^2\theta[b^2 + c^2 + 2bc \cos(2\phi)]}.$$

As a consequence it can be shown that the extrema of $G(\theta,\phi,t)$ with respect to the position on the Bloch sphere (θ,ϕ) coincide with the corresponding extrema of $g(\theta,\phi,t)$. Note, that since $b,c \geqslant 0$, g attains its possible maxima only for $\phi = 0, \pi$. Thus, maximizing g is equivalent to maximizing the expression

$$a^2 \cos^2\theta + [b(t) + c(t)]^2 \sin^2\theta.$$

For time intervals where $a > b(t) + c(t)$ the maxima of the classical correlation appears at the poles of the Bloch sphere $\theta = 0, \pi$. In this time interval, the classical information is constant, as seen from Eqs. (11) and (12). Therefore, this basis of eigenstates of $\hat{\sigma}_z$ corresponds to a basis of pointer states.

On the other hand, if $a < b(t) + c(t)$ the maxima appear at $\theta = \frac{\pi}{2}$ so that the basis corresponds to eigenstates of $\hat{\sigma}_x$. However, the classical information in general is not constant. Only for very large times, when $b(t)$ and $c(t)$ reach their stationary values, the classical information asymptotically

reaches a constant value. This latter case again corresponds to a basis of pointer states. As $b(t)$ and $c(t)$ depend on time via the functions (7) and since these functions scale with temperature, varying the temperature allows a change of the basis of pointer states. This can be seen in the three cases depicted in Fig. 2: In (a) for large times the classical correlation becomes stationary and a basis of pointer states is asymptotically established as eigenstates of $\hat{\sigma}_x$. Increasing temperature, see Fig. 2(b), a metastable regime of $\hat{\sigma}_z$ pointer states is observed for the time interval where C is constant, which is replaced for large times by the $\hat{\sigma}_x$ pointer-state basis. Finally, for even higher temperatures the previously metastable regime becomes stable and the $\hat{\sigma}_z$ eigenstates become the pointer states, see (c).

At intermediate temperatures between cases (b) and (c), i.e., when the metastable $\hat{\sigma}_z$ pointer-state basis gradually becomes stable, an interesting feature can be observed, as shown in Fig. 3. When increasing temperature more than one metastable regime can occur, e.g., three regimes in the case shown in Fig. 3. For long times again a stationary $\hat{\sigma}_x$ pointer-state basis is reached asymptotically. The appearance of one or more metastable regimes is due to the non-Markovian nature of the evolution of the system [17–19]. Indeed, we have checked that increasing the separation between the qubits, the quantum correlations decay monotonically before reaching a stationary (nonzero) value. This dynamics resembles the one in Markovian systems. Also, the metastable pointer states do not appear in this regime. The reason is the following: the probability of a photon emitted by a qubit is absorbed by the other qubit, decreases when increasing separation between qubits. In other words, the phonons are more likely to spread around the lattice, leading to a Markovian dynamics. Related to the work of authors in Ref. [13] where double sudden transitions in geometric quantum correlations are reported, in our case we found multiple sudden transitions for quantum discord [see Fig. 3(b)].

The order of magnitude of the temperature T_P where the abrupt transition between $\hat{\sigma}_z$ and $\hat{\sigma}_x$ pointer states occur, can be estimated from the order of magnitude of the stationary values $b(\infty) \approx p \exp(-16\pi T/T_s)$ and $c(\infty) = (1-p)\exp(-16\pi T/T_s)$, and results from the condition $|a| = b(\infty) + c(\infty)$ as

$$T_P/T_s \approx -\frac{\ln|2p-1|}{16\pi}. \qquad (14)$$

Indeed this estimate agrees with the fact that for the special case of a pure initial state ($p = 1/2$) no abrupt transition can occur.

The appearance of the metastable pointer-state basis is also evidenced by the time evolution of the Von Neumann entropy $S(\hat{\rho}_{AB})$. Within each metastable regime the Von Neumann entropy reaches a local maximum, which is in agreement with the metastability of the pointer-state basis. At large times the entropy, similar to the classical correlation, reaches a stationary value.

We have shown that for a system of two donor-based charge qubits, the decoherence may lead to a time evolution where a series of transitory stages appear, each stage establishing a characteristic basis of pointer states. This scenario is fundamentally different from single abrupt transitions of the classical correlation, as shown in Refs. [9,10]. However, the
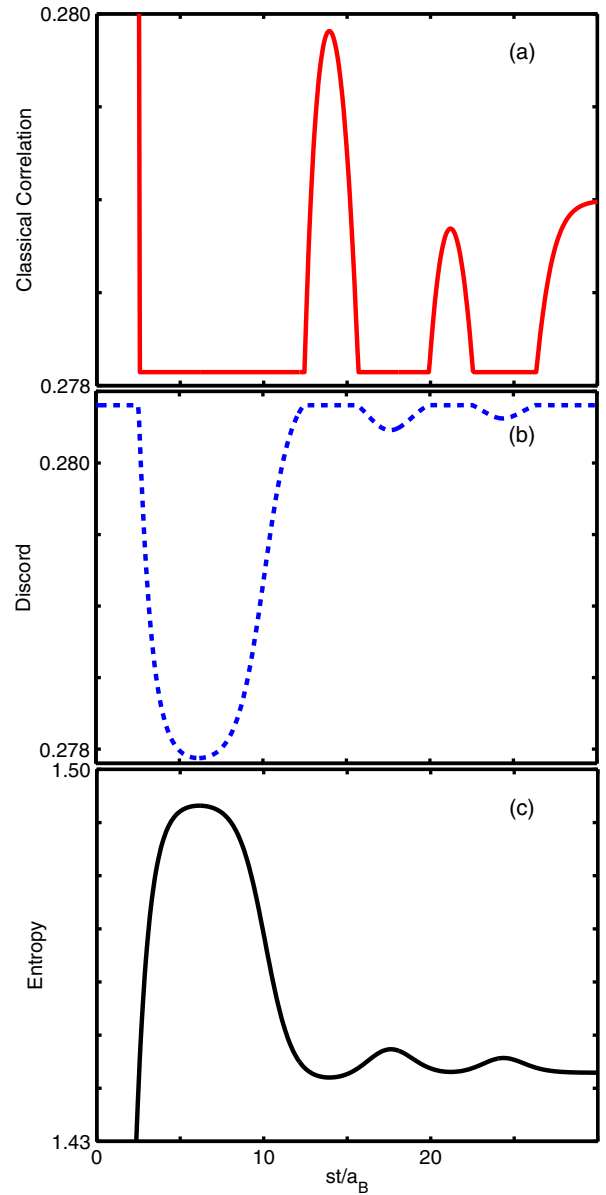

FIG. 3. (Color online) Evolution of the classical correlation (red solid line), the quantum discord (blue dashed line), and Von Neumann entropy (black solid line) for an initial state with mixing parameter $p = 0.8$ and $T/T_B = 0.0384$.

latter case can be observed in our system for the case of higher temperatures, as shown in Fig. 2(c). The system described here, exhibits a phaselike transition with respect to a change of temperature, where the equilibrium basis of pointer states go from $\hat{\sigma}_x$ eigenstates at $T \ll T_P$ to $\hat{\sigma}_z$ eigenstates at $T \gg T_P$, where T_P is estimated in Eq. (14). This feature opens the possibility to engineer the basis of pointer states by tuning the parameters of the physical system.

[1] B. P. Lanyon, M. Barbieri, M. P. Almeida, and A. G. White, Phys. Rev. Lett. **101**, 200501 (2008).

[2] H. Ollivier and W. H. Zurek, Phys. Rev. Lett. **88**, 017901 (2001).

[3] B. Groisman, S. Popescu, and A. Winter, Phys. Rev. A **72**, 032317 (2005).

[4] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).

[5] W. H. Zurek, Ann. Phys. **9**, 855 (2000).

[6] L. Henderson and V. Vedral, J. Phys. A **34**, 6899 (2001).

[7] J. Oppenheim, M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Rev. Lett. **89**, 180402 (2002).

[8] S. Luo, Phys. Rev. A **77**, 042303 (2008).

[9] J. Maziero, L. C. Celeri, R. M. Serra, and V. Vedral, Phys. Rev. A **80**, 044102 (2009).

[10] L. Mazzola, J. Piilo, and S. Maniscalco, Phys. Rev. Lett. **104**, 200401 (2010).

[11] J. S. Xu, C. F. Li, C. J. Zhang, X. Y. Xu, Y. S. Zhang, and G. C. Guo, Phys. Rev. A **82**, 042328 (2010).

[12] M. F. Cornelio, O. J. Farías, F. F. Fanchini, I. Frerot, G. H. Aguilar, M. O. Hor-Meyll, M. C. de Oliveira, S. P. Walborn, A. O. Caldeira and P. H. Souto Ribeiro, Phys. Rev. Lett. **109**, 190402 (2012).

[13] F. M. Paula, I. A. Silva, J. D. Montealegre, A. M. Souza, E. R. deAzevedo, R. S. Sarthour, A. Saguia, I. S. Oliveira, D. O. Soares-Pinto, G. Adesso, and M. S. Sarandy, Phys. Rev. Lett. **111**, 250401 (2013).

[14] W. H. Zurek, Phys. Rev. D **24**, 1516 (1981).

[15] L. C. L. Hollenberg, A. S. Dzurak, C. Wellard, A. R. Hamilton, D. J. Reilly, G. J. Milburn, and R. G. Clark, Phys. Rev. B **69**, 113301 (2004).

[16] J. Eckel, S. Weiss, and M. Thorwart, Eur. Phys. J. B **53**, 91 (2006).

[17] F. Lastra, S. A. Reyes, and S. Wallentowitz, J. Phys. B **44**, 015504 (2011).

[18] F. Lastra, S. A. Reyes, and S. Wallentowitz, Rev. Mex. Fis. S **57**, 148 (2011).

[19] F. Lastra, S. A. Reyes, and S. Wallentowitz, J. Phys. B **45**, 015503 (2012).

[20] M. Ali, A. R. P. Rau, and G. Alber, Phys. Rev. A **81**, 042105 (2010); **82**, 069902(E) (2010).