Generation of quantum correlations at adiabatic demagnetization

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Abstract

Adiabatic demagnetization (AD) is an effective way to achieve low temperatures required for generating quantum correlations. The emergence and behavior of quantum and classical correlations in a one-dimensional dipolar-coupled nuclear spin-1/2 system cooled using the conventional AD technique are theoretically investigated. The case is considered where the Zeeman energy is of the order of or even less than the dipolar interaction one. It is shown that, the mutual information and classical correlations increase monotonically in the AD process and achieve their maxima at switching off the magnetic field. The quantum correlations achieve the maximum at the point where the Zeeman energy is the order of the dipolar energy and decrease to zero with decreasing the field. Discord and classical correlations are asymmetrical with respect to permutation of asymmetrically located spins.

1. Introduction

Spin systems of magnetic and paramagnetic samples are widely used as models in various studies of quantum correlations [1–4]. The spin models constitute, on the one hand, a simple mechanism to produce classical and quantum correlations and, on the other hand, provide a clear physical picture. The spin systems can be relatively easily described theoretically, since spin operators are defined by simple operational expressions and obey simple commutation rules. The systems can find practical applications in the fields of quantum communication [5,6] and quantum amplification [7–9].

In quantum information theory, mutual information $I$ is adopted as a measure of total correlations that include quantum $D$ and classical $C$ parts and can be represented as a sum of these parts $I = D + C$ [10–12]. Quantum discord $D$ is a measure of nonclassical correlations between two subsystems of a quantum system and has been extensively studied recently [13–19]. For a pure state of the spin system, discord $D$ coincides with the entropy of entanglement $E$. In mixed states, $D$ can be nonzero even in the case when entanglement is absent [4].

An important aspect in the realization of quantum computation is the preparation of the system state at which quantum correlations appear. Usually, the quantum correlations appear in a spin system at very low temperature of the order of microkelvin [20–22]. A major part of the performed studies of quantum correlations does not take into consideration the realistic cooling technique for achieving such low temperature. One of the effective ways of deep cooling is the adiabatic demagnetization (AD) which is performed by variation of an external magnetic field [23–28].

Using AD technique in the rotating frame (ADRF) [29–31], entanglement in a dipolar-coupled nuclear spin system was studied [32]. In contrast to the conventional AD method, in ADRF method a radiofrequency external magnetic field is applied and varied. The amplitude of this field is stronger than an internal dipolar field and the frequency differs from the Larmor frequency.

Recently, the appearance of quantum correlation in a one-dimensional system of dipolar-coupled nuclear spins-1/2 was studied at cooling using the conventional AD technique [33]. It was shown that the entangled states can exist between nearest neighbor spins as well as between remote spins. The unexpected behavior of
entanglement for the remote spins is revealed: the entangled states in a spin system can exist in two distinct temperature and magnetic field regions separated by a region of the separable state.

In this paper we consider the discord emergence in a one-dimensional dipolar-coupled nuclear spin-1/2 system (spin chain) cooled using the AD technique. We consider the case where the external field is decreased to a value at which the Zeeman energy is of the order of or even less than the dipolar interaction one.

The structure of the paper is as follows: in the next section, we describe the Hamiltonian for a spin system in an external field, conditions of the AD realization and analyze variations of the spin temperature \( T \) at AD. Then we consider the pairwise correlations. Numerical simulation results for various correlations are presented in section 4. Discussion of the results and conclusion are given in the final section.

2. Spin system under AD

We consider a linear system, chain, of \( N \) dipole-coupling nuclear spins \( I_1, \ldots, I_N \) in an external magnetic field when the Zeeman energy of the order of or less than the dipolar interaction one. The Hamiltonian of the system can be presented in the following form

\[
H = H_z + H_{dd},
\]

where the Hamiltonian \( H_z \) describes the Zeeman interaction between the nuclear spins and external magnetic field directed along the \( z \)-axis

\[
H_z = \omega_0 \sum_{k=1}^{N} I_z^k,
\]

\( \omega_0 = \gamma |\tilde{H}_0| \) is the energy difference between the excited and ground states of an isolated spin, \( \tilde{H}_0 \) is the external magnetic field, \( \gamma \) is the gyromagnetic ratio of a spin, \( \tilde{H}_z \) is the projection of the angular spin momentum operator on the \( z \)-axis. The Hamiltonian \( H_{dd} \) describing dipolar interactions in an external magnetic field can be represented in terms of spherical tensor operators in the following form

\[
H_{dd}(\theta, \varphi) = -\sqrt{6} \sum_{m<n} \gamma^2 \hbar \sum_{k=-2}^{2} (-1)^k R_{(2,k)}(\theta, \varphi) T^{(mn)}_{(2,-k)},
\]

where the quadrupolar irreducible spherical spin tensor components of the spin tensors \( T_{(2,k)} \) are defined as

\[
T^{(m=0)}_{(2,0)} = \frac{1}{\sqrt{6}} [3 I_1^m I_2^m - I_1 I_2],
\]

\[
T^{(m=\pm 1)}_{(2,\pm 1)} = \frac{1}{\sqrt{2}} (I_1^m I_2^m + I_1 I_2),
\]

\[
T^{(m=\pm 2)}_{(2,\pm 2)} = I_1 I_2,
\]

and the spatial tensors \( R_{(2,k)}(\theta_{mn}, \varphi_{mn}) \) are defined by polar \( \theta_{mn} \) and azimuthal \( \varphi_{mn} \) angles

\[
R_{(2,0)}(\theta_{mn}, \varphi_{mn}) = \frac{1}{2} (3 \cos^2 \theta_{mn} - 1),
\]

\[
R_{(2,\pm 1)}(\theta_{mn}, \varphi_{mn}) = \pm \frac{3}{2} \sqrt{\frac{3}{8}} e^{\pm i \varphi_{mn}} \sin 2\theta_{mn},
\]

\[
R_{(2,\pm 2)}(\theta_{mn}, \varphi_{mn}) = \frac{3}{2} \sqrt{\frac{3}{8}} e^{\pm 2i \varphi_{mn}} \sin^2 \theta_{mn},
\]

where \( r_{mn}, \theta_{mn}, \) and \( \varphi_{mn} \) are the spherical coordinates of the vector \( \tilde{r}_{mn} \) connecting the \( m \)th and \( n \)th nuclei. \( I_1^m \) and \( I_2^m \) are the raising and lowering spin angular momentum operators of the \( m \)th spin. We consider AD when \( \omega_0 \) of the order of \( D_{12} = \frac{\gamma^2 \hbar}{\tilde{H}_0^2} \) (here \( D_{12} \) is the dipolar coupling constant for the nearest spins), and it is necessary to take into account all the terms of the Hamiltonian (3).

A spin system can be considered as a system in the thermal equilibrium during evolution and be described by the density matrix [26]

\[
\rho = \frac{1}{Z} \exp \{ -\beta H \},
\]

if

\[
\frac{d\tilde{H}_0}{dt} \ll \gamma \tilde{H}_{loc},
\]
where $\beta$ is the inverse spin temperature in units of $D_{12}$, $T$ is the spin temperature and $Z = \text{Tr} \{ \exp ( - \beta H) \}$ is the partition function, $H^\prime$ is the Hamiltonian normalized by $D_{12}$, $H_{\text{loc}} = \frac{1}{\gamma} \sqrt{\frac{\text{Tr}(H^2_{\text{loc}})}{\text{Tr}I}}$ is the local magnetic field created by the dipolar interactions.

The entropy, $S$, heat capacity $C$, and magnetization $M$ of a spin system can be expressed in terms of the partition function:

$$S = k_B \frac{\partial (\beta \ln Z)}{\partial \beta},$$

$$C = k_B \beta^2 \frac{\partial^2 (\ln Z)}{\partial \beta^2},$$

and

$$M = - \frac{1}{\beta Z} \frac{\partial Z}{\partial B}$$

respectively. In (10) $B$ is the external magnetic flux density normalized by $D_{12}$. In adiabatic processes the entropy $S = \text{const}$.

### 3. Correlations in a spin 1/2 system

The calculation methods for characteristics of various correlation types have been developed for two-spin 1/2 systems [1–4]. One of the methods of the correlation analysis in multi-spin systems is based on consideration of correlation between two spins, the $m$th and $n$th spins, using a reduced density matrix (RDM) which is defined as $\rho_{mn} = \text{Tr}_{\text{mn}} \rho$ where $\text{Tr}_{mn}(...)$ denotes the trace over the degrees of freedom for all spins except the $m$th and $n$th spins. We showed analytically for three-spin systems and numerically for circle and chain spin systems up to 10 spins that the RDM corresponding to the $m$th and $n$th spins of the system described by the Hamiltonian $H(1)$ is given by

$$\rho_{mn} = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{14} \\ 0 & \rho_{22} & \rho_{23} & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} \end{pmatrix},$$

where the matrix elements $\rho_{ij}$ depend on the spin numbers, $i$ and $j$, and all elements noted by $\rho_{ij}$ in (11) are nonzero in the general case.

#### 3.1. Quantum mutual information

If $\rho^{AB}$ denotes the density matrix (operator) of a composite bipartite system $AB$, quantum mutual information is [36]

$$I = S(\rho^A) + S(\rho^B) - S(\rho^{AB}),$$

where $S(\rho) = - \text{tr} (\rho \log_2 \rho)$ is the von Neumann entropy, $\rho^A$ and $\rho^B$ are the density operators of parts $A$ and $B$, respectively. For the density matrix of the $X$-form (9) quantum mutual information is [14]:

$$I = S(\rho^A_x) + S(\rho^B_x) + \sum_{i=1}^{4} \lambda_i \log_2 \lambda_i,$$

where $\rho^A_x$ and $\rho^B_x$ are the marginal states of matrix (11) and

$$S(\rho^A_x) = - \{ (\rho_{11} + \rho_{22}) \log_2 (\rho_{11} + \rho_{22}) + (\rho_{33} + \rho_{44}) \log_2 (\rho_{33} + \rho_{44}) \},$$

$$S(\rho^B_x) = - \{ (\rho_{11} + \rho_{33}) \log_2 (\rho_{11} + \rho_{33}) + (\rho_{22} + \rho_{44}) \log_2 (\rho_{22} + \rho_{44}) \},$$

and the eigenvalues $\lambda_i$ ($i = 1, \ldots, 4$) of density matrix (9) are

$$\lambda_{1,2} = \frac{1}{2} \{ \rho_{11} + \rho_{44} \} \pm \sqrt{(\rho_{11} - \rho_{44})^2 + 4 |\rho_{14}|^2},$$

$$\lambda_{3,4} = \frac{1}{2} \{ \rho_{22} + \rho_{33} \} \pm \sqrt{(\rho_{22} - \rho_{33})^2 + 4 |\rho_{23}|^2}.$$
measures of entanglement: concurrence and entanglement of formation. The concurrence between two, the $m$th and $n$th, spins can be defined as \[ C_{mn} = \max \{ q_{mn}, 0 \} , \] with \( q_{mn} = \lambda_1^{(1)} - \lambda_2^{(2)} = \lambda_3^{(3)} - \lambda_4^{(4)} \). Here \( \lambda_k^{(k)}(k = 1, 2, 3, 4) \) are the square roots of eigenvalues, in descending order, of the following non-Hermitian matrix:

\[
R_{mn} = \rho_{mn} (\sigma_y \otimes \sigma_y) \rho_{mn} (\sigma_y \otimes \sigma_y) .
\]

For maximally entangled states, the concurrence \( C_{mn} \) equals 1 while for separable states \( C_{mn} = 0 \). Our calculation of concurrence for chains containing 2, 3, 4 spins showed that in thermal equilibrium the concurrence \( C_{mn} \) is zero at \( q = 0 \) and \( q = p \), and reaches the maximum values at \( q = \frac{\pi}{2} \) and \( q = 0 \) \cite{41, 42}. Therefore, we will restrict ourselves to the cases corresponding to the maximal concurrence.

We will also characterize the entangled states of the $m$th and $n$th spins by the entanglement of formation \( E_{mn} \):

\[
E_{mn} = -h_+^{m} \log_2 h_+^{m} - h_-^{m} \log_2 h_-^{m},
\]

where \( h_{\pm} = \frac{1}{2} (1 \pm \sqrt{1 - c_{mn}^2}) \).

### 3.3. Discord

Quantum discord can be determined as

\[
D = I - C,
\]

where a measure of the classical correlations is \[ C(\rho) = \sup_{\{B_k\}} \mathcal{I}(\rho | \{B_k\}) , \]

where \( \{B_k\} \) are the projection operators describing a von Neumann measurement on subsystem $B$ only and the conditional density operator $\rho_k$ associated with the measurement result $k$ is

\[
\rho_k = \frac{1}{p_k} (e \otimes B_k) \rho (e \otimes B_k),
\]

and

\[
p_k = tr[(e \otimes B_k) \rho (e \otimes B_k)]
\]

\[ (e \text{ is the } 2 \times 2 \text{ unit matrix}). \] The quantum mutual information associated with this measurement is

\[
\mathcal{I}(\rho | \{B_k\}) = S(\rho^A) - S(\rho | \{B_k\}) ,
\]

where the quantum conditional entropy with respect to the measurement result $k$ is

\[
S(\rho | \{B_k\}) = \sum_k p_k S(\rho_k).\]

Computing quantum discord requires finding the maximal measure of the classical correlations over all possible von Neumann measurements on $B$.

The discord is not a symmetric quantity \cite{44, 45}: it is possible to exist states with discord $D_A$ determined through the measurements on subsystem $A$ does not equal discord $D_B$ calculated using subsystem $B$. In appendix we present analytical results for $D_A$ and $D_B$ obtained using the approach developed in \cite{14, 46}.

### 3.4. Geometric discord

Another measure of the quantum correlations, which is not connected with calculation of the classical correlation and optimization problem, has been proposed in \cite{45}. The authors of \cite{45} introduced so-called the geometric discord $D_G$ as the minimal square norm in the Hilbert–Schmidt space between the two-spin state and zero-discord state:

\[
D_G(\rho) = \min_{\chi \in \Omega_0} \| \rho - \chi \|^2 ,
\]

where \( \Omega_0 \) denotes the set of zero-discord states and \( \|X\|^2 = trX^2 = tr(XX^T) \) is the square norm.

Density matrix $\rho$ can be rewritten in the Bloch representation:

\[
\rho = \frac{1}{4} \left( e \otimes e + \sum_{i=1}^{3} \chi_i \sigma_i \otimes e + \sum_{i=1}^{3} \gamma_i e \otimes \sigma_i + \sum_{i,j=1}^{3} T_{ij} \sigma_i \otimes \sigma_j \right),
\]

where $\chi_i = tr(\rho \sigma_i \otimes e)$, $\gamma_i = tr(\rho e \otimes \sigma_i)$ are the components of the local Bloch vectors, $T_{ij} = tr(\rho \sigma_i \otimes \sigma_j)$ are components of the correlation tensor, and $\sigma_i (i = 1, 2, 3)$ are three Pauli matrices.
The geometric discord $d_{\text{GA}}$ measured on subsystem $A$ is [45]:

$$d_{\text{GA}}(\rho) = \frac{1}{4}(\|X\|^2 + \|T\|^2 - \lambda_{\text{max}}),$$

(25)

where $\lambda_{\text{max}}$ is the largest eigenvalue of matrix $X^T X + TT^T$.

The geometric discord $d_{\text{GB}}$ measured on subsystem $B$ is [47]:

$$d_{\text{GB}}(\rho) = \frac{1}{4}(\|Y\|^2 + \|T\|^2 - \lambda_{\text{max}}),$$

(26)

where now $\lambda_{\text{max}}$ is the the largest eigenvalue of matrix $Y^T Y + T^T T$.

The geometric discords given by equations (25) and (26) are not normalized to 1 [47]: their maximum value is $1/2$ for two-qubit states. Following [47] we will consider the normalized geometric discords $D_{\text{GA}} = 2d_{\text{GA}}$ and $D_{\text{GB}} = 2d_{\text{GB}}$ with the maximum measures of 1 for comparison with other quantum correlations.

4. Correlations under AD

The numerical simulation of correlations under AD is performed using the software based on the MatLab package. The calculation process is as follows. At the initial magnetic field, $\omega_0^{\text{inv}}$, and inverse temperature, $\beta_{\text{inv}}$, the entropy is calculated using equations (6) and (8), the external magnetic field is slightly decreased and a new temperature is determined from the condition $S = \text{const}$. Then, using a new density matrix, heat capacity $C$, and magnetization $M$, are calculated; a new RDM is used to calculate correlations. At the calculation of the correlations, the spin with a lower number in the chain is considered as subsystem $A$ in equations (12), (13), (18), (21), and (22); the spin with a higher number corresponds to subsystem $B$. We have analyzed correlations between various spin pairs in chains with spin numbers from 2 to 10. The results are qualitatively similar for various chains. Below, in figures 1–7, we present the results for the two-spin and seven-spin chains. Figure 1 shows the inverse spin temperature, $\beta$, versus the external magnetic field for the two-spin systems.

The curve can be considered as an AD trajectory on the $\omega_0 - \beta$ phase plane. At relatively high magnetic fields ($\omega_0/D_{12} > 3$ in the considered case), the field decrease leads to an increase in $\beta^{-1}/\omega_0$. At low field $\omega_0/D_{12} < 1$ the inverse temperature does not change much with the magnetic field and the maximum $\beta_{\text{m}} \approx 7.1$.

In contrast to the temperature dependence on the external field magnetic field, the magnetization is about constant at $\omega_0/D_{12} > 3$ and decreases linearly with a magnetic field decrease at $\omega_0/D_{12} < 1$ (figure 1, the inset). The heat capacity increases with decreasing field up to its maximum at $\omega_0/D_{12} = 1.3$ and then fast decreases (figure 1, the inset). The pronounced increase in the capacity and its maximum coincide with the increase and maximum in quantum correlations (compare figure 1, the inset and figure 2).

At initial temperatures and magnetic fields the measures of the correlations have small but finite values and increase with a decrease of the magnetic field (figures 2–5). The quantum mutual information and classical
correlations increase monotonically and achieve their maxima at zero field. Note, that for pure states of a two-spin system the maxima for the quantum mutual information and classical correlations are 2 and 1, respectively, at the same value of the field. In contrast from this, in considered mixed states, the quantum mutual information and quantum correlations have their maxima at different fields. Therefore, the maximal value of the quantum mutual information is less than 2 and is achieved at the point where quantum correlations are very weak or even disappear at $H = 0$. The quantum discords $D$ and $D_{G}$ monotonically increase with a decrease of the magnetic field to their maxima at $\frac{\hbar}{D_{12}} \approx 1$, then decrease and can achieve zero value. The maxima are reduced with an increase of the distance between the considered spins in a chain (compare figures 3, 4, and 5) and with an increase of the number of spins in the system (compare figures 2 and 3). When the quantum correlations are
maximum, the total magnetic field is determined as a sum of the local and nonzero external fields and the magnetization is small but finite (figure 1, the inset).

As was noted above, the calculation results for the classical and quantum correlations, are different for subsystem $A$ and subsystem $B$ (figures 3 and 4), and only for the pairs where the considered spins are under identical conditions give the same results (figures 2 and 5). The difference between these correlation measures, calculated relative different subsystems, increases to the maximum with the decrease of magnetic field and then decreases to zero at zero field. As example, figure 6 presents the normalized difference between quantum discords $D_{AB}$ and $D_{CD}$ for the for the 1st and 2nd spins in a seven-spin chain as a function of the applied magnetic field $\frac{D_{0}}{D_{12}}$ under AD.
Two measures for quantum correlations, discord $D$ and geometric discord $D_G$, are substantially different (figures 2–5). This difference does not change monotonically with the external magnetic field (figure 7). The relationship between $D$ and $D_G$: $D_G \geq D^2$ obtained in [47] holds in the cases considered here.

Behavior of entanglement differs from other correlations. For remote spins the concurrence can have two maxima which are separated by area with zero concurrence (figure 4, the inset, and see also figures 6–9 and their discussion in [33]). The concurrence can exist in the regions where the measures of other quantum correlations are nonzero (figures 2–5). On the other hand, the concurrence can be larger than measures of the classical correlations, quantum discords and even quantum mutual information (figures 2 and 3). For non-adiabatic conditions ($\omega_0 = \text{const}$ and $T = \text{const}$) this phenomenon was discussed early [14, 46, 48]. The entanglement of formation demonstrates the behavior similar to behavior of the concurrence (figures 2–4). The entanglement of formation is less than the quantum mutual information and classical correlations, while can exceed both discords (figures 2–4). Thus, the entanglement of formation is more, than the concurrence, suitable measure for comparison of entanglement with other correlations.
5. Conclusion

The analysis of correlations between various spin pairs in chains with numbers of spins from 2 to 10 under AD shows that the results for different chains are qualitatively similar:
- concurrence and the entanglement of formation appear at temperatures below a critical value which depends on magnetic field while other correlations and quantum mutual information exist at any temperature and magnetic field;
- quantum and geometric discords, $D$ and $D_G$, and classical correlations are asymmetrical and these correlation measures determined relatively to subsystem $A$ and relative subsystem $B$ are the same for spins in the identical states i.e. where the spins are symmetrically located in a chain. The asymmetric behavior of the correlations between $A$ and $B$ subsystems can be used in quantum information processing as an identification marker of the different spins and can provide us a tool for selective control of the spin states.
- at AD, discords $D$ and $D_G$ possess one maxima in all cases, while, for remote spins, the entanglement measures, concurrence and entanglement of formation, possess two maxima.
- the behavior of the correlations are qualitatively similar for various chains and the maxima of the quantum correlations are reduced with an increase of the distance between the considered spins in a chain and with an increase of the number of spins in the system.

Investigation of relation between discord $D$ and geometric $D_G$ discords, classical correlation and entanglement at AD shows that the entanglement of formation is a more, than concurrence, suitable measure for comparison of entanglement with other correlations. All considered measures of quantum correlations are independent, with no simple relation between them.

Quantum correlations are an essential resource for implementations for quantum information processing. It is very useful to study the conditions required to initiate correlations between qubits based on the states of a spin system. The AD technique allows one to generate various correlations in dipolar-coupling spin systems. It opens a simple and effective way to experimental testing of quantum and classical correlations in spin systems. Our investigation demonstrates that the dependence of these correlations on temperature and magnetic field can be much more complicated than might otherwise have been expected from results for two-spin systems. Adiabatic variations of the external field can be applied for controlling of the quantum correlations between qubits and may be used for realization of quantum computation.

Appendix

Here we present analytical results for discords $D_A$ [14, 46] and $D_B$. For analysis of correlations in multi-spin systems we use the RDM. Any von Neumann measurement for subsystem $A$ can be written:

$$A_i = \Pi_i V^\dagger, \quad i = 0, 1,$$

(A1)

where $\Pi_i = |i\rangle\langle i|$ is the projector for subsystem $A$ along the computation base and $V$ is a unitary operator with unit determinant. The measurement on subsystem $B$ can be written in a similar form. After the measurements the density matrix will change to the ensemble $\{p_{ii}, p_{1r}, p_{2r}\}$, where for subsystem $A$

$$\rho_{Ai} = \frac{1}{P_{Ai}} (A_i \otimes e) \rho (A_i \otimes e),$$

(A2)

and for subsystem $B$

$$\rho_{Bi} = \frac{1}{P_{Bi}} (e \otimes B_i) \rho (e \otimes B_i),$$

(A3)

where $P_{Ai} = tr[(A_i \otimes e) \rho (A_i \otimes e)]$ and $P_{Bi} = tr[(e \otimes B_i) \rho (e \otimes B_i)]$.

In both cases we may write $V$ as

$$V = te + i\vec{z} \cdot \vec{\sigma},$$

(A4)

where $t, z_1, z_2, z_3$ are real and $t^2 + z_1^2 + z_2^2 + z_3^2 = 1$. Two eigenvalues of each $\rho_0$ and $\rho_1$ can be presented as

$$\lambda_{i\pm}(\rho_0) = \frac{1}{2} (1 \pm \theta),$$

$$\lambda_{i\pm}(\rho_1) = \frac{1}{2} (1 \pm \theta').$$

(A5)
The corresponding probabilities are for \( A \) case
\[
\begin{align*}
 p_{50} &= (\rho_{11} + \rho_{22}) k + (\rho_{33} + \rho_{44}) l, \\
 p_{41} &= (\rho_{11} + \rho_{22}) l + (\rho_{33} + \rho_{44}) k.
\end{align*}
\] (A6)
and for \( B \) case
\[
\begin{align*}
 p_{20} &= (\rho_{11} + \rho_{33}) k + (\rho_{22} + \rho_{44}) l, \\
 p_{21} &= (\rho_{11} + \rho_{33}) l + (\rho_{22} + \rho_{44}) k.
\end{align*}
\] (A7)
\( \theta \) and \( \theta' \) are defined for \( A \) case
\[
\begin{align*}
\theta_A &= \sqrt{\frac{|(\rho_{11} - \rho_{22}) k + (\rho_{33} - \rho_{44}) l|^2 + \Theta_A}{|(\rho_{11} + \rho_{22}) k + (\rho_{33} + \rho_{44}) l|^2}}, \\
\theta_A' &= \sqrt{\frac{|(\rho_{11} - \rho_{22}) l + (\rho_{33} - \rho_{44}) k|^2 + \Theta_A}{|(\rho_{11} + \rho_{22}) l + (\rho_{33} + \rho_{44}) k|^2}},
\end{align*}
\] (A8)
and for \( B \) case
\[
\begin{align*}
\theta_B &= \sqrt{\frac{|(\rho_{11} - \rho_{33}) k + (\rho_{22} - \rho_{44}) l|^2 + \Theta_B}{|(\rho_{11} + \rho_{33}) k + (\rho_{22} + \rho_{44}) l|^2}}, \\
\theta_B' &= \sqrt{\frac{|(\rho_{11} - \rho_{33}) l + (\rho_{22} - \rho_{44}) k|^2 + \Theta_B}{|(\rho_{11} + \rho_{33}) l + (\rho_{22} + \rho_{44}) k|^2}},
\end{align*}
\] (A9)
where
\[
\begin{align*}
\Theta_A &= 4k[|\rho_{11}|^2 + |\rho_{22}|^2 + 2 \text{Re}(\rho_{14}\rho_{23})] - 16m \text{Re}(\rho_{14}\rho_{23}) + 16n \text{Im}(\rho_{14}\rho_{23}), \\
\Theta_B &= 4k[|\rho_{11}|^2 + |\rho_{33}|^2 + 2 \text{Re}(\rho_{14}\rho_{23}^*)] - 16m \text{Re}(\rho_{14}\rho_{23}^*) + 16n \text{Im}(\rho_{14}\rho_{23}^*),
\end{align*}
\]
Re(\( z \)) and Im(\( z \)) are the real and imaginary parts of the complex number \( z = z^* \) is the complex conjugate value of \( z \).
The parameters \( m, n, k, l \) are defined as \( m = (t_{z1} + z_2 z_3)^2, n = (t_{z2} - z_1 z_3)(t_{z1} + z_2 z_3), k = t^2 + z_3^2, l = z_1^2 + z_2^2 \).

In both cases the entropies of the ensemble \( \{\rho_{ij}, p_i\} \) are
\[
\begin{align*}
S(\rho_{ij}) &= -\lambda_+ (\rho_{ij}) \log \lambda_+ (\rho_{ij}) - \lambda_- (\rho_{ij}) \log \lambda_- (\rho_{ij}), \\
S(\rho_{ij}) &= -\lambda_+ (\rho_{ij}) \log \lambda_+ (\rho_{ij}) - \lambda_- (\rho_{ij}) \log \lambda_- (\rho_{ij}).
\end{align*}
\] (A10)

The classical correlations are for \( A \) case
\[
C_A(\rho) = S(\rho_A^B) - \min_{\{p_i\}} [p_{50} S(\rho_{50}^B) + p_{41} S(\rho_{41}^B)]
\] (A11)
and for case \( B \)
\[
C_B(\rho) = S(\rho_B^A) - \min_{\{p_i\}} [p_{20} S(\rho_{20}^A) + p_{21} S(\rho_{21}^A)]
\] (A12)

With \( k + l = 1 \) and \( m^2 + n^2 = kl \) the probabilities, eigenvalues, and, hence, the classical correlations for a given density matrix depend on two real parameters \( m \) and \( k: k \in [0, 1] \) and \( m \in [0, 1/4] \). To minimize note that the expressions are symmetric under the interchange of \( k \) and \( l = 1 - k \). The minimized functions are even functions of \( (k - l) \) and the extrema at \( k = l = 1/2 \) or at the end points \( k = 0 \) or \( k = 1 \). According to the definitions of these parameters and the correlation between them at \( k = 0: l = 1, m = 0, n = 0 \); at \( k = 1: l = 0, m = 0, n = 0 \). At \( k = l = 1/2 \) the minimization task is reduced to finding the extrema of expression
\[
-16m \text{Re}(\rho_{14}\rho_{23}) + K n \text{Im}(\rho_{14}\rho_{23})
\]
and for subsystem \( A: M = 16 \text{Re}(\rho_{14}\rho_{23}) \) and \( K = 16 \text{Im}(\rho_{14}\rho_{23}) \) and for subsystem \( B: M = 16 \text{Re}(\rho_{14}\rho_{23}^*) \) and \( K = 16 \text{Im}(\rho_{14}\rho_{23}^*) \). The extrema are at
\[
m = \frac{1}{8} \left( 1 + \sqrt{\frac{M^2}{M^2 + K}} \right)
\]
or at the end points \( m = 0 \) or \( m = 1/4 \). The classical correlations are determined as the smallest value of (A11) and (A12) at:
\[
k = 0; \quad l = 1; \quad m = 0; \quad n = 0;
k = 1; \quad l = 0; \quad m = 0; \quad n = 0;
k = 1/2; \quad l = 1/2; \quad m = 0; \quad n = 0;
k = 1/2; \quad l = 1/2; \quad m = 1/4; \quad n = 0;
k = 1/2; \quad l = 1/2; \quad m = \frac{1}{8} \left( 1 + \sqrt{\frac{M^2}{M^2 + k^2}} \right) n = \pm \frac{1}{4} m - m^2;
k = 1/2; \quad l = 1/2; \quad m = \frac{1}{8} \left( 1 - \sqrt{\frac{M^2}{M^2 + k^2}} \right) n = \pm \frac{1}{4} m - m^2.
\]

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