Quantum correlations in a system of nuclear $s = 1/2$ spins in a strong magnetic field

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Abstract

Entanglement and quantum discord for a pair of nuclear spins $s = 1/2$ in a nanopore filled with a gas of spin-carrying molecules (atoms) are studied. The correlation functions describing dynamics of dipolar-coupled spins in a nanopore are found. The dependence of spin-pair entanglement on the temperature and the number of spins is obtained from the reduced density matrix, which is centrosymmetric (CS). An analytic expression for the concurrence is obtained for an arbitrary CS density matrix. It is shown that the quantum discord as a measure of quantum correlations attains a significant value at low temperatures. It is also shown that the discord in the considered model has ‘flickering’ character and disappears periodically in the course of time evolution of the system. The geometric discord is studied for arbitrary $4 \times 4$ CS density matrices.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Quantum correlations in many-particle systems are responsible for the performance of the quantum devices (in particular, quantum computers) and give them significant advantages over their classical counterparts [1, 2]. Until recently it was believed [3] that entanglement is responsible for quantum correlations [4], and quantum devices can be created only on the basis of materials which can be easily prepared in entangled states [2]. However, it turned out that one can work out quantum algorithms [4, 5] that significantly outperform their classical counterparts by mixing separable (non-entangled) states. It also turned out that quantum non-locality can be observed in systems without entanglement [6]. From this, one can conclude that entanglement describes only a part of quantum correlations but not all of them.

According to the current understanding [1], total correlations, quantum and classical, are determined by the mutual information [7]. The problem is how to divide the correlations into
quantum and classical ones. The problem was solved independently by Henderson and Vedral [8] as well as Ollivier and Zurek [9]. The classical correlation in a binary system is determined by the total set of projective measurements carried out only for its one subsystem [8]. Then the quantum correlation measure (the quantum discord) is determined as the difference between the mutual information and its classical part optimized over all possible projective measurements [8, 9]. The quantum discord is determined completely by quantum properties of the system and equals zero for classical systems.

The calculation of the quantum discord is a complex problem because it is necessary to execute many-parametric optimization. Therefore, analytic calculations for the discord are possible only in simple two-qubit systems [10, 11].

Special attention was devoted to a connection of the quantum discord and physical parameters of the system [12, 13]. Such investigations open a direct way to experimental measurements of the discord. In this paper, we investigate theoretically the entanglement and quantum discord in a thin silicon film containing closed nanopores filled with a gas of spin-carrying molecules (atoms) with spin $s = 1/2$ in a strong external magnetic field. NMR line shape in such films was studied experimentally [14] and theoretically [15, 17]. Fast molecular motion in nanopores does not average the dipole–dipole interactions (DDIs) completely (space confinement) and the residual DDI is described by one coupling constant which is the same for all pairs of interacting spins [14, 15]. Reducing the density matrix (which describes the time evolution of the system with the residual DDI) over all spins except the chosen pair, one can obtain information about the pair entanglement and quantum discord in the system. The main goal of this paper is the investigation of entanglement and quantum discord of spin pair in the nanopore filled with a gas of spin-carrying molecules (atoms).

It is also significant that the reduced density matrix in the considered model is centrosymmetric (CS) [18]. In this paper, we obtain an analytic expression for the concurrence [19] of an arbitrary $4 \times 4$ CS density matrix. The geometric discord for an arbitrary $4 \times 4$ CS matrix is also calculated.

### 2. The reduced density matrix of the spin pair in a nanopore

We consider a system consisting of $N$ spin-carrying molecules (atoms) of a gas with spin $s = 1/2$ in a closed nanopore in a strong external magnetic field $B$ (figure 1). Molecular motions lead to a partial averaging of the secular DDI, $H_{dc}$ [14, 15] and the Hamiltonian of the residual (averaged) DDI is [15]

$$H_{dc} = \frac{D}{2}(3I_z^2 - I^2),$$

(1)

where $D$ is the coupling constant, which is the same for all spin pairs [14, 15], $I^2$ is the square of the total angular momentum, $I_\alpha = \sum_{i=1}^{N} I^\alpha_i$, $I^\alpha_i$ is the operator of the momentum projection of spin $i$ ($i = 1, 2, \ldots, N$) on the axis $\alpha$ ($\alpha = x, y, z$). In the initial moment of time, the resonance $\pi/2$-pulse, turning spins by the angle $\pi/2$ about the axis $y$ (figure 1), acts on the system. It is the usual method of creating a nonequilibrium state in the NMR spectroscopy [16]. As a result, the equilibrium density matrix, $\rho_0$, in a strong external magnetic field is given by

$$\rho_0 = \frac{1}{Z} e^{\beta H},$$

(2)

where $Z = \text{Tr}(e^{\beta H}) = 2^N \cosh^N \frac{\beta}{2}$ is the partition function, $\beta = \frac{k_B T}{\omega_0}$ is the inverse dimensionless temperature, $\omega_0 = \gamma B_0$ ($\gamma$ is the gyromagnetic ratio) is the Larmour frequency
Figure 1. A gas of spin-carrying molecules (atoms) in a nanopore in the external magnetic field.

and $T$ is the temperature of the system. The time evolution of the density matrix is described as

$$
\rho(t) = e^{-iH_d t} \rho_0 e^{iH_d t} = \frac{1}{Z} e^{-i\alpha I^x_0} e^{i\beta I^z_0},
$$

where we took into account that $[I^\alpha, I^\beta] = 0$ ($\alpha = x, y, z$) and set $a = \frac{3D}{2}$. The density matrix (3) describes the free induction decay and NMR line shape [15, 17]. In order to solve our problems, it is convenient to rewrite the density matrix $\rho(t)$ as [20]

$$
\rho(t) = \sum_{\xi_1, \xi_2, \ldots, \xi_N = 0}^3 \alpha_{1, 2, \ldots, N}(t) I_1^{\xi_1} \otimes I_2^{\xi_2} \otimes \cdots \otimes I_N^{\xi_N},
$$

where $\xi_j = 0, 1, 2, 3$ ($j = 1, 2, \ldots, N$), $I_j^0 = E_j$ ($E_j$ is the $2 \times 2$ matrix), $I_j^1 = I_j^y$, $I_j^2 = I_j^z$, $I_j^3 = I_j^y$ and $\alpha_{1, 2, \ldots, N}(t)$ is a function of time. Since $\text{Tr}(I_j^{3\xi^j}) = 0$ ($j = 1, 2, \ldots, N, \xi_j = 1, 2, 3$), the condition of the normalization of the density matrix leads to

$$
\alpha_{0, 0, \ldots, 0}^{1, 2, \ldots, N} = \frac{1}{2^N}.
$$

Consider an arbitrary spin pair. Without loss of generality, we can assume that it includes spins 1 and 2. We will investigate the entanglement and the quantum discord for that pair. The reduced over spins 3, 4, \ldots, $N$ density matrix $\rho^{(1,2)}(t)$ is

$$
\rho^{(1,2)}(t) = \sum_{\xi_1, \xi_2 = 0}^3 \alpha_{1, 2}^{\xi_1, \xi_2}(t) I_1^{\xi_1} \otimes I_2^{\xi_2},
$$
where \( \alpha_{1,2}^{\xi_1,\xi_2}(t) = \alpha_{1,2}^{\xi_1,\xi_2,0,...,0}(t) \). One can verify that \( \text{Tr}(\rho^{(1,2)}) = 1 \). Functions \( \alpha_{1,2}^{\xi_1,\xi_2}(t) \) can be expressed via the correlation functions of the spin system as follows:

\[
\alpha_{1,2}^{\xi_1,\xi_2}(t) = \begin{cases} 
4\text{Tr}\{\rho(t)(I_1^{\xi_1} \otimes I_2^{\xi_2} \otimes E_3 \otimes \cdots \otimes E_N)\}, & \xi_1, \xi_2 = 1, 2, 3,\\ 
\text{Tr}\{\rho(t)(I_1^{\xi_1} \otimes I_2^{\xi_2} \otimes E_3 \otimes \cdots \otimes E_N)\}, & \xi_1 = 0, \xi_2 = 1, 2, 3 \text{ or } \xi_1 = 1, 2, 3, \xi_2 = 0,\\ 
\frac{1}{4}\text{Tr}\{\rho(t)(I_1^{\xi_1} \otimes I_2^{\xi_2} \otimes E_3 \otimes \cdots \otimes E_N)\}, & \xi_1 = 0, \xi_2 = 0. 
\end{cases}
\]

(7)

One can find from equation (5) that \( \alpha_{12}^{00} = 1/4 \). Relationships (3) and (7) lead to

\[
\alpha_{12}^{03} = \alpha_{12}^{30} = \alpha_{12}^{21} = \alpha_{12}^{31} = \alpha_{12}^{23} = \alpha_{12}^{32} = 0.
\]

(8)

Taking into account the permutation symmetry over the numbers of spins 1 and 2, it is convenient to introduce the correlation functions

\[
p = \text{Tr}\{\rho(t)(I_1^{i} \otimes E_2 \otimes E_3 \otimes \cdots \otimes E_N)\}
\]

\[
= \text{Tr}\{\rho(t)(I_2^{i} \otimes E_1 \otimes E_3 \otimes \cdots \otimes E_N)\},
\]

(9)

\[
q = \text{Tr}\{\rho(t)(I_1^{j} \otimes I_2^{j} \otimes E_3 \otimes \cdots \otimes E_N)\},
\]

(10)

\[
r = \text{Tr}\{\rho(t)(I_1^{j} \otimes I_2^{j} \otimes E_3 \otimes \cdots \otimes E_N)\},
\]

(11)

\[
\sigma = \text{Tr}\{\rho(t)(I_1^{j} \otimes I_2^{j} \otimes I_3 \otimes \cdots \otimes E_N)\}.
\]

(12)

Using equation (3) for the density matrix \( \rho(t) \) and executing the unitary transformation \( U_1 = \exp(i t I_1) \otimes E_2 \otimes E_3 \otimes \cdots \otimes E_N \) under the sign of the trace (13) we obtain that \( \sigma = 0 \). Using equations (7)–(13) the reduced density matrix can be written as

\[
\rho^{(1,2)}(t) = \begin{pmatrix}
\frac{1}{4} & \frac{p}{2} - iu & \frac{p}{2} - iu & q - r \\
\frac{p}{2} + iu & \frac{1}{4} & q + r & \frac{p}{2} + iu \\
\frac{p}{2} + iu & q + r & \frac{1}{4} & \frac{p}{2} + iu \\
q - r & \frac{p}{2} - iu & \frac{p}{2} - iu & \frac{1}{4}
\end{pmatrix}.
\]

(14)

It is obvious that the density matrix elements \( \rho^{(1,2)}_{i,j}(t) \) \( (i, j = 1, 2, 3, 4) \) satisfy the relationship \( \rho^{(1,2)}_{i,j}(t) = \rho^{(1,2)}_{j,i}(t) \). Such matrices are called CS [18]. One can show that the general expression for the Hermitian CS 4 × 4 matrix is

\[
\rho = \begin{pmatrix}
p_1 & p_2 + ip_3 & p_4 + ip_5 & p_6 \\
p_2 - ip_3 & \frac{1}{2} - p_1 & p_7 & p_4 - ip_5 \\
p_4 - ip_5 & p_7 & \frac{1}{2} - p_1 & p_2 - ip_3 \\
p_6 & p_4 + ip_5 & p_2 + ip_3 & p_1
\end{pmatrix}.
\]

(15)
where $p_i$ ($i = 1, \ldots, 7$) are real parameters. Because the density matrix must be non-negatively defined, all its eigenvalues are greater or equal to zero:

$$\Lambda_{1,2} = \frac{1}{2}(p_6 + p_7 + 1) \pm \sqrt{\frac{1}{4} (2p_1 + p_6 - p_7 - 1/2)^2 + (p_2 + p_4)^2 + (p_3 + p_5)^2} \geq 0,$$

$$\Lambda_{3,4} = \frac{1}{2}(1/2 - p_6 - p_7) \pm \sqrt{\frac{1}{4} (2p_1 - p_6 + p_7 - 1/2)^2 + (p_2 - p_4)^2 + (p_3 - p_5)^2} \geq 0. \quad (16)$$

These inequalities restrict the range of values for the parameters $p_1, \ldots, p_7$.

3. Calculation of the correlation functions

To calculate the correlation functions (9)–(13), we use the commutation relations for spin-1/2
\[ e^{-i\alpha I_z I} e^{i\beta I_z I} = e^{-i\alpha (2I_z - 1/2) I}, \quad (17) \]
where $I^z = I_x + iI_y$. As a result, the expressions under the trace sign in equations (7)–(12) can be represented as products of two operators. One of them depends only on spins 1 and 2, while the other operator depends on spins 3, 4, ..., $N$ and equals the product of one-spin operators. Such approach allows us to rewrite the correlation functions as follows:

$$p = \frac{1}{2} \tanh \frac{\beta}{2} \cos^{N-1}(at), \quad (18)$$

$$q + r = \frac{1}{4} \tanh^2 \frac{\beta}{2}, \quad q - r = \frac{1}{4} \tanh^2 \frac{\beta}{2} \cos^{N-2}(2at) \quad (19)$$

$$u = \frac{1}{4} \tanh \frac{\beta}{2} \cos^{N-2}(at) \sin(at). \quad (20)$$

The correlation functions (18)–(20) depend on time periodically and do not decay up to zero at $t \to \infty$. This is because the coupling constants for all spin pairs are the same in the considered model.

4. Entanglement of spin pairs in a nanopore

In our model, elements of the CS matrix of equation (15) are given by the expressions

$$p_1 = \frac{1}{4}, \quad p_2 = p_4 = \frac{p}{2}, \quad p_3 = p_5 = -u, \quad p_6 = q - r, \quad p_7 = q + r. \quad (21)$$

Using equation (A.9), one can find that for the system with the density matrix (14) the parameters $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ needed to calculate the concurrence are

$$\lambda_1 = \frac{\sqrt{z}}{2} + w, \quad \lambda_2 = \frac{\sqrt{z}}{2} - w, \quad \lambda_3 = \frac{1}{4} - q - r, \quad \lambda_4 = \frac{1}{4} - q + r, \quad (22)$$

where

$$z = \frac{(1 + 4q)^2 - 16p^2}{4}, \quad w = \sqrt{r^2 + 4u^2}. \quad (23)$$

Using equations (18)–(20), (22) and (23) one can show that $\lambda_1$ is the maximal value in the set \{$\lambda_1, \lambda_2, \lambda_3, \lambda_4$\}. Then the concurrence (see equation (A.4)) is

$$C(\rho^{(1,2)}) = \max \left\{0, 2(\sqrt{r^2 + 4u^2} + q) - \frac{1}{2} \right\}. \quad (24)$$
The dependence of the concurrence on the inverse temperatures and dimensionless time for different numbers of spins is represented in figure 2. It is evident from figure 2 that the concurrence equals zero at $t = 0$. Then the concurrence emerges and its evolution has periodic character. One can see in figure 2 that the concurrence disappears at shorter times (inside a period $\pi/a$) when the number of the spins increases. In particular, one can obtain from equation (24) that the concurrence is absent in the system at $N \to \infty$.

5. Quantum discord in spin pairs in a nanopore

An investigation of the quantum discord in the system described by the density matrix (14) is a technically complex problem. First we consider the case $N \gg 1$, $at \neq \pi l$, $2at \neq \pi n$ ($l$, $n$ are positive integers). Then the correlation functions (18)–(20) are getting simple and equal

$$ p = u = 0, \quad q = r = \frac{1}{8} \tanh^2 \frac{\beta}{2}. \quad (25) $$

Thus, the density matrix (14) has the diagonal Bell form for which the discord $Q$ was evaluated in [10]. Using the technique [10], we find that the discord $Q$ for the spin pair in a nanopore equals

$$ Q = \frac{1}{4} \left[ (1 + 8q) \log_2 (1 + 8q) + (1 - 8q) \log_2 (1 - 8q) \right] $$

$$ - \frac{1 + 4q}{2} \log_2 (1 + 4q) - \frac{1 - 4q}{2} \log_2 (1 - 4q). \quad (26) $$
Figure 3. The dependences of the quantum and geometric discord for a spin pair in a nanopore on the temperature at \( N \gg 1 \), at \( a \neq \pi l \), \( 2a \neq \pi n \) \((l, n\) are positive integers). The Larmour frequency \( \omega_0 = 2\pi \times 500 \times 10^{6} \text{s}^{-1} \).

At a low temperature \( T \to 0 \) \((\beta \to \infty)\), the asymptotic behavior of the discord is determined as

\[
Q \approx \frac{3}{4} \log_2 \frac{4}{3} - \frac{\beta e^{-\beta}}{\sqrt{2}}. \tag{27}
\]

Note that for the temperature limit \( T = 0 \), \((\beta = \infty)\), we have the expression \( Q = \frac{3}{4} \log_2 \frac{4}{3} \cong 0.3113 \). Surprisingly, the same analytical result was obtained in [22] for another special mixed state in which four nonorthogonal states of the first qubit are correlated with four nonorthogonal states of the second qubit (see equation (1) and page 2 of [22]). At a high temperature \( T \to \infty \) \((\beta \to 0)\), the asymptotic behavior of the quantum discord is the following:

\[
Q \approx \frac{1}{128 \ln 2} \beta^4 = \frac{1}{128 \ln 2} \left( \frac{\hbar \omega_0}{k_B T} \right)^4. \tag{28}
\]

The dependence of the quantum discord on the temperature is represented in figure 3. One can see from figure 3 that quantum correlations are relatively large only at milli-kelvin temperatures for the Larmour frequency \( \omega_0 = 2\pi \times 500 \times 10^{6} \text{s}^{-1} \).

The considered model allows us to investigate some peculiarities of the time evolution of the discord. At the time moments \( t_l = (1 + 2l)\pi / (2a) \), \( l = 0, 1, 2, \ldots \), the correlation functions are

\[
p = u = 0, \quad q = \frac{1}{8} \tanh^2 \frac{\beta}{2} [1 + (-1)^{N-2}], \quad r = \frac{1}{8} \tanh^2 \frac{\beta}{2} [1 - (-1)^{N-2}]. \tag{29}
\]

Essentially one of the correlation functions, \( q \) or \( r \), equals zero depending on the parity of the number of spin-carrying molecules in the nanopore. Here the structure of the density matrix coincides with the so-called \( X \)-matrix for which the method of the calculation of the discord was worked out in [11]. The method [11] allows us to conclude that the quantum discord equals zero at the time moments \( t_l = (1 + 2l)\pi / (2a) \) \((l = 0, 1, 2, \ldots)\). Such is the case, because one of the correlation functions equals zero in these time moments. Thus, we have ‘flickering’ quantum discord which equals zero periodically.
The geometric discord can be expressed through $T$ where

\[ k = 8 \]

The geometric discord \cite{23} simplifies calculations of the quantum discord. In particular, it allows us to find the discord for the CS matrix \eqref{15}. Using the Pauli matrices $\sigma_i^j (j = 1, 2; i = x, y, z)$, we can rewrite the density matrix \eqref{15} in the Bloch form:

\[
\rho = \frac{1}{4} \left[ 1 + \sum_{i,j=1}^{3} T_{ij} \sigma_i^j \otimes \sigma_j^i + \sum_{i=1}^{3} x_i \sigma_i^i \otimes 1 + \sum_{i=1}^{3} y_i 1 \otimes \sigma_i^i \right]
\]

where $T$ is the correlation matrix, equal to

\[
T = \begin{pmatrix}
2(p_6 + p_7) & 0 & 0 \\
0 & 2(p_7 - p_6) & -4p_5 \\
0 & -4p_3 & 4p_1 - 1
\end{pmatrix}
\]

and $\vec{x}$ and $\vec{y}$ are the Bloch vectors

\[
\vec{x}_T = (4p_4, 0, 0), \quad \vec{y}_T = (4p_2, 0, 0).
\]

The geometric discord $Q_\rho$ for the two-qubit system is given by \cite{23}

\[ Q_\rho = \frac{1}{2} ||\vec{x}||^2 + ||T||^2 - k_{max}, \]

where the spheric (Hilbert–Schmidt) norm $||A||$ is

\[ ||A|| = \sqrt{\text{Tr}(AA^T)}, \]

and $k_{max}$ is the maximal eigenvalue of the matrix $K = \vec{x} \vec{x}^T + TT^T$.

The geometric discord can be expressed through $k_1, k_2, k_3$ as

\[ Q_\rho = \frac{1}{2}(k_1 + k_2 + k_3 - k_{max}). \]

Simple calculations yield the eigenvalues $k_1, k_2, k_3$ of the matrix $K$:

\[
k_1 = 16p_2^2 + 4(p_6 + p_7)^2,
\]

\[
k_{2,3} = 8p_2^2 + 2(p_7 - p_6)^2 + 8p_3^2 + \frac{1}{4}(4p_1 - 1)^2
\]

\[ \pm \left[ 8p_2^2 + 2(p_7 - p_6)^2 - 8p_3^2 - \frac{1}{4}(4p_1 - 1)^2 \right]^{1/2} + 16p_3(4p_1 - 1) - 1 + 2p_3(p_7 - p_6)^2 \]

In the case of a nanopore, using \eqref{21}, we can obtain the expressions

\[
k_1 = 4(p^2 + 4q^2),
\]

\[
k_{2,3} = 8[2a^2 + r^2 \pm r\sqrt{r^2 + 4a^2}].
\]

As a result, the geometric discord has the form

\[ Q_\rho = \frac{1}{8} \tanh^4 \frac{\beta}{2}. \]

In the limit $T \to 0$, the geometric discord $Q_\rho = 1/8 = 0.125$. At a high temperature $T \to \infty, (\beta \to 0)$, the asymptotic behavior of the geometric discord is the following:

\[ Q_\rho \approx \frac{1}{128} \beta^4 = \frac{1}{128} \left( \frac{\hbar \omega_0}{k_B T} \right)^4. \]
7. Conclusion

We investigated the entanglement and quantum discord in a nanopore filled with a gas of spin-carrying molecules (atoms). Even when the entanglement is absent, the quantum discord can reach large values in the considered system. It reveals significant quantum correlations in the system. They exhibit ‘flickering’ character and equal zero periodically in the process of the time evolution of the system.

The density matrix in the considered model belongs to the so-called CS matrices. We evaluated the analytic expression for the concurrence of a general two-qubit CS density matrix. We studied the geometric discord for systems with CS density matrices and obtained an analytic expression for the geometric discord in the considered model.

The model under question confirms once more that entanglement describes only a part of quantum correlations, while the discord is a measure of total quantum correlations [1].

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Appendix. Entanglement of the CS 4 × 4 density matrix

To calculate the entanglement for the general two-qubit density matrix, one should find the ‘spin-flip transformed’ density matrix which is [19]

\[
\tilde{\rho} = (\sigma_1^y \otimes \sigma_2^y) \rho^* (\sigma_1^y \otimes \sigma_2^y),
\]

(A.1)

where \(\rho^*\) is the complex conjugate matrix to \(\rho\) in the standard basis \{|00\}, |01\}, |10\}, |11\}\], and \(\sigma_j^y (j = 1, 2)\) is the Pauli matrix. Then it is necessary to calculate the concurrence \(C(\rho)\) which determines unambiguously the entanglement \(E(\rho)\) [19]

\[
E(\rho) = H \left( \frac{1 + \sqrt{1 - C^2(\rho)}}{2} \right),
\]

(A.2)

where \(H(x)\) is the Shannon function [25]

\[
H(x) = -x \log_2 x - (1 - x) \log_2 (1 - x).
\]

(A.3)

The concurrence is given as [19]

\[
C(\rho) = \max \{0, 2 \lambda - \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}
\]

\[
\lambda = \max \{\lambda_1, \lambda_2, \lambda_3, \lambda_4\},
\]

(A.4)

where \(\lambda_1, \lambda_2, \lambda_3, \lambda_4\) are the square roots of the eigenvalues of the matrix product \(\rho \tilde{\rho}\).

One can show that the matrix \(\tilde{\rho}\) is a CS matrix if the density matrix \(\rho\) is a CS one. It means that the matrix \(\rho \tilde{\rho}\) is also a CS one. Under the orthogonal transformation

\[
S = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 0 & 0 & 1 \\
0 & 1 & 1 & 0 \\
0 & 1 & -1 & 0 \\
1 & 0 & 0 & -1
\end{pmatrix} = S^T,
\]

(A.5)
any 4 \times 4 CS matrix takes the block-diagonal form consisting of two 2 \times 2 subblocks. As a result, the square roots of the eigenvalues of the matrix product \( \rho \tilde{\rho} \) can be written as follows:

\[
\lambda_{1,2} = \frac{1}{\sqrt{2}} \left( (p_1 + p_6)^2 - 2(p_2 + p_4)^2 + 2(p_3 + p_5)^2 + \left( \frac{1}{2} - p_1 + p_7 \right)^2 \right) \\
\pm \sqrt{\left[ (2p_1 + p_6 - \frac{1}{2} - p_7)^2 + 4(p_3 + p_5)^2 \right] \left[ \left( \frac{1}{2} + p_6 + p_7 \right)^2 - 4(p_2 + p_4)^2 \right]}^{\frac{1}{2}},
\]

(A.6)

\[
\lambda_{3,4} = \frac{1}{\sqrt{2}} \left( (p_1 - p_6)^2 - 2(p_2 - p_4)^2 + 2(p_3 - p_5)^2 + \left( \frac{1}{2} - p_1 - p_7 \right)^2 \right) \\
\pm \sqrt{\left[ (2p_1 - p_6 - \frac{1}{2} + p_7)^2 + 4(p_3 - p_5)^2 \right] \left[ \left( \frac{1}{2} - p_6 - p_7 \right)^2 - 4(p_2 - p_4)^2 \right]}^{\frac{1}{2}}.
\]

(A.7)

Using identities

\[
2\left[ (p_1 + p_6)^2 + \left( \frac{1}{2} - p_1 + p_7 \right)^2 \right] = (2p_1 + p_6 - \frac{1}{2} - p_7)^2 + \left( \frac{1}{2} + p_6 + p_7 \right)^2,
\]

\[
2\left[ (p_1 - p_6)^2 + \left( \frac{1}{2} - p_1 - p_7 \right)^2 \right] = (2p_1 - p_6 - \frac{1}{2} + p_7)^2 + \left( \frac{1}{2} - p_6 - p_7 \right)^2,
\]

(A.8)

we can rewrite finally \( \lambda_1, \lambda_2, \lambda_3, \lambda_4 \) as

\[
\lambda_1 = \frac{1}{2} \left[ \sqrt{\left( 2p_1 + p_6 - \frac{1}{2} - p_7 \right)^2 + 4(p_3 + p_5)^2} + \sqrt{\left( \frac{1}{2} + p_6 + p_7 \right)^2 - 4(p_2 + p_4)^2} \right],
\]

\[
\lambda_2 = \frac{1}{2} \left[ \sqrt{\left( 2p_1 + p_6 - \frac{1}{2} - p_7 \right)^2 + 4(p_3 + p_5)^2} - \sqrt{\left( \frac{1}{2} + p_6 + p_7 \right)^2 - 4(p_2 + p_4)^2} \right],
\]

\[
\lambda_3 = \frac{1}{2} \left[ \sqrt{\left( 2p_1 + p_6 - \frac{1}{2} + p_7 \right)^2 + 4(p_3 - p_5)^2} + \sqrt{\left( \frac{1}{2} - p_6 + p_7 \right)^2 - 4(p_2 + p_4)^2} \right],
\]

\[
\lambda_4 = \frac{1}{2} \left[ \sqrt{\left( 2p_1 + p_6 - \frac{1}{2} + p_7 \right)^2 + 4(p_3 - p_5)^2} - \sqrt{\left( \frac{1}{2} - p_6 + p_7 \right)^2 - 4(p_2 + p_4)^2} \right].
\]

(A.9)

These relationships together with equations (A.2)–(A.4) give an analytical formula only through the square radicals for calculating the entanglement of formation for the arbitrary two-qubit density matrix (15).

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