Relationship between probabilities of the state transfers and entanglements in spin systems with simple geometrical configurations.

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Abstract

In this paper we derive analytical relations between probabilities of the excited state transfers and entanglements calculated by both the Wootters and positive partial transpose (PPT) criteria for the arbitrary spin system with single excited spin in the external magnetic field and Hamiltonian commuting with $I_z$. We apply these relations to study the arbitrary state transfers and entanglements in the simple systems of nuclear spins having two- and three-dimensional geometrical configurations with $XXZ$ Hamiltonian. It is shown that High-Probability State Transfers (HPSTs) are possible among all four nodes placed in the corners of the rectangle with the proper ratio of sides as well as among all eight nodes placed in the corners of the parallelepiped with the proper ratio of sides. Entanglements responsible for these HPSTs have been identified.

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I. INTRODUCTION

This paper is devoted to the problem of the high probability state transfer (HPST) among many nodes of the spin system and to the relationship between probabilities of HPSTs and entanglements responsible for these transfers. We consider nuclear spin-1/2 systems with XXZ-Hamiltonian and different geometrical configurations. However, the above relationship remains valid for any Hamiltonian $H$ commuting with the total projection operator $I_z$.

By ”state transfer” we mean the following phenomenon \[2, 3\]. Consider the chain of spin-1/2 with dipole-dipole interaction in the strong external magnetic field. Let all spins be directed along the external magnetic field except the $i$th one whose initial state is arbitrary. In other words, let the spin system be prepared in the state

$$\psi_{ii} = \cos(\theta/2)|0\rangle + e^{-i\phi}\sin(\theta/2)|i\rangle,$$

where $|0\rangle$ is a ground state, i.e. all spins are directed along the magnetic field and $|i\rangle$ means that only $i$th spin is directed opposite to the external magnetic field (i.e. $i$th spin is excited). Let the energy of the ground state be zero. If the state becomes

$$\psi_{ij} = \cos(\theta/2)|0\rangle + e^{-i\phi}\sin(\theta/2)|j\rangle$$

with $|\tilde{f}_{ij}| = 1$ at the time moment $t = t_{ij}$ then we say that the initial state has been transferred from the $i$th to the $j$th node with the phase shift $\tilde{\Gamma}_{ij} = \arg\tilde{f}_{ij}$. Since $|\tilde{f}_{ij}| = 1$, all other spins are directed along the field at $t = t_{ij}$.

Here $\tilde{f}_{ij} = f_{ij}(t_{ij})$ and $f_{ij}(t)$ is the transition amplitude of an excited state from the $i$th to the $j$th node: $f_{ij}(t) = \langle j|e^{-itH}|i\rangle$. It is known \[2\] that the effectiveness of the state transfer between the $i$th and $j$th nodes may be characterised by the fidelity $F_{ij}(t)$

$$F_{ij}(t) = \frac{|f_{ij}(t)| \cos \Gamma_{ij}(t)}{3} + \frac{|f_{ij}(t)|^2}{6} + \frac{1}{2}.$$  \hspace{1cm} (1)

We see that the fidelity is maximal for $\Gamma_{ij} = 0 \mod 2\pi$. If the external magnetic field is homogeneous and we are interested in the state propagation between two nodes, say between $s$th and $r$th nodes at the moment $t_{rs}$, then condition $\tilde{\Gamma}_{rs} = \Gamma_{rs}(t_{rs}) = 0$ may be simply satisfied by the proper choice of the constant magnetic field value \[2\]. In this case the fidelity $\tilde{F}_{rs} = F_{rs}(t_{rs})$ takes maximal value together with absolute value of the transition amplitude $|\tilde{f}_{rs}| = |f_{rs}(t_{rs})|$. For this reason, namely $|\tilde{f}_{rs}|$ (rather then $\tilde{F}_{rs}$) is considered as the characteristic of the state transfer in many refs, see, for instance, \[3, 4, 5\]. It is clear that $|\tilde{f}_{rs}(t)|$ may be replaced by the probability of the excited state transfer $P_{rs}(t) = |f_{rs}(t)|^2$ and $\tilde{P}_{rs} = |\tilde{f}_{rs}|^2$ \[1, 6\].

More general case of the HPSTs among many nodes of the $N$ node spin chain has been studied in \[6\]. In this case any particular state transfer between the $i$th and $j$th nodes is
associated with its own phase shift $\bar{\Gamma}_{ij}, i, j = 1, \ldots, N$ (note that $i$ may be equal to $j$ which means return of the state to the $i$th node). However, it is important that all these shifts may be eliminated using magnetic field properly depending on time [6]. For this reason the effectiveness of the state transfer between the $i$th and the $j$th nodes may be equivalently described either by the fidelity $\bar{F}_{ij}$ or by the probability of the excited state transfer $\bar{P}_{ij}$ even in this generalized case. Namely optimization of $\bar{P}_{ij}$ allows us to find all necessary parameters of the geometrical spin configuration providing HPSTs among many nodes while phases $\bar{\Gamma}_{ij}$ may be removed by the appropriate time dependent external magnetic field as it was done in [6]. For this reason, we will study the probability of the single excited state transfer instead of the fidelity (1) of arbitrary state transfer in the subsequent sections of this paper. This means that the spin $1/2$ system of $N$ nodes is prepared in the initial state

$$\psi_{ii} = |i\rangle,$$

where $i$ takes one of the values $i = 1, \ldots, N$.

The problem of the perfect state transfers (PSTs), HPSTs and entanglements in the spin systems is very attractive and different aspects of this problem have been studied in many details [3, 4, 5, 7, 8, 9, 10, 11, 12, 13, 14, 16]. Nevertheless, most of the results are devoted to the linear and circular spin chains, which are considered as communication channels in the quantum information systems. Different Hamiltonians describing these chains have been studied, such as $XY$, $XYZ$, Heisenderg Hamiltonians. Usually, the approximation of the nearest neighbour interactions is taken as a basic tool for such studies. Note, that this is a good approximation in the case of, for instance, exchange interaction, when coupling constants decrease exponentially with increase in the distance. However, this approximation is not satisfactory for the spin systems with dipole-dipole interaction (such as nuclear spin systems in solids) and a wide spread of the coupling constants.

Most efforts have been turned to the study of two phenomena: the state transfer along chains [2, 3, 4, 5, 7, 8, 11, 13] and two-qubit entanglements in chains (such as entanglement between end nodes or between nearest nodes [2, 8, 12, 15]). The Wootters criterion is applicable in this case allowing one to describe the entanglement in terms of so-called concurrence [22]. It is important that there is an analytical dependence of the concurrence between two nodes on the probability of the state transfer between these nodes which was derived in [4, 17] for the system with single excited spin. However, complicated system of
N spins exhibits entanglements not only between two nodes, but also between arbitrary two subsystems. These entanglements may be effectively described by the positive partial transpose (PPT) criterion \[18,19\] introducing so-called double negativity as a measure of entanglement. Explicit relations of the double negativity associated with two subsystems on the probabilities of the excited state transfers between different nodes will be derived in this paper for the spin system with single excitation.

Although the PST would be preferable in the quantum communication chains, it is hardly realizable in experiments with long chains because of the following two basic reasons:

1. Theoretical prediction of the PST in the long chains is associated with the approximation of the Hamiltonian by the nearest neighbour interaction, while the complete Hamiltonian must be used in practice. As we have already noted, this approximation is well applicable to the systems with exchange interaction and is not always valid for the systems with dipole-dipole interaction.

2. Coupling constants may not be always known as accurately as we want in the case of both exchange and dipole-dipole interaction.

Thus, HPST between different nodes of the spin system \[1\] seems to be more realistic in comparison with PST.

In this paper we will study the spin systems with dipole-dipole interaction in the external magnetic field with single excited node described by the XXZ Hamiltonian. We will study the spin systems with different geometrical configurations of nodes and initial state \[2\] which may provide the HPSTs of the excited state among all of nodes. We will show which parts of the spin system must be entangled in order to provide each of these transfers. The study of two- and three-dimensional spin systems is important because they are more compact and consequently they are more promising as quantum registers and/or short communication channels. It will be shown in this paper, that namely such configurations (more precisely, spin configurations with nodes placed in the corners of either rectangle or parallelepiped) provide the HPSTs among several different nodes of the spin system during relatively short time interval in comparison with the line systems \[6\] which is important for the development of the quantum information systems and/or short communication channels. Our study is also stimulated by the experiments on the quantum information processes in solids \[24,25\].
This paper is organized as follows. In Sec.II (and in Appendices A and B) we obtain analytical dependence of the either concurrences (Wootters criterion) or double negativities (PPT criterion) between different two subsystems of the spin system on the probabilities of the state transfers, generalizing the results of refs. [4, 17]. In Sec.IV we consider the simplest one-dimensional model of two nodes where the relationship between entanglement and probability of the state transfer is most transparent and an equivalent result may be obtained using either the Wootters [4] or PPT criterion. Two-dimensional spin systems will be considered in Sec.V, see also Appendix C. We arrange HPST among all nodes of the four-node spin system (rectangular geometry) and show that the external magnetic field directed along one of the sides of the rectangle decreases significantly (more then twice) the time intervals needed for the HPSTs among nodes in comparison with the case when the field is perpendicular to the plane of the rectangle. Similar study of the three-dimensional eight-node system (with spins placed in the corners of the parallelepiped) is represented in Sec.VI, see also Appendix D. It is evident that HPSTs may not be effectively arranged in the arbitrary system of nodes. Detailed algorithm allowing one to obtain parameters of the rectangle spin system (namely, the ratio of sides of the rectangle) with the HPSTs among all four nodes is given in Appendix C. Particular example of the eight-node three-dimensional spin system with HPSTs among all nodes (parallelepiped configuration) is represented in Appendix D.

II. SPIN-1/2 SYSTEMS WITH SINGLE EXCITED NODE AND XXZ HAMILTONIAN

We study the HPSTs and entanglements among the nodes of the spin-1/2 system in the external magnetic field described by the XXZ Hamiltonian with zero Larmor frequencies:

\[ \mathcal{H} = \sum_{i,j=1}^{N} D_{ij} (I_{i,x} I_{j,x} + I_{i,y} I_{j,y} - 2I_{i,z} I_{j,z}), \]

\[ D_{ij} = \frac{1 - 3 \cos^2 \theta_{ij}}{r_{ij}^3} \gamma^2 \hbar, \]

where \( \gamma \) is gyromagnetic ratio, \( r_{ij} \) is the distance between \( i \)th and \( j \)th spins, \( \theta_{ij} \) is the angle between the external magnetic field and \( r_{ij} \), \( I_{i,\alpha} \) is the projection operator of the \( i \)th spin on the \( \alpha \) axis, \( \alpha = x, y, z \), \( D_{ij} \) are the dipole-dipole coupling constants. This Hamiltonian
describes the secular part of the dipole-dipole interaction in the strong external magnetic field [20]. We denote $D_n \equiv D_{n,n+1}$, $n = 1, \ldots, N - 1$. Taking into account the definition of $D_{ij}$, for description of the spin system with arbitrary geometrical configuration we use the coordinates of each node, i.e. the set of the following triads

$$(x_i, y_i, z_i), \ i = 1, \ldots, N, \ (5)$$

so that

$$r_{ij} = \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2 + (z_j - z_i)^2}, \ (6)$$

$$\cos^2 \theta_{ij} = \frac{(z_j - z_i)^2}{r_{ij}^2}.$$  

It is important, that the Hamiltonian (3) commutes with $I_z$ ($z$-projection of the total spin):

$$[\mathcal{H}, I_z] = 0. \ (7)$$

This means that both $\mathcal{H}$ and $I_z$ have the common set of eigenvectors. It is convenient to write the eigenvectors of the operator $I_z$ in terms of the Dirac notations. Let

$$|n_1 \ldots n_N\rangle \ (8)$$

be the eigenvector of the operator $I_z$ where the $i$th spin is directed opposite to the external magnetic field if $n_i = 1$ and along the field if $n_i = 0$. For the sake of brevity, hereafter we will use notations $|0\rangle$ for the eigenvector associated with the state when all spins are directed along the external field and $|i_1 \ldots i_k\rangle$ for the eigenvectors associated with the state when $i_1$, ..., $i_k$th spins are directed opposite to the external field, i.e. these spins are excited. Thus eigenvector $|i\rangle$ means that only $i$th spin is excited. Using these notations, the basis (8) may be ordered as follows:

$$|i_1\rangle, \ |0\rangle, \ |i_1i_2\rangle, \ldots, \ |i_1 \ldots i_N\rangle, \ i_1 < i_2 < \ldots < i_N, \ i.e. \ (9)$$

$$i_1 = 1, \ldots, N, \ i_k = i_{k-1} + 1, \ldots, N, \ k = 2, \ldots, N.$$

The matrix representation $H$ of the Hamiltonian $\mathcal{H}$ in basis (9) gets the following diagonal block structure:

$$H = \text{diag}(H_1, H_0, H_2, H_3, \ldots, H_N), \ (10)$$
where the block $H_i$ is associated with the set of states of the whole spin system having $i$ spins directed opposite to the field.

Hereafter we will study the problem of the single excited quantum state transfer among nodes of the spin-$1/2$ system with the XXZ Hamiltonian in the external magnetic field. We say, that the $k_0$th node is excited initially. It is important that only the block $H_1$ is nonzero in this case:

$$H_1 = \frac{1}{2}(D - \Gamma I),$$

(11)

$$D = \begin{pmatrix}
A_{11} & D_1 & D_{13} & \cdots & D_{1(N-2)} & D_{1(N-1)} & D_{1N} \\
D_1 & A_{22} & D_2 & \cdots & D_{2(N-2)} & D_{2(N-1)} & D_{2N} \\
D_{13} & D_2 & A_{33} & \cdots & D_{3(N-3)} & D_{3(N-1)} & D_{3N} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
D_{1(N-2)} & D_{2(N-2)} & D_{3(N-2)} & \cdots & A_{(N-2)(N-2)} & D_{j-1} & D_{(N-2)N} \\
D_{1(N-1)} & D_{2(N-1)} & D_{3(N-1)} & \cdots & D_{j-1} & A_{(N-1)(N-1)} & D_j \\
D_{1N} & D_{2N} & D_{3N} & \cdots & D_{(N-2)N} & D_j & A_{NN}
\end{pmatrix},$$

$$A_{nn} = 2 \sum_{i=1}^{N} D_{in}, \quad \Gamma = \sum_{i,j=1}^{N} D_{ij},$$

where $I$ is $N \times N$ identity matrix. This simplification of the Hamiltonian allows one to

1. derive explicit analytical dependence of concurrence and/or double negativity (as measures of entanglement between any two subsystems of the spin system) on the probabilities of the state transfers between different nodes of the system, which is hardly realizable in the case of the Hamiltonian with general structure (10);

2. perform the numerical simulations of the state transfers in the big spin systems, which is hardly realizable in general case [21].

Hereafter we will use the dimensionless time $\tau$, coupling constants $d_{nm}$ and distances $\xi_{nm}$:

$$\tau = D_{12} t, \quad d_{nm} = \frac{D_{nm}}{D_{12}}, \quad \xi_{nm} = \frac{r_{nm}}{r_{12}}.$$

(12)

Using definitions (12) and taking into account that $D_{12} = \gamma^2 \hbar / r_{12}^3$ in all our examples, Hamiltonian (3) may be written as follows:

$$\mathcal{H} = D_{12} \mathcal{H}, \quad \mathcal{H} = \sum_{i,j=1}^{N} d_{ij}(I_{i,x}I_{j,x} + I_{i,y}I_{j,y} - 2I_{i,z}I_{j,z}),$$

(13)
\[ d_{ij} = \frac{1 - 3 \cos^2 \theta_{ij}}{\mathcal{E}_{ij}^3}. \] (14)

III. PROBABILITIES OF THE STATE TRANSFERS AND ENTANGLEMENTS BETWEEN DIFFERENT SUBSYSTEMS OF THE ARBITRARY NUCLEAR SPIN SYSTEM

First of all, in order to establish the relationships between probabilities of the state transfers among nodes and entanglements among them we will need density matrix \( \rho \) introduced as follows:

\[ \rho = e^{-i\vec{H}\tau}|k_0\rangle\langle k_0|e^{i\vec{H}\tau}, \] (15)

where \( k_0 \) means that \( k_0 \)th spin was directed opposite to the field initially. Only such initial states will be considered hereafter. It is important, that this matrix may be written in the following block form using basis (9)

\[
\rho = \begin{pmatrix}
A & 0_{N,2^N-N} \\
0_{2^N-N,N} & 0_{2^N-N,2^N-N}
\end{pmatrix},
A = \begin{pmatrix}
a_{11} & \cdots & a_{1N} \\
\vdots & \ddots & \vdots \\
a_{N1} & \cdots & a_{NN}
\end{pmatrix},
\] (16)

where \( 0_{n,m} \) means \( n \times m \) zero matrix and nonzero elements \( a_{ij} \) are defined as follows:

\[ a_{ij} \equiv \langle i|\rho|j\rangle = f_{koi}f^*_{koj}, \quad a_{ji} = a_{ij}^*, \quad i,j = 1,\ldots,N, \] (17)

where \( f_{nm} \) are transmission amplitudes,

\[ f_{nm} = \langle m|e^{-i\vec{H}\tau}|n\rangle = \sum_{j=1}^{N} u_{nj}u_{mj}e^{-i\lambda_j\tau/2}, \quad f_{nm} = f_{mn}. \] (18)

Here \( u_{ij}, i,j = 1,\ldots,N, \) are the components of the normalized eigenvector \( u_j \) corresponding to the eigenvalue \( \lambda_j \) of the matrix \( D: Du_j = \lambda_j u_j. \)

A. Probability of the state transfer from the \( k_0 \)th to the \( m \)th node of the \( N \)-node spin chain

The probability \( P_{km} \) of the state transfer from the \( k_0 \)th to the \( m \)th node as a function of time is defined by the diagonal element \( a_{mm} \) of the density matrix. In fact [11],

\[ P_{km}(\tau) = |\langle m|e^{-i\vec{H}\tau}|k_0\rangle|^2 = |f_{km}|^2 \equiv a_{mm}. \] (19)
Throughout this paper we will use notations $\bar{P}_{km}$ and $\tau_{km}$ for the probability of the HPST and for the time interval required for the HPST from the $k_0$th to the $m$th node of the $N$-node chain:

$$\bar{P}_{km} \equiv P_{km}(\tau_{km}).$$

(20)

By our definition, the state transfer from the $k_0$th node to the $m$th node will be referred to as HPST if

$$\bar{P}_{km} \geq P_0.$$

(21)

The value $P_0$ is conventional, in our paper we take $P_0 = 0.9$. In addition, there is an important parameter of the HPSTs, namely the time interval $T$ during which the excited state may be detected in all nodes of the system [1]:

$$T = \max_{n=1,...,N} \tau_{kn}.$$

(22)

B. Wootters criterion: two-node entanglements in the spin system

It is well known that the entanglement between two nodes $i$ and $j$ of the $N$-node spin system may be described by the Wootters criterion [22], which introduces the so-called concurrence $C_{ij}$ as a measure of the entanglement:

$$C_{ij} = \max \left( 0, 2\lambda - \sum_{n=1}^{4} \lambda_n \right), \quad \lambda = \max(\lambda_1, \lambda_2, \lambda_3, \lambda_4).$$

(23)

Here $\lambda_n$, $n = 1, 2, 3, 4$ are the square roots of the eigenvalues of the $4 \times 4$ matrix $\tilde{\rho}_{ij}$

$$\tilde{\rho}_{ij} = (\tilde{\rho}_{ij}^{red})^{*} \rho_{ij}^{red},$$

(24)

where * means complex conjugate, $\rho_{ij}^{red}$ is the reduced density matrix, i.e.

$$\rho_{ij}^{red} = \text{Tr}_{n \neq i,j} \rho.$$

(25)

Matrix $\tilde{\rho}_{ij}^{red}$ is defined as

$$\tilde{\rho}_{ij}^{red} = \sigma^y_i \otimes \sigma^y_j \rho_{ij} \sigma^y_j \otimes \sigma^y_i.$$

(26)

After simple calculations (see Appendix [A] for details) one derives the following formula:

$$C_{ij} = 2|a_{ij}| = 2\sqrt{P_{kai}P_{kaj}}, \quad i \neq j.$$

(27)

This relation is valid for the system with any number of spins and for any Hamiltonian commuting with $I_z$ [4, 17].
C. PPT criterion: entanglement between two arbitrary subsystems

PPT criterion describes the entanglement between any two subsystems $A$ and $B$ of the system $S$ in terms of the so-called double negativity $N_{A,B}$ [19, 23], which is the absolute value of the doubled sum of the negative eigenvalues of the matrix $\rho_{AB}^{T_A}$:

$$\rho_{AB:C} = (\rho_{A,B})^{T_A}, \quad S = A \cup B \cup C,$$

where the reduced density matrix $\rho_{A,B}$ is defined as follows:

$$\rho_{A,B} = Tr_C \rho,$$

and $T_A$ means the transposition with respect to the subsystem $A$. In particular, the subsystem $C$ may be empty. It is important that one can write the explicit formulae for $N_{A,B}$ for the spin system in the magnetic field with single excited spin described by any Hamiltonian commuting with the total projection $I_z$ (see Appendix B for details):

$$N_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} = - \left( \sigma_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} - \sqrt{\sigma_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}}^2 + 4 \sum_{n=1}^{M_1} \sum_{m=1}^{M_2} |a_{i_n j_m}|^2} \right) = \left( \sigma_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} - \sqrt{\sigma_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}}^2 + 4 \sum_{n=1}^{M_1} \sum_{m=1}^{M_2} P_{i_n j_m} P_{j_n i_m}} \right),$$

where $A = \{i_1 \ldots i_{M_1}\}$, $B = \{j_1 \ldots j_{M_2}\}$,

$$\sigma_{i_1 \ldots i_{N_0}} = \sum_{n=1}^{N} a_{nn} = \sum_{n=1}^{N} P_{k_n n} = 1 - \sum_{n=1}^{N_0} P_{k_n n},$$

(we use the identity $\sum_{n=1}^{N} P_{k_n n} \equiv 1$). In particular,

$$N_{i,j} = - \left( \sigma_{ij} - \sqrt{\sigma_{ij}^2 + 4 |a_{ij}|^2} \right) = - \left( \sigma_{ij} - \sqrt{\sigma_{ij}^2 + 4 P_{k_i j} P_{k_j i}} \right) = - \left( 1 - P_{k_i j} - P_{k_j i} - \sqrt{(1 - P_{k_i j} - P_{k_j i})^2 + 4 P_{k_i j} P_{k_j i}} \right),$$

$$N_{i,rest} = 2 \sqrt{\sum_{j \neq i} |a_{ij}|^2} = 2 \sqrt{P_{k_i j} \sum_{j \neq i} P_{k_j o} = 2 \sqrt{P_{k_i j}(1 - P_{k_i j})}},$$

$$N_{i_1 i_2, j_1 j_2} = - \left( \sigma_{i_1 i_2 j_1 j_2} - \sqrt{\sigma_{i_1 i_2 j_1 j_2}^2 + 4 \sum_{n=1}^{2} \sum_{m=1}^{2} |a_{i_n j_m}|^2} \right) = - \left( \sigma_{i_1 i_2 j_1 j_2} - \sqrt{\sigma_{i_1 i_2 j_1 j_2}^2 + 4 (P_{k_{i_1 j_1} + P_{k_{i_2 j_2}}}(P_{k_{i_1 j_2} + P_{k_{i_2 j_1}}})) \right).$$
where $N_{i,\text{rest}}$ is double negativity associated with the entanglement between $i$th spin and the rest part of the spin system. It has the most simple expression depending only on $P_{k_0i}$.

Eqs. (30, 32-34) are simple relations between two important characteristics of the spin system: entanglement between arbitrary subsystems $A$ and $B$ (characterized by the double negativity) and probabilities of the state transfers from the $k_0$th node to other nodes of the subsystems $A$ and $B$. However, since (a) both these characteristics have rather complicated oscillating behaviour and (b) it is difficult to "inverse" relation (30) (i.e. to write probabilities as functions of double negativities), it is hard to get answers to the following questions:

1. Which geometrical configurations of the spin system provide HPSTs among all nodes?
2. Which entanglements are responsible for the HPSTs among different nodes of the spin system?

We will answer these questions for the particular systems of two, four and eight nodes in Secs. IV, V, VI.

IV. PERFECT STATE TRANSFER AND ENTANGLEMENT IN THE SYSTEM OF TWO NODES

It was shown in [3] that the probabilities for the excited state to be detected in the first and in the second nodes are following ($k_0 = 1$):

$$P_{11}(\tau) = \cos^2(\tau/2), \quad P_{12}(\tau) = \sin^2(\tau/2),$$  \hfill (35)

while the double negativity $N_{1,2}$ is defined by eq. (32):

$$N_{1,2}(\tau) \equiv C_{12}(\tau) = 2\sqrt{P_{11}(\tau)P_{12}(\tau)} = |\sin \tau|,$$  \hfill (36)

i.e. $P_{12} = 1$ at $\tau_{12} = \pi + 2\pi n, \ n = 0, \pm 1, \pm 2, \ldots$. We compare the graphs of $P_{11}(\tau)$ and $P_{12}(\tau)$ with double negativity $N_{1,2}(\tau)$, see Fig. [I] and observe that maxima of $N_{1,2}$ correspond to $P_{11} = P_{12} = 1/2$ while the minima of $N_{1,2}$ correspond to the maxima and minima of $P_{1i}$, $i = 1, 2$. This result is not surprising. In fact, the wave function associated with the two-node spin system is following:

$$\Psi(\tau) = f_{11}(\tau)|10⟩ + f_{12}(\tau)|01⟩, \quad P_{11} = |f_{11}|^2, \quad P_{12} = |f_{12}|^2.$$  \hfill (37)
However, if $P_{11} = 0$ or $P_{12} = 0$ this function reduces to $\Psi = |01\rangle$ or $\Psi = |10\rangle$ respectively. It is well known that these states are separable and their entanglements are zero. Vice-versa, if $P_{11} = P_{12} = 1/2$, then we have the singlet state $\Psi = 1/\sqrt{2}(|01\rangle - |10\rangle)$ which is the most entangled one.

We see from Fig.1 that the relation between the probability of the state transfer and the entanglement in the two-node system is very transparent. Moreover, we will see that relations between probabilities of state transfers and entanglements in more complicated systems are very similar. However, the system with $N > 2$ requires additional analysis in order to find such geometrical configuration of the spin system which allows the HPSTs among all nodes (or, may be, among some of them). Algorithms allowing us to perform this analysis for the rectangular system of four nodes and for the eight-node system with spins placed in the corners of the parallelepiped are represented in Appendices C and D.

V. HPSTS AND ENTANGLEMENTS IN THE SYSTEM OF FOUR NODES WITH RECTANGULAR GEOMETRY

We consider the rectangle shown in Fig.2. Here $\xi_{12} = 1$ while the length of another side is a parameter of the system, $\xi_{14} = b$. However, it is more convenient for us to introduce parameter

$$\delta = \frac{1}{b^3}. \quad (38)$$
FIG. 2: The rectangular system of four nodes. Here $\xi_{12} = 1$ while $\xi_{14}$ is a parameter: $\xi_{14} = b$. We will use parameter $\delta = 1/b^3$ instead of $b$.

Instead of $b$. Due to the symmetry of the spin system, matrix $D$ in eq. (11) reads:

$$
D = \begin{pmatrix}
2\tilde{\Gamma} & 1 & d_{13} & d_{14} \\
1 & 2\tilde{\Gamma} & d_{14} & d_{13} \\
d_{13} & d_{14} & 2\tilde{\Gamma} & 1 \\
d_{14} & d_{13} & 1 & 2\tilde{\Gamma}
\end{pmatrix}, \quad \tilde{\Gamma} = 1 + d_{13} + d_{14}.
$$

(39)

The structure of the matrix $D$ helps us to guess the following set of independent normalized eigenvectors:

$$
u_1 = 1/2(1 \ -1 \ 1 \ -1)^T, \quad u_2 = 1/2(1 \ 1 \ 1 \ 1)^T,$$

$$u_3 = 1/2(1 \ -1 \ -1 \ 1)^T, \quad u_4 = 1/2(1 \ 1 \ -1 \ -1)^T$$

with the appropriate eigenvalues:

$$
\lambda_1 = 2\tilde{\Gamma} - 1 - d_{14} + d_{13}, \quad \lambda_2 = 2\tilde{\Gamma} + 1 + d_{14} + d_{13},
$$

$$
\lambda_3 = 2\tilde{\Gamma} - 1 + d_{14} - d_{13}, \quad \lambda_4 = 2\tilde{\Gamma} + 1 - d_{14} - d_{13}.
$$

(41)

It is remarkable that

1. these eigenvectors do not depend on $b$ and

2. any component of any eigenvector is either 1 or -1.

Namely the latter property guaranties the HPSTs among all nodes of the four-node system.

Due to the symmetry of the rectangular cluster, it is enough to consider the case with initial excited state in the first node, i.e. $k_0 = 1$. Eq. (19) yields explicit expressions for the
probabilities $P_{ij}$:

$$P_{11} = \frac{1}{4} \left( 1 + \cos \tau \left( \cos(d_{14}\tau) + \cos(d_{13}\tau) \right) + \cos(d_{14}\tau) \cos(d_{13}\tau) \right),$$

(42)

$$P_{12} = \frac{1}{4} \left( 1 - \cos \tau \left( \cos(d_{14}\tau) + \cos(d_{13}\tau) \right) + \cos(d_{14}\tau) \cos(d_{13}\tau) \right),$$

$$P_{13} = \frac{1}{4} \left( 1 + \cos \tau \left( \cos(d_{14}\tau) - \cos(d_{13}\tau) \right) - \cos(d_{14}\tau) \cos(d_{13}\tau) \right),$$

$$P_{14}^{(i)} = \frac{1}{4} \left( 1 + \cos \tau \left( -\cos(d_{14}\tau) + \cos(d_{13}\tau) \right) - \cos(d_{14}\tau) \cos(d_{13}\tau) \right).$$

The explicit formulae relating the coupling constants $d_{1j}$ and $b$ depend on the direction of the external magnetic field in accordance with the definition of $d_{ij}$, see eq. (14). We consider two following cases:

1. The external magnetic field is perpendicular to the rectangle, so that

$$d_{14} = \delta, \quad d_{13} = \frac{1}{(1 + b^2)^{3/2}}.$$  

(43)

2. The external magnetic field is directed along the side $b$ of the rectangle, so that

$$d_{14} = -2\delta, \quad d_{13} = \left( 1 - \frac{3b^2}{1 + b^2} \right) \left( 1 + b^2 \right)^{-3/2}.$$  

(44)

Remark that both cases (43) and (44) allow equality $|d_{14}| = 1$ if $b = b_0 = 1$ for case (43) and $b = b_0 = 2^{1/3}$ for case (44). Rectangles with these special values of $b$ may not provide HPSTs to all nodes. In fact, the appropriate expressions for $P_{ij}$ become simpler in this case:

$$P_{11} = \frac{1}{4} \left( 1 + \cos^2 \tau + 2 \cos \tau \cos (d_{13}\tau) \right),$$

(45)

$$P_{12} = P_{14} = \frac{\sin^2 \tau}{4} \leq \frac{1}{4} < P_0 = 0.9,$$

$$P_{13} = \frac{1}{4} \left( 1 + \cos^2 \tau - 2 \cos \tau \cos (d_{13}\tau) \right).$$

We see that in this case max $P_{12} = max P_{14} = 1/4$, i.e. HPST exists only between 1st and 3rd nodes. Any rectangular configuration with $b \neq b_0$ provides HPSTs among all nodes, although the appropriate time interval $T$ may be long.

A. Relationships between probabilities and double negativities

As we noted above, any rectangle with $b \neq b_0$ provides HPST among all nodes. However, in general, the time interval $T$ is long. An important problem is to find such values of $b$.
which provide relatively short time interval $\mathcal{T}$. This problem is solved in Appendix C for the rectangular configuration of four nodes, where we have found the values of $b$ such that $\mathcal{T} \leq 10$ and $\mathcal{T} \leq 15$ for the case with magnetic field perpendicular to the plane of rectangle:

$$\delta \in [5.56, 9.62] \quad \text{for } \mathcal{T} \leq 10,$$

$$\delta \in [5.56, 17.79] \quad \text{for } \mathcal{T} \leq 15.$$  \hspace{1cm} (46)

and values of $b$ such that $\mathcal{T} \leq 3.5$ and $\mathcal{T} \leq 6$ for the case with magnetic field directed along the side $b$:

$$\delta \in [2.62, 6.08] \quad \text{for } \mathcal{T} \leq 3.5,$$

$$\delta \in [2.32, 6.08] \cup [14.89, 30.63] \quad \text{for } \mathcal{T} \leq 6.$$  \hspace{1cm} (47)

Thus we see that $\mathcal{T}$ is longer in the first case (magnetic field perpendicular to the plane of the rectangle), i.e. the second case is more preferable for the organization of the HPSTs.

To demonstrate the qualitative relationship between the probabilities of the state transfers and the double negativities (see eqs. 30-34) we show their graphs corresponding to the case \((44)\) and $\delta = 4.3$ in Fig.3 during the interval $\mathcal{T} = [0, 3.5]$. We see that the whole interval may be separated into three parts. During the first part, $0 \leq \tau \lesssim 1.1$, the probabilities $P_{11}$ and $P_{14}$ have big amplitudes. The associated big amplitude double negativity is $N_{1,4}$, showing that the first and the 4th nodes are most entangled during this interval. During the last part, $2.2 \lesssim \tau \leq 3.5$, the probabilities $P_{12}$ and $P_{13}$ have big amplitudes. The appropriate big amplitude double negativity is $N_{2,3}$ showing that the second and the third nodes are most entangled during this interval. The middle part, $1.1 \lesssim \tau \leq 2.2$, is characterized by the small values of $P_{1j}$ and considerable double negativity $N_{14,23}$ showing us that two opposite sides (namely sides 1-4 and 2-3) of the rectangle are well entangled. Two more double negativities, $N_{1,2}$ and $N_{3,4}$, are also considerable during the middle interval but they are not represented in the figure because their role is equivalent to the role of $N_{14,23}$. The double negativities $N_{1,3}$ and $N_{2,4}$ remain small during the whole interval $\mathcal{T}$, see Fig.3(c). We conclude that the time interval $\mathcal{T} = \tau_{13} \approx 3.29$. 

15
FIG. 3: Four-node system with the external field directed along $\xi_{14}$. (a) The probabilities $P_{1i}$, $(\tau_{14}, \bar{P}_{14}) = (0.36, 0.97)$, $(\tau_{12}, \bar{P}_{12}) = (2.92, 0.96)$, $(\tau_{13}, \bar{P}_{13}) = (3.29, 0.96)$; (b) the double negativities which provide HPSTs in the system; (c) the two-node double negativities which are not associated with HPSTs;

VI. THREE-DIMENSIONAL SPIN SYSTEM OF EIGHT NODES WITH HPSTS AMONG ALL OF THEM

In this section we consider the parallelepiped with spin-1/2 nodes in its corners, see Fig 4. Matrix $D$ in eq. (11) has the following block structure:

$$D = \begin{pmatrix} R_1 & R_2 & R_3 & R_4 \\ R_2 & R_1 & R_4 & R_3 \\ R_3 & R_4 & R_1 & R_2 \\ R_4 & R_3 & R_2 & R_1 \end{pmatrix},$$

(48)

$$R_1 = \begin{pmatrix} 2\tilde{\Gamma} & 1 \\ 1 & 2\tilde{\Gamma} \end{pmatrix}, \quad R_2 = \begin{pmatrix} d_{13} & d_{14} \\ d_{14} & d_{13} \end{pmatrix}, \quad R_3 = \begin{pmatrix} d_{15} & d_{16} \\ d_{16} & d_{15} \end{pmatrix}, \quad R_4 = \begin{pmatrix} d_{17} & d_{18} \\ d_{18} & d_{17} \end{pmatrix},$$
FIG. 4: The three-dimensional eight-node system. The external magnetic field $\vec{h}$ is directed along the side $\xi_{15}$. Here $\xi_{12} = 1$, while two other sides are parameters of this configuration: $\xi_{14} = b_1$, $\xi_{15} = b_2$. We will use parameters $\delta_i = 1/b_i^3$, $i = 1, 2$ instead of $b_1$ and $b_2$.

\[d_{13} = (1 + b_1^2)^{-3/2}, \quad d_{14} = b_1^{-3}, \quad d_{15} = -2b_2^{-3},\]
\[d_{16} = \left(1 - 3\frac{b_2^2}{1 + b_2^2}\right)(1 + b_2^2)^{-3/2}, \quad d_{17} = \left(1 - 3\frac{b_2^2}{1 + b_2^2 + b_1^2}\right)(1 + b_2^2 + b_1^2)^{-3/2},\]
\[d_{18} = \left(1 - 3\frac{b_2^2}{b_2^2 + b_1^2}\right)(b_2^2 + b_1^2)^{-3/2}, \quad \tilde{\Gamma} = \sum_{i=2}^{8} d_{1j}, \quad d_{12} = 1.\]

Again, the structure of the matrix $D$ allows us to find the following set of normalized independent eigenvectors:

\[u_1 = \frac{1}{2\sqrt{2}}(1 1 1 1 1 1 1 1)^T, \quad u_2 = \frac{1}{2\sqrt{2}}(1 1 1 1 1 1 1 1)^T,\]  
\[u_3 = \frac{1}{2\sqrt{2}}(1 1 1 -1 -1 1 1 -1)^T, \quad u_4 = \frac{1}{2\sqrt{2}}(1 1 1 -1 -1 1 1 -1)^T,\]  
\[u_5 = \frac{1}{2\sqrt{2}}(1 -1 1 -1 -1 -1 1 1)^T, \quad u_6 = \frac{1}{2\sqrt{2}}(1 -1 1 -1 -1 -1 1 1)^T,\]  
\[u_7 = \frac{1}{2\sqrt{2}}(1 -1 -1 1 -1 -1 -1 1)^T, \quad u_8 = \frac{1}{2\sqrt{2}}(1 -1 -1 1 -1 -1 -1 1)^T.\]

Similar to the case of four nodes, the eigenvectors do not depend on $b_i$, $i = 1, 2$. The correspondent set of eigenvalues reads:

\[\lambda_1 = 3\tilde{\Gamma}, \quad \lambda_2 = 3\tilde{\Gamma} - 2(d_{15} + d_{16} + d_{17} + d_{18}),\]  
\[\lambda_3 = 3\tilde{\Gamma} - 2(d_{13} + d_{14} + d_{17} + d_{18}), \quad \lambda_4 = 3\tilde{\Gamma} - 2(d_{13} + d_{14} + d_{15} + d_{16}),\]  
\[\lambda_5 = 3\tilde{\Gamma} - 2(1 + d_{14} + d_{16} + d_{18}), \quad \lambda_6 = 3\tilde{\Gamma} - 2(1 + d_{14} + d_{15} + d_{17}),\]  
\[\lambda_7 = 3\tilde{\Gamma} - 2(1 + d_{13} + d_{16} + d_{17}), \quad \lambda_8 = 3\tilde{\Gamma} - 2(1 + d_{13} + d_{15} + d_{18}),\]

Due to the symmetry of our cluster, it is enough to study the case with the initial excited state in the first node, i.e. $k_0 = 1$ similar to Sec. V. The expressions (19) for the probabilities
$P_{ij}$ in terms of the coupling constants $d_{ij}$ are rather complicated so that we do not represent them here. Note, however, that the cube does not allow the HPSTs among all nodes. In fact, in the case $b_1 = b_2 = 1$ one has

$$P_{12} = P_{14} = \frac{\sin^2(2\tau)}{16} \leq \frac{1}{16},$$

$$P_{11} = \frac{1}{32} \left( 7 + \cos(4\tau) + 8 \cos \frac{\tau}{4\sqrt{2}} \left( \cos \tau + \cos(2\tau) \cos \frac{\tau}{4\sqrt{2}} \right) + 4 \left( \cos \tau + \cos(3\tau) \right) \cos \frac{3\tau}{4\sqrt{2}} \right),$$

$$P_{13} = \frac{1}{32} \left( 7 + \cos(4\tau) - 8 \cos \frac{\tau}{4\sqrt{2}} \left( \cos \tau - \cos(2\tau) \cos \frac{\tau}{4\sqrt{2}} \right) - 4 \left( \cos \tau + \cos(3\tau) \right) \cos \frac{3\tau}{4\sqrt{2}} \right),$$

$$P_{15} = \frac{\sin^2 \tau}{8} \left( 3 + \cos(2\tau) + 4 \cos \tau \cos \frac{3\tau}{4\sqrt{2}} \right),$$

$$P_{16} = P_{18} = \frac{1}{32} \left( 3 + \cos(4\tau) - 2 \cos \left( \frac{\sqrt{2} - 8}{4} \right) - 2 \cos \left( \frac{\sqrt{2} + 8}{4} \right) \right) \leq \frac{1}{4},$$

$$P_{17} = \frac{\sin^2 \tau}{8} \left( 3 + \cos(2\tau) - 4 \cos \tau \cos \frac{3\tau}{4\sqrt{2}} \right),$$

so that the probabilities $P_{12}, P_{14}, P_{16}$ and $P_{18}$ may not approach $P_0 = 0.9$.

The study of the HPSTs and entanglements in this system requires finding such subspace of the two-dimensional space of positive parameters $\delta_1$ and $\delta_2$ that any pair $(\delta_1, \delta_2)$ from this subspace provides the HPSTs among all nodes. This computational problem will not be considered in this paper in the full extend. Instead, we consider an example. Namely, we will show (see Appendix D for details) that the HPSTs among all nodes are possible for $\delta_1 = 9$ and $\delta_2 = 26.20$ during the $\tau$-interval $T \leq 25$.

We demonstrate that the relationship between probabilities and double negativities is very similar to one considered in Sec.V. For this purpose, let us refer to Figs.5(a) and (b) collect all probabilities and all double negativities involved into the state transfer process. Similar to the four-node system considered in Sec.V we select three parts of the whole interval $T = [0, 25]$: $0 < \tau \lesssim 0.5$, $0.5 \lesssim \tau \lesssim 23$ and $23 \lesssim \tau \lesssim 24$. It is clear from Fig.5(a), that the HPSTs take place in the first and in the third parts of $T$. All probabilities of the state transfers are not high during the second part of the above interval. Amplitudes of the probabilities $P_{1i}, i = 1, 4, 5, 8$, are big during the first part of the interval, while amplitudes of the probabilities $P_{1i}, i = 2, 3, 6, 7$, are big during the third part of the interval.
FIG. 5: Eight-node system. The probabilities and double negativities corresponding to $\delta_1 = 9$, $\delta_2 = 26$. The HPSTs take place during the first and the last parts of the time interval $0 \leq \tau \leq 25$.

Similarly, Fig. 5(b) shows that double negativities $N_{1,5}$, $N_{4,8}$ and $N_{15,48}$ are significant during the first part of the interval $T$ while double negativities $N_{2,6}$, $N_{3,7}$ and $N_{26,37}$ are significant during the third part of this interval. One more double negativity $N_{1458,2367}$ is significant during the second part of the interval $T$ and is not high during the first and the last parts. This means that namely $N_{1458,2367}$ is responsible for the HPSTs from the plane 1-4-5-8 to the plane 2-3-6-7.

The probabilities and double negativities during the first and the third parts of the interval $T$ are represented in Figs. 6 and 7 respectively in more details. We show only those probabilities whose amplitudes exceed the value $P_0 = 0.9$. One can see from Fig. 6(a, b) that the HPSTs to the 4th, 5th and 8th nodes occur during the interval $0 \leq \tau \leq \tau_4 = 0.36$. Functions $N_{1,5}$ and $N_{4,8}$ provide the HPSTs between the first and the 5th and between the 4th and the 8th nodes respectively, while $N_{15,48}$ provides the HPST from the side 1-5 to the side 4-8.
Similarly, we see from Fig. 7(a, b) that the HPSTs to the 2nd, 3rd, 6th and 7th nodes occur during the time interval \((\tau_{16} = 23.23) \leq \tau \leq (\tau_{12} = 23.89)\). Functions \(N_{2,6}\) and \(N_{3,7}\) provide the HPSTs between the 2nd and the 6th and between the 3rd and the 7th nodes respectively, while \(N_{26,37}\) provides HPST from the side 2-6 to the side 3-7. We also conclude that \(T = \tau_{12} = 23.89\).

**FIG. 6:** Eight-node system. The probabilities and double negativities corresponding to \(\delta_1 = 9\), \(\delta_2 = 26.20\) and HPSTs during the time interval \(0 \leq \tau \leq 0.5\); \((\tau_{15}, \bar{P}_{15}) = (0.06, 0.93)\), \((\tau_{18}, \bar{P}_{18}) = (0.30, 0.91)\), \((\tau_{14}, \bar{P}_{14}) = (0.36, 0.93)\)

**FIG. 7:** Eight-node system. The probabilities and double negativities corresponding to \(\delta_1 = 9\), \(\delta_2 = 26.20\) and HPSTs during the time interval \(23.1 \leq \tau \leq 24\); \((\tau_{16}, \bar{P}_{16}) = (23.23, 0.90)\), \((\tau_{13}, \bar{P}_{13}) = (23.53, 0.95)\), \((\tau_{17}, \bar{P}_{17}) = (23.59, 0.95)\) , \((\tau_{12}, \bar{P}_{12}) = (23.89, 0.91)\)
VII. CONCLUSIONS

We have derived simple relations between the probabilities of the excited state transfers to different nodes of the spin system and the entanglements between different parts of this system described by PPT criterion for the arbitrary spin system in the external magnetic field with single excited spin and any Hamiltonian preserving the number of excitations, such as $XXZ$ Hamiltonian. Although similar relations for the concurrence (which is a measure of the entanglement between two nodes in accordance to Wootters criterion) has been found [4, 17], the PPT criterion allows one to involve entanglements between two arbitrary subsystems of nodes which is important for the systems with HPSTs among many nodes as has been illustrated in this paper.

We have found examples of 4- and 8-node spin systems which provide HPSTs among all nodes. We have seen that the HPSTs between two subsystems require the high entanglement between them. This is illustrated in all examples considered in this paper: two-node, four-node and eight-node nuclear spin systems, see Figs.1, 3, 5-7 respectively.

In all spin systems considered in this paper, the HPSTs among many nodes are possible due to the remarkable property of the eigenvectors of the matrix $D$ (see eq. (11)): all their elements are real, equal by absolute value and differ only by sign. It is important that four- and eight-nodes systems with this property have simple geometrical configuration: either rectangle (four nodes) or parallelepiped (eight nodes). It is possible to construct the higher dimensional eigenvectors with this property using the following simple algorithm.

Consider the eigenvector spaces with the above mentioned property: all elements of all eigenvectors are real and have the same absolute value. Suppose that we have $M$-dimensional space $\mathcal{B}_M$ of such vectors. Then we may construct $2M$ dimensional space by the formula

$$\mathcal{B}_{2M} = 1/\sqrt{2} \left( (1,1) \otimes \mathcal{B}_M \cup (1,-1) \otimes \mathcal{B}_M \right).$$

Thus we are able to construct $2^s$-dimensional basis with the above property. However it is difficult to find appropriate spin configurations different from those which have been described above. Of course, it is quite possible that the HPSTs among many nodes may be arranged using completely different mechanism allowing one, for instance, to handle the coupling constants in complicated spin systems [5, 16], which is one of the open problems for further study.
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APPENDIX A: WOOTTERS CRITERION. DERIVATION OF EQ. (27)

Our calculations are based on eqs. (23-25). By construction, the reduced density matrix \( \rho_{\text{red}}^{ij} \) defined by eq. (25) takes a simple \( 4 \times 4 \)-dimensional form in the following basis

\[
|10\rangle, \ |01\rangle, \ |00\rangle, \ |11\rangle, \tag{A1}
\]

where the first and the second elements are associated with the \( i \)th and the \( j \)th nodes respectively. One has

\[
\rho_{\text{red}}^{ij} = \begin{pmatrix}
  a_{ii} & a_{ij} & 0 & 0 \\
  a_{ji} & a_{jj} & 0 & 0 \\
  0 & 0 & \sigma_{ij} & 0 \\
  0 & 0 & 0 & 0
\end{pmatrix}, \quad \sigma_{ij} = \sum_{n=1}^{N} a_{nn} = \sum_{n=1 \neq i,j}^{N} P_{kn} = 1 - P_{k1i} - P_{k1j}. \tag{A2}
\]

Then

\[
\tilde{\rho}_{\text{red}}^{ij} = \begin{pmatrix}
  a_{jj} & a_{ji} & 0 & 0 \\
  a_{ij} & a_{ii} & 0 & 0 \\
  0 & 0 & 0 & 0 \\
  0 & 0 & 0 & \sigma_{ij}
\end{pmatrix}. \tag{A3}
\]

Direct calculation shows that the matrix \( \tilde{\rho}_{ij} \) has only one non-zero eigenvalue: \( \lambda_1 = 4|a_{ij}|^2 = 4P_{k1i}P_{k1j} \), which yields eq. (27).

APPENDIX B: PPT CRITERION. DERIVATION OF EQ. (30)

We derive formulae (30) in this section. First of all, in order to calculate \( N_{i_1 \ldots i_{M_1}, j_1 \ldots j_{M_2}} \) one needs the reduced density matrix \( \rho_{i_1 \ldots i_{M_1}, j_1 \ldots j_{M_2}} \) calculated in accordance with eq. (29), where

\[
A = \{i_1, \ldots, i_{M_1}\}, \quad B = \{j_1, \ldots, j_{M_2}\}. \tag{B1}
\]

This is \( 2^{M_1} \times 2^{M_1} \times 2^{M_2} \times 2^{M_2} \) matrix. However, most of elements of this matrix are zeros. All nonzero elements are collected in the \( K \times K \) \( (K = M_1 + M_2 + M_1M_2 + 1) \) block on the
diagonal of $\rho_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}}$. This block corresponds to the subspace spanned by the following set of vectors (we use notations equivalent to ones introduced for basis (9)):

$$|i_n\rangle, \ |j_m\rangle, \ |0\rangle, \ |i_n j_m\rangle, \ n = 1, \ldots, M_1, \ m = 1, \ldots, M_2. \quad (B2)$$

We refer to this block as $\tilde{\rho}_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}}$:

$$\tilde{\rho}_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} = \begin{pmatrix} Q_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} & 0_I & 0_{II} \\ 0_I^T & \sigma_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} & 0_{III} \\ 0_{II}^T & 0_{III}^T & 0_{IV} \end{pmatrix}, \quad (B3)$$

where $Q_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}}$ is $(M_1 + M_2) \times (M_1 + M_2)$ square matrix

$$Q_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} = \begin{pmatrix} R_{i_1 \ldots i_{M_1}} & R_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} \\ R_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}}^T & R_{j_1 \ldots j_{M_2}} \end{pmatrix}, \quad (B4)$$

$$R_{i_1 \ldots i_{M_1}} = \begin{pmatrix} a_{i_1 i_1} & \cdots & a_{i_1 i_{M_1}} \\ \cdots & \cdots & \cdots \\ a_{i_{M_1} i_1} & \cdots & a_{i_{M_1} i_{M_1}} \end{pmatrix}, \ R_{j_1 \ldots j_{M_2}} = \begin{pmatrix} a_{j_1 j_1} & \cdots & a_{j_1 j_{M_2}} \\ \cdots & \cdots & \cdots \\ a_{j_{M_2} j_1} & \cdots & a_{j_{M_2} j_{M_2}} \end{pmatrix},$$

$$R_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} = \begin{pmatrix} a_{i_1 j_1} & \cdots & a_{i_1 j_{M_2}} \\ \cdots & \cdots & \cdots \\ a_{i_{M_1} j_1} & \cdots & a_{i_{M_1} j_{M_2}} \end{pmatrix}, \ q_{i_k j_1 \ldots j_{M_2}} = (a_{i_k j_1} \text{ cdots } a_{i_k j_{M_2}}),$$

$0_I$ is the column of $M_1 + M_2$ zeros, $0_{II}$ is the $(M_1 + M_2) \times M_1 M_2$ zero matrix, $0_{III}$ is the row of $M_1 M_2$ zeros, $0_{IV}$ is the $M_1 M_2 \times M_1 M_2$ square matrix of zeros.

Now we have to transpose the matrix $\rho_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}}$ with respect to the nodes $i_1, \ldots, i_{M_1}$. The nonzero diagonal block of the resulting matrix is associated with transposition of the block $\tilde{\rho}_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}}$ with respect to the nodes $i_1, \ldots, i_{M_1}$:

$$\tilde{\rho}_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} = \begin{pmatrix} \tilde{Q}_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} & 0_I & 0_{II} \\ 0_I^T & \sigma_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} & 0_{III} \\ 0_{II}^T & 0_{III}^T & 0_{IV} \end{pmatrix}, \quad (B5)$$

where $^*$ means hermitian conjugation,

$$\tilde{Q}_{i_1 \ldots i_{M_1} j_1 \ldots j_{M_2}} = \begin{pmatrix} R_{i_1 \ldots i_{M_1}}^T & 0_V \\ 0_V^T & R_{j_1 \ldots j_{M_2}} \end{pmatrix}, \ R_I = (q_{i_1 j_1 \ldots j_{M_2}} \cdots q_{i_{M_1} j_1 \ldots j_{M_2}}), \quad (B6)$$
0_\nu is the $M_1 \times M_2$ zero matrix. By construction, both blocks $R_{i_1...i_{M_1}}^T$ and $R_{j_1...j_{M_2}}$ are density matrices and, as a consequence, have non-negative eigenvalues. Thus, all eigenvalues of the matrix $\tilde{Q}_{i_1...i_{M_1}j_1...j_{M_2}}^{red}$ are non-negative. For this reason, looking for the negative eigenvalues of the matrix $\tilde{\rho}_{i_1...i_{M_1}j_1...j_{M_2}}$, we stay with the matrix

$$
\begin{pmatrix}
\sigma_{i_1...i_{M_1}j_1...j_{M_2}} & R_I \\
R_I^+ & 0_{IV}
\end{pmatrix}.
$$

(B7)

Its characteristics equation reads:

$$
(-\lambda)^{M_1M_2-1} \left( \lambda^2 - \lambda \sigma_{i_1...i_{M_1}j_1...j_{M_2}} - \sum_{n=1}^{M_1} \sum_{m=1}^{M_2} |a_{i_nj_m}|^2 \right) = 0,
$$

(B8)

which has two nonzero roots one of which is negative:

$$
\lambda_1 = \frac{1}{2} \left( \sigma_{i_1...i_{M_1}j_1...j_{M_2}} - \sqrt{\sigma_{i_1...i_{M_1}j_1...j_{M_2}}^2 + 4 \sum_{n=1}^{M_1} \sum_{m=1}^{M_2} |a_{i_nj_m}|^2} \right).
$$

(B9)

Consequently,

$$
N_{i_1...i_{M_1}j_1...j_{M_2}} = 2|\lambda_1|,
$$

(B10)

which generates the formulae (30).

**APPENDIX C: OPTIMIZATION OF THE RECTANGULAR SYSTEM. VALUES OF THE PARAMETER $\delta$ PROVIDING THE HPSTS AMONG ALL NODES**

There are four functions characterizing HPSTs in the system of four spin-1/2 nodes:

$$
P_{i_1}(\tau), \quad i = 1, 2, 3, 4.
$$

(C1)

As for the entanglements, the situation is more complicated. We have the following lists of all possible double negativities in the four-node system:

$$
N_{1,1} \equiv \{N_{i,j}, \quad i, j = 1, 2, 3, 4, \quad i \neq j \},
$$

(C2)

$$
N_{2,2} \equiv \{N_{12,34}, \quad N_{13,24}, \quad N_{14,23}, \quad N_{13,24} \},
$$

(C3)

$$
N_{1,3} \equiv \{N_{1,234}, \quad N_{2,134}, \quad N_{3,124}, \quad N_{4,123} \}.
$$

(C4)

We will show that $N_{1,1}$ and $N_{2,2}$ are responsible for the HPSTs among all nodes.
Our system has one geometrical parameter \( b \) or \( \delta \) (see eq.(38)) completely describing the rectangular geometry. We represent an algorithm allowing one to find such values of the parameter \( \delta \) which provide inequality (21) with the short time interval \( T \) (22). For this purpose we consider the functions \( P_{1i} \) and \( N_{i,j} \) as functions of two arguments, \( \tau \) and \( \delta \).

Let us fix some time interval \( T \) and check whether the state may be transferred with high probability from the 1st node to any other node and whether the entanglements between any two nodes are significant during this time interval. For this purpose we construct two following functions:

\[
F^P(\delta, T) = \lim_{\Delta \tau \to 0} F^P(\delta, T, \Delta \tau), \tag{C5}
\]

\[
F^N(\delta, T) = \lim_{\Delta \tau \to 0} F^N(\delta, T, \Delta \tau), \tag{C6}
\]

where

\[
F^P(\delta, T, \Delta \tau) = \min_{k=1,2,3,4} \left[ \max_{i=0,\ldots,K} P_{1k}(\tau_i, \delta) \right], \tag{C7}
\]

\[
F^N(\delta, T, \Delta \tau) = \min_{n,m=1,2,3,4, n \neq m} \left[ \max_{i=0,\ldots,K} N_{n,m}(\tau_i, \delta) \right], \quad \tau_i = i\Delta \tau, \quad \Delta \tau = \frac{T}{K}, \quad K \in \mathbb{N}.
\]

The HPSTs among all nodes of the system are possible if there is such \( \delta = \delta_0 \) that

\[
F^P(\delta_0, T) \geq P_0. \tag{C8}
\]

Then

\[
T \leq T. \tag{C9}
\]

Function \( F^N \) tells us how significant is the entanglement between any two nodes of the system.

First, we consider the case when the external magnetic field is perpendicular to the rectangle. Functions \( F^P(\delta, T, \Delta \tau) \) and \( F^N(\delta, T, \Delta \tau) \) with \( \Delta \tau = 0.01 \) corresponding to the intervals \( T = 10 \) and \( 15 \) are represented in Fig.8. The HPSTs among all nodes are possible for the parameter \( \delta \) inside of the intervals (46).

The interval of \( \delta \) corresponding to the HPSTs among all nodes increases with increase in \( T \). If \( T \) is big enough (we have found that \( T \gtrsim 40 \)), then the HPSTs among all nodes exist even for \( \delta < 1 \). If \( \delta = \delta_0 = 1 \), then \( F^P \) may not exceed \( 1/4 \) in accordance with eqs.(45).

Fig.8 shows that the function \( F^N \sim 0.8 \div 0.9 \) when \( F^P \gtrsim 0.9 \). This means, that the HPSTs...
among all nodes during the interval $T$ entangle any two nodes in this case, i.e. functions $N_{i,j}$ (for $i, j = 1, 2, 3, 4, i \neq j$) must have big amplitudes during the time interval $T$.

Similarly, the functions $F^P(\delta, T, \Delta \tau)$ and $F^N(\delta, T, \Delta \tau)$ for the case with the magnetic field directed along $\xi_{14}$ are represented in Fig.9 for, $T = 3.5, \Delta \tau = 0.01$ and $T = 6, \Delta \tau = 0.001$. The HPSTs among all nodes are possible for $\delta$ inside of the intervals $[\delta_{i}, \delta_{i + 1}]$. In this case the function $F^N$ does not necessary take a big value when $F^P \gtrsim 0.9$. This means, that not any two nodes must be entangled in order to provide the HPSTs among all nodes during the time interval $T$. Note that exceptional value of $\delta$ is $\delta = \delta_0 = 1/2$, when $F^P$ does not exceed $1/4$ in accordance with eqs.(45).

![Comparison of Figs.8(a) and 9(a) shows that the second case (i.e. external field is directed](image)

FIG. 8: Four-node system with the external field perpendicular to the plane of the rectangle. Functions $F^P(\delta, T, 0.01)$ and $F^N(\delta, T, 0.01)$. (a) $T = 10$, $\delta_1 = 5.56$, $\delta_2 = 9.62$; (b) $T = 15$, $\delta_1 = 5.56$, $\delta_2 = 17.79$.

FIG. 9: Four-node system with the external field directed along $\xi_{14}$. Functions $F^P(\delta, T)$ and $F^N(\delta, T)$; (a) $T = 3.5$, $\delta_1 = 2.62$, $\delta_2 = 6.08$, $\delta_0 = 4.3$. $F^P(\delta_0, 3.5) = 0.96$ (b) $T = 6$, $\delta_1 = 2.32$, $\delta_2 = 6.08$, $\delta_3 = 14.89$, $\delta_4 = 30.63$. Comparison of Figs.8(a) and 9(a) shows that the second case (i.e. external field is directed...
along $\xi_{14}$) is more preferable for the organization of the HPSTs because appropriate interval $T$ is almost three times shorter.

Figs. 8 and 9 show that the intervals of the parameter $\delta$ providing the HPSTs among all nodes increase with increase in $T$, i.e. the system becomes more “stable” with respect to variations in $b$ (compare the interval $\delta_1 \leq \delta \leq \delta_2$ in Fig.8 and the intervals $\delta_1 \leq \delta \leq \delta_2$, $\delta_3 \leq \delta \leq \delta_4$ in Fig.9).

Finally, remark that function (C7) are decreasing functions of $\Delta \tau$. Thus, one may expect that the graphs of the functions $F^P(\delta, T)$ and $F^N(\delta, T)$ are above of the appropriate curves shown in Figs.8 and 9. However, further decrease in $\Delta \tau$ negligibly effects the shapes of the above curves in all examples of this section.

**APPENDIX D: ON THE OPTIMIZATION OF THE EIGHT-NODE SYSTEM. VALUES OF THE PARAMETERS $\delta_1$ AND $\delta_2$ PROVIDING THE HPSTS AMONG ALL NODES**

We introduced functions $F^P$ and $F^N$ in Appendix C, see eqs.(C5,C6). However, we have seen that $F^N$ is not as helpful as $F^P$ in defining the optimal parameter $\delta$. In fact, Figs.8 and 9 show us that $F^N$ may be either big or small when $F^P \gtrsim 0.9$ reflecting the fact that not all entanglements between two nodes are important for the HPSTs during the interval $T$. For this reason we consider only $F^P$ in this section:

$$F^P(\delta, T) = \lim_{\Delta \tau \to 0} F^P(\delta, T, \Delta \tau),$$  \hspace{1cm} (D1)

where

$$F^P(\delta, T, \Delta \tau) = \min_{k=1, \ldots, 8} \left[ \max_{i=0, \ldots, K} P_{1k}(\tau_i, \delta) \right], \quad \tau_i = i \Delta \tau, \quad \Delta \tau = \frac{T}{K}, \quad K \in \mathbb{N},$$  \hspace{1cm} (D2)

and $P_{1k}$ are given by eqs.(19,49,50).

Function $F^P(\delta, T, \Delta \tau)$ is shown in Fig.10 for $T = 25$ and $\Delta \tau = 0.01$. We see from Fig.10(b) that the HPSTs among all nodes are possible, for instance, for $\delta = \delta_0 = 26.20$.

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[1] E.I.Kuznetsova and A.I.Zenchuk, Phys.Lett.A, 372, 6134 (2008)
FIG. 10: Function $F^P(\delta, T, 0.01)$ for $T = 25; \delta_0 = 26.20.$

[2] S.Bose, Phys.Rev.Lett, 91 (2003) 207901
[3] M.Christandl, N.Datta, A.Ekert and A.J.Landahl, Phys.Rev.Lett. 92, 187902 (2004)
[4] G.Gualdi, I.Marzoli, P.Tombesi, [arXiv:0812.2404v1] [quant-ph]
[5] D.I.Tsomokos, M.B.Plenio, I. de Vega and S.F.Huelga, Phys.Rev.A, 78 062310 (2008)
[6] E.B.Fel’dman and A.I.Zenchuk, Phys.Lett.A, 373 (2009) 1719, [arXiv:0809.1967v1] [quant-ph]
[7] E.B.Fel’dman, R.Brüschweiler and R.R.Ernst, Chem.Phys.Lett. 294, 297 (1998)
[8] G.Gualdi, V.Kostak, I.Marzoli and P.Tombesi, Phys.Rev. A, 78, 022325 (2008)
[9] C.Albanese, M.Christandl, N.Datta and A.Ekert, Phys.Rev.Lett., 93, 230502 (2004)
[10] E.B.Fel’dman and M.G.Rudavets, JETP Letters, 81, 47 (2005)
[11] E.I.Kuznetsova and E.B.Fel’dman, J.Exp.Theor.Phys., 102, 882 (2006)
[12] L.Campos Venuti, S.M.Giampaolo, F.Illuminati and P.Zanardi, Phys.Rev.A 76, 052328 (2007)
[13] P.Karbach and J.Stolze, Phys.Rev.A, 72, 030301(R) (2005)
[14] D.Burgarth, V.Giovannetti and S.Bose, Phys.Rev.A 75 062327 (2007)
[15] S.I.Doronin, A.N.Pyrkov, E.B.Fel’dman, J.Exp.Theor.Phys., 105, 953 (2007)
[16] S.Bose, A.Casaccino, S.Mancini and S.Severini, [arXiv:0808.0748] [quant-ph]
[17] L.Amico, A.Osterloh, F.Plastina, R.Fazio, G.M.Palma, Phys.Rev. A, 69, 022304 (2004)
[18] A.Peres, Phys.Rev.Lett., 77, 1413 (1996)
[19] G.Vidal and R.F.Werner, Phys.Rev.A, 65, 032314 (2002)
[20] Abragam A. The principles of nuclear magnetism, Oxford, Clarendon Press, 1961
[21] S.I.Doronon, E.B.Fel’dman, I.Ya.Guinsbourg and I.I.Maximov, Chem.Phys.Lett., 341, 144 (2001)
[22] S.Hill and W.K.Wootters, Phys.Rev.Lett., 78, 5022 (1997)
[23] K. Zyczkowski, P. Horodecki, A. Sanpera and M. Lewenstein, Phys. Rev. A, 58, 883 (1998)
[24] H. G. Krojanski and D. Suter, Phys. Rev. Lett. 93, 090501 (2004)
[25] H. J. Cho, P. Cappellaro, D. G. Cory and C. Ramanathan, Phys. Rev. B 74, 224434 (2006)