Systems with stationary distribution of quantum correlations: open spin-1/2 chains with XY interaction

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Abstract Although quantum correlations in a quantum system are characterized by the evolving quantities (which are entanglement and discord usually), we reveal such basis (i.e. the set of virtual particles) for the representation of the density matrix that the entanglement and/or discord between any two virtual particles in such representation are stationary. In particular, dealing with the nearest neighbor approximation, this system of virtual particles is represented by the $\beta$-fermions of the Jordan–Wigner transformation. Such systems are important in quantum information devices because the evolution of quantum entanglement/discord leads to the problems of realization of quantum operations. The advantage of stationary entanglement/discord is that they are completely defined by the initial density matrix and by the Hamiltonian governing the quantum dynamics in the system under consideration. Moreover, using the special initial condition together with the special system’s geometry, we construct large cluster of virtual particles with the same pairwise entanglement/discord. In other words, the measure of quantum correlations is stationary in this system and correlations are uniformly “distributed” among all virtual particles. As examples, we use both homogeneous and non-homogeneous spin-1/2 open chains with XY-interaction although other types of interactions might be also of interest.

Keywords Stationary quantum discord · Quantum entanglement · Spin chain · XY Hamiltonian · Quantum register
1 Introduction

An attractive problem in quantum information processing is that of revealing of quantum correlations in a system. Presently, two measures are most acknowledged as characteristics of quantum correlations: the quantum entanglement [1–5] and the quantum discord [6–9]. The so-called quantum entanglement must be noted as the first quantitative measure of quantum correlations. However, it was shown that the quantum discord involves more quantum correlations. As justification of this statement, there are quantum systems with zero entanglement revealing the non-zero discord. Therefore, it is considered [10] that namely discord is a proper measure responsible for advantages of quantum information devices (quantum speed-up and others).

In general, the calculation of discord is a very cumbersome optimization problem. In spite of intensive study of discord, only very special cases have been treated analytically [11–14]. Nevertheless, namely these cases correspond to the reduced binary density matrix in spin-1/2 chains governed by different Hamiltonians with either the thermal equilibrium initial state [15,16], the initial state with the single excited node [17] and the initial state with the single polarized node [18–20].

Let us notice, that the problem of a proper initial state is one of the fundamental problems in study of quantum correlations in different physical systems because of the technical difficulties in realization of a particular state. The so-called thermal equilibrium initial state [15] is most popular because of its simple realization. However, the initial state with a single excited node is more relative, for instance, to quantum communication lines [17,21–25]. Another example is the state with a single polarized node which was produced experimentally [18]. The evolution of a quantum system with this initial state at high temperatures was studied, for instance, in [19], where the quantum echo was found.

In spite of intensive study, the problem of identification of quantum correlations is not resolved yet. In particular, the measure of quantum correlations depends on the basis which is taken for the density matrix representation. The reason is that, considering different bases, we involve different types of virtual particles. A possible way to avoid this ambiguity is suggested in ref. [26], where the unitary invariant discord is introduced. This measure takes into account correlations among all possible virtual particles so that there is no privilege of any particular density matrix representation.

In [20], instead of counting the correlations among all virtual particles (like in the unitary invariant discord [26]), the problem of preferable virtual particles was formulated. Namely, the quantum correlations among three types of particles are considered separately and compared with each other. These particles are following: (i) the fermions, which appear in a spin-1/2 system with the nearest neighbor interaction after the diagonalization via the Jordan–Wigner transformation [27] (we call them as the β-fermions), (ii) the fermions which are the Fourier representations of the β-fermions (the c-fermions), and (iii) the physical spin-1/2 particles with the basis of eigenvectors of the operators $I_{jz}$ ($z$-projection of the $j$th spin, $j = 1, \ldots, N$). It is shown, that the distributions of quantum correlations among eigenstates corresponding to three above bases are completely different. Remind that the β-representation is most attractive owing to its several remarkable properties. First of all, it yields the stationary pairwise discord (i.e. the discord between any two nodes $n$ and $m$), which might be convenient
for the realization of quantum operations. Second, the discord might be nonzero even between the states with zero entanglement, which confirms the privilege of the discord as a measure of quantum correlations. Third, the stationary discord is completely defined by the initial density matrix (for the given type of quantum interactions) [20], which provides a simple tool to handle the stationary discord distribution. Thus, if the first node in the odd-node spin chain is initially polarized, then all nodes of the chain are correlated and the pairwise stationary discord increases to the center node of the chain [20]. If the middle node is initially polarized, then the system of odd nodes forms a cluster of correlated fermions with equal pairwise discord. This is the remarkable fact which was not observed in the systems of real physical particles and may be useful for formation of large quantum registers.

It is interesting to note that the dependence of quantum correlations on the particular basis of eigenstates is considered in [28–33] from another standpoint. Namely, the whole space of quantum states of a given system (the open spin-1/2 chain in the above case) may be split into two subspaces. The quantum correlations are considered in the first one (the subsystem $A$) while another subsystem $B$ is referred to as the environment. In the above references, the dependence of quantum correlations on the particular selected subsystem of quantum states is demonstrated. In our case the subsystem $A$ is represented by the eigenstates of two virtual particles of a particular density matrix representation, while the eigenstates of the rest of particles form the environment.

This paper is devoted to the problem of study of such system of virtual particles in a given quantum system that possesses the stationary discord. We substantially extend a particular rather qualitative result of ref. [20] concerning the stationary discord in the system of Jordan–Wigner $\beta$-fermions corresponding to the single initially polarized node in a homogeneous spin-1/2 chain governed by the XY Hamiltonian with the nearest neighbor interactions. Namely

1. Along with the single initially polarized node, we consider the single initially excited node in a spin-1/2 chain.
2. We show analytically that the pairwise discord/entanglement are stationary in the system of virtual particles corresponding to the eigenstates of the Hamiltonian if only the initial state with the single excited/polarized node is considered. If we deal with the nearest neighbor interactions, then this virtual particles are the $\beta$-fermions of the Jordan–Wigner representation, which agrees with ref. [20].
3. We find out that both entanglement and discord are stationary and nonzero in the above basis if the initial state with the single excited node is taken (remember that the entanglement is zero in the $\beta$-fermion system considered in ref. [20]).
4. We represent the detailed analytical and numerical study of the discord/entanglement distribution in dependence on the position of the initially excited/polarized node in the chain. Subsystems with (almost) uniform pairwise discord/entanglement distribution have been revealed with analytical formulas for some of them. Examples of large subsystems are among them.
5. We refer to the inhomogeneous chains (alternating, 3-alternating and completely inhomogeneous chain of ref. [21]) and have found several peculiar subsystems with nonzero discord/entanglement. The diamerization effect is studied in the alternating chain.
6. Along with the approximation of nearest neighbor interaction, we consider the case of dipole–dipole interactions among all nodes (the case of a single initially excited node) and show that the remote interactions do not significantly deform the overall pairwise discord/entanglement distribution. Emphasize that this is an important advantage in comparison with the discord/entanglement in the system of usual spin-1/2 particles, where the remote interactions crucially change this distribution. The reason is that the remote interactions significantly affect the spin dynamics and, consequently, on the dynamics of quantum correlations. However, these correlations are stationary in our system of virtual particles.

Systems with the stationary discord/entanglement are important for construction of the quantum information devices where the stationary distribution of quantum correlations simplifies the realization of quantum operations. The matter is that the quantum operations in a given cluster of correlated particles may be performed only during the period of its existence (which is defined by the decoherence time associated with a given quantum system) and only provided that the quantum correlations are properly distributed among all nodes of a cluster. However, even if the quantum correlations are properly distributed at some instant $t_0$, this distribution will be destroyed owing to the quantum evolution. Alternately, in a system with the stationary discord, we only have to take care about the proper initial quantum correlations. Consequently, we receive the relatively simple tool to handle the quantum correlations varying the initial state and perhaps the type of quantum interactions in a system.

Note that the nodes in the system of the above virtual particles with stationary pairwise discord/entanglement are not localized in the physical space, which makes obstacles in organization of the impact on the state of a particular virtual particle using the classical environment. For this reason, the interface between the operator and quantum device must be significantly modified, which is a subject of further study. However, all representations are equivalent from the standpoint of interactions inside of a quantum system. Thus, we assume that the systems of virtual particles with stationary distribution of discord/entanglement will be useful in organization of those parts of quantum algorithms where the interaction with the operator is absent (“inner” quantum algorithms).

The paper is organized as follows. In Sect. 2, we formulate general statements on the existence of systems of virtual particles with the stationary pairwise discord in an arbitrary quantum system. Generalizing the idea of ref. [20], we show that the stationary entanglement/discord is associated with the system of virtual particles whose eigenstates diagonalize the Hamiltonian governing the dynamics of a quantum system. In Sect. 3, we consider the spin dynamics in the spin-1/2 system governed by the XY-Hamiltonian and reveal general properties of the stationary entanglement/discord in this case. Then, in Sect. 4, using the numerical simulations, we construct the stationary pairwise discord distributions among the virtual particles in the open spin-1/2 chain of $N = 41$ nodes (odd $N$) governed by the XY Hamiltonian using two types of initial conditions: (i) a single initially excited node and (ii) a single initially polarized node. In the case of a single initially excited node, we consider both the approximation of nearest neighbor interactions and the model with the dipole–dipole interactions (DDIs) among all nodes and demonstrate that the later does not significantly deform the
distribution of the stationary pairwise quantum entanglement/discord in the system. In the case of a single initially polarized node, we consider only the nearest neighbor approximation. In this case the entanglement is zero for the long chains $N > 4$ so that the discord is a proper measure of quantum correlations in this case. We discuss our results in Sect. 5. Some auxiliary calculations are given in the “Appendix”, Sect. 6.

2 Basis of virtual particles with stationary pairwise discord

The discord and entanglement in a quantum system are evolving quantities in general. Their evolution is determined by the Hamiltonian $H$ governing the dynamics of a quantum system. However, there is a basis of virtual particles possessing the stationary discord. Below we consider the Hamiltonian commuting with the $z$-projection of the total spin momentum $I_z$ and show that such basis is that of eigenvectors of Hamiltonian $H$ provided that one of two following types of initial density matrices $\rho_0$ is considered: (i) the initial state with a single excited spin and (ii) the initial state with a single polarized spin.

First, we represent the evolution of the density matrix as

$$\rho(t) = e^{-iHt} \rho_0 e^{iHt},$$

where $\rho_0$ is the initial density matrix. Diagonalizing $H$ we have

$$H = U \Lambda U^+,$$

where $\Lambda$ is the diagonal matrix of eigenvalues of the Hamiltonian $H$ and $U^+$ is the matrix of its eigenvectors. In the basis of these eigenvectors, the evolution of the density matrix reads

$$\rho^H(t) = \hat{E} \rho_0^H \hat{E}^+, \quad \rho_0^H = U^+ \rho_0 U, \quad \hat{E} = e^{-i\Lambda t}.$$

To proceed further one has to fix a particular initial density matrix $\rho_0$.

2.1 Single initially excited node in system of spin-1/2 particles

In this section we derive the formulas for the stationary entanglement/discord in a system of spin-1/2 particles with a single initially excited spin. The dynamics of the quantum system of $N$ nodes governed by any Hamiltonian commuting with $I_z$ (the $z$-projection of the total spin) can be described in the $N$-dimensional basis $|n\rangle$, $n = 1, \ldots, N$, where $n$ means that $n$th spin is excited (i.e. directed opposite to the strong magnetic field) while other spins are arranged along the magnetic field. The initial density matrix $\rho_0$ corresponding to the $j$th initially excited spin is defined by its elements as

$$(\rho_0)_{nm} = \delta_{nj} \delta_{mj}.$$
Then we can write

\[
(\rho^H_{0})_{nm} = U^*_jn U_{jm}.
\]  

(5)

As a consequence, we have the relation

\[
|(|\rho^H_{0})_{nm}\rangle|^2 = (\rho^H_{0})_{nn}(\rho^H_{0})_{mm}.
\]  

(6)

Since the evolution of the density matrix elements \(\rho^H_{nm}\) reads as

\[
\rho^H_{nm}(t) = (\rho^H_{0})_{nm} \exp(-i(\Lambda_n - \Lambda_m)t),
\]  

(7)

then, taking into account Eq. (6), we have

\[
|\rho^H_{nm}|^2 = \rho^H_{nn}\rho^H_{mm},
\]  

(8)

so that the diagonal elements do not evolve as well as \(|\rho^H_{nm}|\) for any \(n\) and \(m\). This property of the density matrix \(\rho^H\) results in the stationary discord and entanglement.

Next, we reduce the density matrix \(\rho^H\) with respect to all nodes except for the \(n\)th and \(m\)th ones. Emphasize that now we deal with the system of virtual particles rather than with the system of spin-1/2 particles. Introduce the standard notations for the basis of two particles

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

(9)

where \(n\) and \(m\) in \(|nm\rangle\) mean the different filling numbers for the fermion-like particles. In this basis, the reduced density matrix reads [34]:

\[
\rho^{(nm)} = \begin{pmatrix}
\sigma_{nm} & 0 & 0 & 0 \\
0 & \rho_{nn} & \rho_{nm} & 0 \\
0 & \rho_{mn} & \rho_{mm} & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}, \quad \sigma_{nm} = \sum_{i \neq n,m} \rho_{ii} = 1 - \rho_{nn} - \rho_{mm}, \quad n \neq m.
\]

(10)

Note that the last zero in the main diagonal of the reduced density matrix \(\rho^{(nm)}\) appears because the single node was excited initially and the total projection \(I_z\) commutes with the XY Hamiltonian.

2.1.1 Concurrence

We characterize the entanglement by the Wootters criterion in terms of the concurrence [1,2]. According to [1,2], one needs to construct the spin-flip density matrix

\[
\tilde{\rho}_{(nm)}(\tau) = (\sigma_y \otimes \sigma_y)(\rho^{(nm)})^*(\tau)(\sigma_y \otimes \sigma_y),
\]  

(11)
where the asterisk denotes the complex conjugation and the Pauli matrix \( \sigma_y = 2I_y \). The concurrence for the density matrix \( \rho_{nm}(\tau) \) is equal to

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

where \( \lambda_1, \lambda_2, \lambda_3 \) and \( \lambda_4 \) are the square roots of the eigenvalues of the matrix product \( \rho_{nm}(\tau)\tilde{\rho}_{nm}(\tau) \). For the density matrix \( \rho \) given by Eq. (10) we have only one nonzero \( \lambda \):

\[
\lambda = \lambda_1 = 2\sqrt{\rho_{nn}\rho_{mm}}
\]

Substituting Eqs. (13) into (12) we obtain

\[
C_{nm} = \max \left(0, 2\sqrt{\rho_{nn}\rho_{mm}}\right), \quad n \neq m.
\]

2.1.2 Discord

The matrix (10) is so-called the X-matrix whose discord has been studied in [12]. Although this reference contains a mistake concerning the number of arbitrary optimization parameters in the calculation of the classical part of mutual correlations (see erratum in refs. [12] and [35]), this mistake has no value in our case because the element \( \rho_{14} \) is zero in all density matrices considered below and relation (8) holds. As a consequence, we have only one optimization parameter, which we denote by \( \eta \) [see Eqs. (21, 22)]. Thus, we use the algorithm developed in the above reference for the calculation of discord. Remind that the discord between the particles \( n \) and \( m \) of a biparticle quantum system may be calculated as

\[
Q_m = I(\rho) - C^m(\rho),
\]

provided that the von Neumann type measurements are performed over the particle \( m \). Here, \( I(\rho) \) is the total mutual information [8] which may be written as follows:

\[
I(\rho) = S(\rho^{(n)}) + S(\rho^{(m)}) + \sum_{j=0}^{1} \lambda_j \log_2 \lambda_j,
\]

where \( \lambda_j (j = 0, 1) \) are the non-zero eigenvalues of the density matrix \( \rho^{(nm)} \),

\[
\lambda_0 = \rho_{mm} + \rho_{nn}, \quad \lambda_1 = 1 - \lambda_0,
\]

\( \rho^{(n)} = \text{Tr}_m \rho^{(nm)} \) and \( \rho^{(m)} = \text{Tr}_n \rho^{(nm)} \) are the reduced density matrices and the appropriate entropies \( S(\rho^{(n)}) \) and \( S(\rho^{(m)}) \) are given by the following formulas:

\[
S(\rho^{(n)}) = -(1 - \rho_{mm}) \log_2 (1 - \rho_{mm}) - \rho_{mm} \log_2 \rho_{mm},
\]

\[
S(\rho^{(m)}) = -(1 - \rho_{nn}) \log_2 (1 - \rho_{nn}) - \rho_{nn} \log_2 \rho_{nn}.
\]
The so-called classical counterpart $C^B(\rho^{(nm)})$ of the mutual information can be found considering the minimization over the projective measurements performed on the subsystem $B$ as follows [12]:

\[
C^{(m)}(\rho) = S(\rho^{(n)}) - \min_{\eta \in [0,1]} (p_0 S_0 + p_1 S_1),
\]

where

\[
S(\theta_i) \equiv S_i = -\frac{1 - \theta_i}{2} \log_2 \frac{1 - \theta_i}{2} - \frac{1 + \theta_i}{2} \log_2 \frac{1 + \theta_i}{2},
\]

\[
p_i = \frac{1}{2} \left( 1 + (-1)^i \eta (1 - 2 \rho_{nn}) \right),
\]

\[
\theta_i = \frac{1}{p_i} \left[ (1 - \eta^2) \rho_{nn} \rho_{mm} + \frac{1}{4} \left( 1 - 2 \rho_{mm} + (-1)^i \eta (1 - 2 (\rho_{nn} + \rho_{mm})) \right) \right]^{1/2}, i = 0, 1.
\]

Here we introduce the parameter $\eta$ instead of $k$ in [12], $k = (1 + \eta)/2$. It is simple to show that the quantum discord $Q_n$ obtained performing the von Neumann type measurements on the particle $n$ can be calculated as follows:

\[
Q_n = Q_m \big|_{\rho^{(nn)} \leftrightarrow \rho^{(mm)}},
\]

for the system with the density matrix $\rho^{(nm)}$ given by Eq. (10). Then we define the discord $Q_{nm}$ as the minimum of $Q_n$ and $Q_m$ [36]

\[
Q_{nm} = \min(Q_n, Q_m), \ n \neq m
\]

with the obvious property $Q_{nm} = Q_{mn}$. We see that, since $\rho_{nn}$ and $\rho_{mm}$ do not depend on time, the discord does not evolve as well.

Similar to [20], we can show that the minimum in Eq. (19) corresponds to $\eta = 0$ (the proof of this statement is given in “Appendix”, Sect. 6), so that we result in the following explicit formula for the discord between any two nodes:

\[
Q_m = 1 - \rho_{nn} \log_2 \rho_{nn} - (1 - \rho_{nn}) \log_2 (1 - \rho_{nn}) + (\rho_{nn} + \rho_{mm}) \log_2 (\rho_{nn} + \rho_{mm})
+ (1 - \rho_{nn} - \rho_{mm}) \log_2 (1 - \rho_{nn} - \rho_{mm})
- \frac{1}{2} \left( 1 - \sqrt{1 - 4 \rho_{mm}(1 - \rho_{nn} - \rho_{mm})} \right) \log_2 (1 - \sqrt{1 - 4 \rho_{mm}(1 - \rho_{nn} - \rho_{mm})})
- \frac{1}{2} \left( 1 + \sqrt{1 - 4 \rho_{mm}(1 - \rho_{nn} - \rho_{mm})} \right) \log_2 (1 + \sqrt{1 - 4 \rho_{mm}(1 - \rho_{nn} - \rho_{mm})})
\]

We see that both the discord $Q_m$ and the concurrence $C_m$ are zero if either $\rho_{nn}$ or $\rho_{mm}$ is zero.
2.2 Single initially polarized node

The initial state with a single excited spin considered in Sect. 2.1 is hard for the realization in the experiment and is associated with low temperatures. On the contrary, the initial state with a single polarized node is realizable even at high temperatures [18,19]. This is a motivation to consider the discord in a chain with the initially polarized spin.

The stationary discord in the homogeneous spin-1/2 chain with single initially polarized node governed by the XY-Hamiltonian was introduced in [20]. Here we represent the more detailed analysis of that case and generalize results on the non-homogeneous spin-1/2 chain keeping the approximation of nearest neighbor interactions.

For a non-homogeneous chain, similar to ref. [20], we take advantage of the Jordan–Wigner transformation [27]. Let us emphasize that this transformation is applicable to any Hamiltonian at the approximation of the nearest neighbor interactions. Let $I_{i\alpha}$ ($i = 1, \ldots, N, \alpha = x, y, z$) be the $i$th spin projection on the $\alpha$-axis. The initial density matrix $\rho_0$ corresponding to the initial state of the spin system with the single polarized $j$th node ($1 \leq j \leq N$) at arbitrary temperature reads [19,20]

$$\rho_0 = \frac{e^{\beta I_{jz}}}{Z} = \frac{1}{2^N} \left(1 + 2 I_{jz} \tanh \frac{\beta}{2}\right), \quad Z = \text{Tr}(e^{\beta I_{jz}}) = 2^N \cosh \frac{\beta}{2}, \quad (26)$$

where $\beta = \frac{\hbar \omega_0}{k T}$ is the dimensionless inverse temperature, $\hbar$ is the Planck constant, $k$ is the Boltzmann constant, and $T$ is the temperature of the system. The evolution of the density matrix reads:

$$\rho(t) = e^{-itH} \rho_0 e^{itH} = \frac{1}{2^N} e^{-iHt} \left(1 + 2 I_{jz} \tanh \frac{\beta}{2}\right) e^{iHt}. \quad (27)$$

Diagonalizing the Hamiltonian using the Jordan–Wigner transformation method [27] we result in the following operator representation of the Hamiltonian $H$:

$$H = \sum_k \varepsilon_k \beta_k^+ \beta_k, \quad (28)$$

where the fermion operators $\beta_k$ are defined in terms of the other fermion operators $c_j$ by means of the transformation (which reduces to the Fourier transformation in the case of homogeneous spin-1/2 chain)

$$\beta_k = \sum_{j=1}^{N} U_{kj} c_j, \quad (29)$$

and the fermion operators $c_j$ are defined as [27]

$$c_j = (-2)^{j-1} I_1 I_2 \ldots I_{j} I_{j+1} \ldots I_{N}, \quad (30)$$
Here the eigenvalues $\varepsilon_k$ and the matrix of eigenvectors $U_{kj}$ depend on the particular Hamiltonian. Then the density matrix (27) can be transformed to the following form [19]

$$
\rho(t) = \frac{1 - \tanh \frac{\beta}{2} t}{2^N} + \tanh \frac{\beta}{2} \frac{t}{2^{N-1}} \sum_{k,k'} e^{-it(\varepsilon_k - \varepsilon_{k'})} U_{kj} U_{k'j} \beta_k^+ \beta_{k'},
$$

(31)

(here we take into account reality of $U_{kj}$). Similar to [20], we will study the quantum correlations between any two $\beta$-fermions.

The first step in calculation of the discord between the $n$th and $m$th nodes is the construction of the reduced density matrix with respect to all nodes except for the $n$th and $m$th ones. We use notations (9) for the vectors of the $\beta$-fermion basis. Reducing density matrix (31) we obtain:

$$
\rho^{(nm)}(t) = \frac{1}{4} - \frac{\tanh \frac{\beta}{2}}{4} (U_{nj}^2 + U_{mj}^2) + \frac{\tanh \frac{\beta}{2}}{2} \sum_{k,k'=n,m} e^{-it(\varepsilon_k - \varepsilon_{k'})} U_{kj} U_{k'j} \beta_k^+ \beta_{k'}^+.
$$

(32)

Its matrix representation in the basis (9) reads

$$
\rho^{(nm)} = \begin{pmatrix}
J_{00}^\beta + J_{mm}^\beta + J_{nn}^\beta & 0 & 0 & 0 \\
0 & J_{00}^\beta + J_{mm}^\beta & J_{mn}^\beta & 0 \\
0 & J_{nm}^\beta & J_{00}^\beta + J_{nn}^\beta & 0 \\
0 & 0 & 0 & J_{00}^\beta
\end{pmatrix},
$$

(33)

where

$$
J_{00}^\beta = \frac{1}{4} - \frac{\tanh \frac{\beta}{2}}{4} (U_{nj}^2 + U_{mj}^2),
$$

(34)

$$
J_{nn}^\beta = \frac{\tanh \frac{\beta}{2}}{2} e^{-it(\varepsilon_n - \varepsilon_m)} U_{nj} U_{mj}
$$

It is obvious that

$$
J_{nn}^\beta = \frac{\tanh \frac{\beta}{2}}{2} U_{nj}^2,
$$

(35)

which does not depend on the time $t$. Then [20]

$$
Q_m = -\frac{1}{2} \left( (1 - 2J_{nn}) \log_2 (1 - 2J_{nn}) + (1 + 2J_{nn}) \log_2 (1 + 2J_{nn}) \\
- (1 - 2J_{mm} - 2J_{nn}) \log_2 (1 - 2J_{mm} - 2J_{nn}) \\
- (1 + 2J_{mm} + 2J_{nn}) \log_2 (1 + 2J_{mm} + 2J_{nn}) \\
+ (1 - 2\sqrt{J_{mm}(J_{mm} + J_{nn})}) \log_2 (1 - 2\sqrt{J_{mm}(J_{mm} + J_{nn})}) \\
+ (1 + 2\sqrt{J_{mm}(J_{mm} + J_{nn})}) \log_2 (1 + 2\sqrt{J_{mm}(J_{mm} + J_{nn})}) \right).
$$

(36)
The discord $Q_{nm}$ is defined by Eq. (24) with $Q_n$ from Eq. (23). Similar to Sect. 2.1, the discord $Q_{nm}$ is zero if either $J_{nn}$ or $J_{mm}$ is zero. Emphasize, that the formula (36) for the pairwise discord $Q_n$ in the arbitrary non-homogeneous chain coincides with that derived for the homogeneous chain in [20] up to the definition of elements $J_{nn}$ (35) where $U_{nj}$ are the elements of the $j$th eigenvector of the Hamiltonian $H$ governing the dynamics of the non-homogeneous chain.

3 Dynamics in spin-1/2 chain with XY Hamiltonian and general properties of stationary discord

We consider a one-dimensional open chain of spin-1/2 particles in the strong external magnetic field governed by the XY Hamiltonian

$$H = \sum_{i,j=1}^{N} \sum_{j>i} D_{i,j} (I_{i,x} I_{j,x} + I_{i,y} I_{j,y}), \quad D_{i,j} = \frac{\gamma^2 \hbar}{2 r_{i,j}^2}. \quad (37)$$

Here $D_{i,j}$ is the coupling constant between the $i$th and the $j$th nodes. Hereafter we will use the dimensionless time $\tau$, distances $\xi_{n,m}$, coupling constants $d_{n,m}$ defined as follows:

$$\tau = D_{1,2} t, \quad \xi_{n,m} = \frac{r_{n,m}}{r_{1,2}}, \quad d_{n,m} = \frac{D_{n,m}}{D_{1,2}} = \frac{1}{\xi_{n,m}^3}, \quad d_{1,2} = 1. \quad (38)$$

Using definitions (38), the Hamiltonian (37) may be written as follows:

$$H = D_{1,2} H, \quad H = \sum_{i,j=1}^{N} \sum_{j>i} d_{i,j} (I_{i,x} I_{j,x} + I_{i,y} I_{j,y}). \quad (39)$$

For the nearest neighbor interaction approximation we write $d_{i,j} = d_1 \delta_{j,i+1}, \ j > i$.

3.1 Homogeneous chain with nearest neighbor interaction approximation

First, we consider the homogeneous spin-1/2 chain, i.e. $d_i = d \equiv 1, \ i = 1, \ldots, N - 1$. In this case we have the following formulas for the eigenvalues and eigenvectors of the Hamiltonian [19]:

$$\varepsilon_k = \cos \frac{\pi k}{N + 1}, \quad U_{kj} = \sqrt{\frac{2}{N + 1}} \sin \frac{\pi k j}{N + 1}, \quad (40)$$

which hold for the initial state with both a single excited node and a single polarized node. Consequently,
\begin{align}
\rho_{nn} = U_{nj}^2 &= \frac{2}{N + 1} \sin^2 \frac{\pi nj}{N + 1}, \quad \text{(41)} \\
J_{nn} = \tanh \frac{\beta}{2} U_{nj}^2 &= \tanh \frac{\beta}{2} \frac{N + 1}{\sin^2 \frac{\pi nj}{N + 1}}, \quad \text{(42)}
\end{align}

These expressions must be substituted into Eqs. (14), (25) and (36). The most simple is the expression for the concurrence in the case of the XY Hamiltonian with a single excited node (remember that the concurrence in the case of a single polarized node is zero for long chains [20]):

\begin{equation}
C_{nm}(j) = \frac{4}{N + 1} \sin \frac{\pi nj}{N + 1} \sin \frac{\pi mj}{N + 1}.
\end{equation}

Now we reveal some properties of the pairwise entanglement/discord distribution among the virtual particles. We can always write

\begin{equation}
\frac{j}{N + 1} = \frac{m_1}{m_2},
\end{equation}

where \(m_1\) and \(m_2\) are integers. If \(m_2 < N + 1\), i.e. the integers \(j\) and \(N + 1\) have the common factor, then the discord and the concurrence reveal the periodic behavior with zeros at such nodes \(n\) that

\begin{equation}
\frac{n_j}{N + 1} = 1.
\end{equation}

In the periodic case, the concurrence \(C_{nm}\) and/or the discord \(Q_{nm}\) take several different values depending on \(n\) and \(m\). The number of these values is defined by the number of different pairs of values of \(\rho_{nn}\) and \(\rho_{nm}\) (41), \(n, m = 1, \ldots, N\).

For our convenience, let us use superscripts \(\text{ex}\) and \(\text{pol}\) to mark quantities associated with the initially excited and the initially polarized single node respectively, i.e. we will write \(Q_{nm}^{\text{ex}}, Q_{nm}^{\text{pol}}, C_{nm}^{\text{ex}}\) (while \(C_{nm}^{\text{pol}} \equiv 0\) for long chains). Next, we formulate several statements on existence of large clusters of nodes with equal pairwise discord (concurrence) for odd \(N\).

1. If \(N\) is odd and \(j = (N + 1)/2\), then Eq. (41) yields only one non-zero value for \(\rho_{nn}\):

\begin{equation}
\rho_1 \equiv \rho_{nn} = \frac{2}{N + 1}, \quad n = 1, 3, 5, \ldots \quad \text{(46)}
\end{equation}

In this case the nonzero pairwise discord appears only among the odd nodes and its value is the same for any pair of odd nodes:

\begin{equation}
Q_{1, k_1+1,k_2+1}^{\text{ex, pol}} = Q_{13}^{\text{ex, pol}}, \quad k_1, k_2 = 1, 3, \ldots k_2 > k_1 \quad \text{(47)}
\end{equation}

(we do not represent the explicit formula for discord). The concurrence reads in this case:
\[ C_{1}^{ex} = C_{2k_1+1,2k_2+1}^{ex} = C_{13}^{ex} = \frac{4}{N+1}, \quad k_1, k_2 = 0, 1, 2, \ldots, k_2 > k_1. \] (48)

2. If \( N = 5 + 6i, i = 1, 2, \ldots \), and \( j = \frac{N+1}{3} = 2(i + 1) \), then again we have only one nonzero value for \( \rho_{nn} \),

\[ \rho_1 = \rho_{nn} = \frac{2}{N+1} \sin^2 \frac{\pi}{3} = \frac{3}{2(N+1)}, \quad n = 3k - 1, \ 3k - 2, \]
\[ k = 0, 1, 2, \ldots, 2i + 2, \] (49)

The nonzero discord will be only among the nodes from the set \( \{3k - 1, \ 3k - 2, \ k = 1, \ldots, 2i + 2\} \) and is the same for any pair from this set. It reads:

\[ Q_{1, pol}^{ex} = Q_{12, pol}^{ex}, \] (50)

and is given by Eqs. (23, 24, 25, 36) with proper substitutions for \( J_{ii}, \rho_{ii}, i = n, m \).

The concurrence between any pair from this set reads:

\[ C_{1}^{ex} = C_{12}^{ex} = \frac{3}{N+1}. \] (51)

3. In general, if \( \frac{j}{N+1} = \frac{m_1}{m_2} \), then

\[ \rho_{nn} = \frac{2}{N+1} \sin^2 \frac{\pi mn_1}{m_2}, \] (52)

which is nonzero if the ratio \( \frac{mn_1}{m_2} \) is not integer. Therewith for any \( n_1 \) and \( n_2 \) such that \( \frac{n_1m_1}{m_2} = 1 \pm \frac{n_2m_1}{m_2} \) we have \( \rho_{n_1n_1} = \rho_{n_2n_2} \).

3.2 Alternating chain with odd \( N \) and nearest neighbor interaction approximation

In this case \( d_1 = d_{2n-1} = 1, d_2 = d_{2n}, n = 1, 2, \ldots \) and we use the parameter \( \delta = d_2/d_1 = d_2 \) as the dimerization degree. It is known that the Hamiltonian is analytically diagonalizable in this case for both odd [37] and even \( N \) [40].

It can be readily shown that, if \( N \) is odd and the excited node \( j \) is even, then the discord coincides with that calculated for the homogeneous chain [20]. In fact, using formulas for the eigenvalues and the eigenvectors of the XY Hamiltonian derived in ref. [37], we conclude that both eigenvalues and eigenvectors of the XY Hamiltonian involved in the calculation of the concurrence/discord in this case coincide with those used for the calculation of the pairwise discord in the homogeneous chain, see Eq. (40). If \( j \) is odd, then the discord depends on the dimerization degree \( \delta \). However, we have found that if \( \delta \to 0 \) (the limit of the non-interacting dimers) then the following expressions for the eigenvalues follow from the formulas of ref. [37]
2\varepsilon_k = \lambda_k = \begin{cases} \frac{d_1}{\sqrt{2}}, & k = 1, 2, \ldots, \frac{N-1}{2} \\ 0, & k = \frac{N+1}{2} \\ -\frac{d_1}{\sqrt{2}}, & k = \frac{N+1}{2} + 1, \frac{N+1}{2} + 2, \ldots, N \end{cases}.

(53)

For the elements of the eigenvectors at $k \neq \frac{N+1}{2}$ we have

$$U_{kj} = \begin{cases} \frac{d_1}{\sqrt{2}} \sin \left( \frac{\pi k(j+1)}{N+1} \right), & j = 1, 3, 5, \ldots, N \\ \sqrt{\frac{2}{N+1}} \sin \left( \frac{\pi kj}{N+1} \right), & j = 2, 4, \ldots, N - 1 \end{cases},$$

(54)

Finally, at $k = \frac{N+1}{2}$, we obtain

$$U_{j,(N+1)/2} = \begin{cases} 1, & j = N \\ 0, & j \neq N \end{cases}.$$

(55)

Formulas (54, 55) demonstrate that, in this case, the eigenvectors corresponding to the odd and even initially excited node $j$ are very similar up to the shift $j \to j + 1$. Consequently, for small dimerization parameter $\delta$, discords corresponding to $j = 2n$ and $j = 2n - 1$ are very similar. In addition, the discord vanishes if $j = N$.

We shall emphasize that, considering the stationary discord in the basis of the Hamiltonian eigenstates, we obtain quantum correlations even in a system of non-interacting dimers, $\delta \to 0$. This is consequence of the diagonalization process, which involves all nodes regardless of the values of their interactions.

### 4 Numerical simulations of the dynamics in spin chain with odd $N$, $N = 41$

All calculations of this section are performed for the spin chain with odd $N$. The stationary pairwise discord distribution for the even $N$ is essentially the same.

Both models with the nearest neighbor interaction approximation and with the dipole–dipole interactions (DDIs) among all nodes are considered. In this regard, it is important to note that the interactions among the remote nodes effect significantly on the entanglement between the spin-1/2 particles and on the state transfer process along the spin-1/2 chains [25]. However, the stationary discord is much less sensitive to the remote node interactions, which only deform the distribution of the pairwise stationary discord among the nodes, see Sect. 4.1. This happens because the time evolution of the entanglement (and the polarization) is very sensitive to the interactions of the remote nodes. In general, these interactions speed up the signal propagation. However, the evolution is “averaged” in the stationary discord so that the effect of remote nodes is suppressed.

Hereafter we study the pairwise discord using different initial states with either single excited or single polarized spin. We say that two nodes are correlated if the corresponding concurrence and/or discord are non-vanishing.
4.1 Single excited node: homogeneous spin chain

Now we apply formulas (46–52) to the homogeneous spin chain of \( N = 41 \) nodes. Because of the symmetry, it is enough to consider the initially excited nodes \( j \leq \frac{N+1}{2} \) (for odd \( N \)). First we calculate the discord using the nearest neighbor interaction approximation. The basic results are following:

1. If \( j = 1 \), then all nodes are correlated. Both the discord and the concurrence increase to the center of the chain of virtual particles, Fig. 1a.

2. From Eqs. (41–43) it follows that the discord and the concurrence are the periodic function of \( n \) if \( j = 6, 7, 12, 14, 18, 21 \). For instance, if \( j = 7 \) (see Fig. 1b) than we have three different values for \( \rho_{nn} \):

\[
\rho_{nn} = \rho_1 = \frac{1}{84}, \quad n = 6i + 1, 6i + 5, \quad i = 0, 1, \ldots, 6, \\
\rho_{nn} = \rho_2 = \frac{1}{28}, \quad n = 6i + 2, 6i + 4, \quad i = 0, 1, \ldots, 6, \\
\rho_{nn} = \rho_3 = \frac{1}{21}, \quad n = 6i + 3, \quad i = 0, 1, \ldots, 6.
\]

They produce six different values of the discord

\[
Q_{1ex} = Q_{15ex} \approx 0.023, \quad Q_{2ex} = Q_{24ex} \approx 0.067, \quad Q_{3ex} = Q_{39ex} \approx 0.088, \\
Q_{4ex} = Q_{12ex} \approx 0.036, \quad Q_{5ex} = Q_{13ex} \approx 0.040, \quad Q_{6ex} = Q_{23ex} \approx 0.076, \quad (57)
\]

and of the concurrence

\[
C_{1ex} = C_{15ex} = \frac{1}{42}, \quad C_{2ex} = C_{24ex} = \frac{1}{14}, \quad C_{3ex} = C_{39ex} = \frac{2}{21}, \\
C_{4ex} = C_{12ex} = \frac{1}{14\sqrt{3}}, \quad C_{5ex} = C_{13ex} = \frac{1}{21}, \quad C_{6ex} = C_{23ex} = \frac{1}{7\sqrt{3}}. \quad (58)
\]

Fig. 1 The distribution of the stationary pairwise discord \( Q_{nm} \) among the virtual particles in the homogeneous spin-1/2 chain with \( N = 41 \) at the nearest neighbor interaction approximation. For convenience, we take \( Q_{nn} \) equal to zero which is indicated in all pictures below. The initially excited nodes are following. a \( j = 1 \), the discord distribution is bell-shaped. b \( j = 7 \), the discord takes six different values given in Eq. (57), nodes \( n = 6i, i = 1, \ldots, 6 \), do not correlate with others.
Fig. 2 The distribution of the stationary pairwise discord $Q_{nm}$ among the virtual particles in the homogeneous spin-1/2 chain with $N = 41$; interactions among all nodes are taken into account; the initially excited node is $j = 7$. This distribution only slightly differs from that shown in Fig. 1b.

We see that the correlations are most strong among the nodes from the set $\{6i + 3; \ i = 0, 1, \ldots, 6\}$. The set of nodes $\{6i + 2, 6i + 4; \ i = 0, 1, \ldots, 6\}$ is less correlated with the first one. The correlations with the set $\{6i + 1, 6i + 5; \ i = 0, 1, \ldots, 6\}$ are minimal. Nevertheless, all nodes are correlated except for the nodes $n = 6i, i = 1, \ldots, 6$ because all the pairwise discords involving these nodes are zeros.

3. If $j = 14$, then we have one nonzero value for the elements $\rho_{nn}$ with $n = 3i - 1, 3i - 2, i = 1, \ldots, 13$:

$$\rho_{nn} = \rho_1 = \frac{1}{28}.$$  \hfill (59)

The appropriate nonzero discord and concurrence are following:

$$Q^e_1 = 0.067, \quad C^e_1(\rho_1, \rho_1) = \frac{1}{14}. \hfill (60)$$

Thus, the pairwise concurrences and/or discords are nonzero and take the same values for any pair of nodes from the cluster $\{3i - 1, 3i - 2; \ i = 1, 2, \ldots, 13\}$.

4. If $j = 21$, then, again, there is only one nonzero value $\rho_{nn}$ for all odd $n$:

$$\rho_1 \equiv \rho_{nn} = \frac{1}{21}, \quad n = 2i - 1, \quad i = 0, 1, \ldots, 21.$$  \hfill (61)

The appropriate values of the discord and concurrence are

$$Q^e_1 = 0.088, \quad C^e_1 = \frac{2}{21}. \hfill (62)$$

Thus, the pairwise concurrences/discords are nonzero and equal each other for any pair from the family of odd nodes.

It is remarkable, that the concurrence has the same distribution among nodes as discord. For this reason we do not represent the figures with the concurrence distribution. In addition, we verify that, involving the interactions among all nodes, the discord distribution does not become significantly deformed, which confirms the arguments given in the beginning of Sect. 4. As an example, in Fig. 2, we represent the discord distribution corresponding to the 7th initially excited spin (i.e. $j = 7$) and the Hamiltonian involving the DDIs among all nodes of the spin chain.
Fig. 3 The stationary pairwise discord $Q_{nm}$ among the virtual particles in the alternating spin-$1/2$ chain with $N = 41$, $\delta = 0.1$; a the distribution of the discord for the initially excited node $j = 14$; b the distribution of $\text{abs}(Q_{nm}|j=14 - Q_{nm}|j=13)$

4.2 Single excited node: non-homogeneous spin chains

In this section we show that varying either the coupling constants in the Hamiltonian or the initially excited node we may handle the size of the cluster of the correlated particles. Having this possibility, we may select the cluster of required nodes from the whole chain of virtual particles which is necessary for flexibility of the quantum algorithms. In this regards we notice that the problem of variation of the coupling constants may be effectively resolved using, for instance, the optical lattice [38]. In addition, the effect of variable coupling constants in spin chains may be effectively replaced with the variable magnetic field [39] surrounding the spin chain.

4.2.1 Alternating spin chain

As was mentioned in Sect. 3.2, the diagonalization of the alternating XY Hamiltonian $H$ describing the nearest neighbor interaction approximation may be performed analytically [37,40]. Remember also that, for even initially excited nodes $j$, the discord/entanglement distribution coincides with that obtained for the homogeneous spin-$1/2$ chain. The basic novelty of the alternating chain is that related with the small dimerization parameter $\delta$. We verify the conclusion of Sect. 3.2 that the discord distributions corresponding to $j = 2i$ and $2i - 1$ are very similar, $i = 1, 2, \ldots, 20$. As an example, in Fig. 3a, we represent the discord distribution corresponding to $j = 14$ for the small dimerization parameter $\delta = 0.1$. To confirm that this distribution is very similar to the distribution found for $j = 13$, we turn to Fig. 3b, where the distribution of the absolute values of the differences between both discords, $\text{abs}(Q_{nm}|j=14 - Q_{nm}|j=13)$, is depicted. In both cases, the strongly correlated nodes are $3i - 1, 3i - 2, i = 1, 2, \ldots$. Again, taking into account the DDIs among all nodes we only deform the stationary pairwise discord distribution.

4.2.2 3-alternating chain

Consider the 3-alternating chain $d_{3i+1} = d_1 \equiv 1, d_{3i+2} = d_2 = 1/2$ and $d_{3i} = d_3 = 1/4, i = 0, 1, 2, \ldots, 13$ [41]. We show only the discord distributions corresponding
The distribution of the stationary pairwise discord $Q_{nm}$ among the virtual particles in the 3-alternating spin-1/2 chain with $N = 41$ at the approximation of the nearest neighbor interactions. The initially excited spins are following: a $j = 2$, nodes $k = 14 – 28$ are excluded from the cluster of correlated virtual particles, b $j = 20$, the cluster involves nodes $k = 1, 3, 5, 7, 9, 11, 13, 15, 29, 31, 33, 35, 37, 39, 41$, c $j = 21$, the cluster involves nodes $k = 15, 17, 19, 21, 23, 25, 27$, d $j = 40$, nodes 14 and 28 are strongly correlated between themselves.

Thus, adding one more parameter (the coupling constant $d_3$) allows us to create additional types of the correlated clusters.

4.2.3 Symmetric chain with $d_i = \sqrt{\frac{i(N-i)}{\sqrt{Nn-1}}}$, $1 \leq i \leq 20$ [21]

Considering other variants of alternating chains we may achieve a large variety of different clusters of virtual particles. We represent one more example of the spin chain introduced in [21] for the purpose of realization of the perfect state transfer along the long spin-1/2 chain governed by the XY Hamiltonian at the nearest neighbor interactions.

---

**Fig. 4** The distribution of the stationary pairwise discord $Q_{nm}$ among the virtual particles in the 3-alternating spin-1/2 chain with $N = 41$ at the approximation of the nearest neighbor interactions. The initially excited spins are following: a $j = 2$, nodes $k = 14 – 28$ are excluded from the cluster of correlated virtual particles, b $j = 20$, the cluster involves nodes $k = 1, 3, 5, 7, 9, 11, 13, 15, 29, 31, 33, 35, 37, 39, 41$, c $j = 21$, the cluster involves nodes $k = 15, 17, 19, 21, 23, 25, 27$, d $j = 40$, nodes 14 and 28 are strongly correlated between themselves.
**Fig. 5** The distribution of the stationary pairwise discord \( Q_{nm} \) among the virtual particles in the symmetrical spin-1/2 chain, \( d_i = \frac{\sqrt{i(N-i)}}{N-1}, 1 \leq i \leq 20, \) with \( N = 41 \) at the nearest neighbor interaction approximation; the initially excited nodes are following: a \( j = 1, \) the distribution is bell shaped with smaller cluster of the correlated nodes than in the homogeneous chain with \( j = 1, \) Fig. 1; b \( j = 21, \) the family of odd nodes forms the cluster of correlated nodes.

interaction approximation. It is remarkable that the dimensionless time interval needed for the perfect excited state transfer between end nodes does not depend on the length of the chain and equals \( \pi. \)

The most interesting pairwise discord distributions are following.

1. \( j = 1, \) the cluster of nodes \( n = 11 - 29 \) is formed, Fig. 5a, which is similar (but smaller) to the cluster in Figs. 1a and 4a

2. \( j = 21, \) the cluster of odd nodes is formed, Fig. 5b, but, unlike the homogeneous chain with the initially excited spin \( j = 21, \) the pairwise discord is not the same for all pairs.

### 4.3 Spin-1/2 chains with a single initially polarized node

As mentioned in Sect. 2.2, this initial state is more realistic and may be created at high temperatures. However, one has to remember the overall effect of the temperature on the value of the discord and entanglement. It is well known that both vanish with the increase in the temperature, i.e. the quantum correlations are significant only at low temperatures. In our calculations we take the dimensionless inverse temperature \( \beta = 10. \)

Notice that the distribution of the pairwise discord among the virtual particles is very similar to that obtain for the single initially excited spin in Sect. 4.1. This fact simplifies study of the discord for this more practically realizable initial state. Nevertheless, we underline basic differences of the discord distribution in this case to show that initially polarized state can be preferable in some situations. In addition, unlike the initial state with the single excited spin, the entanglement is identical to zero for long chains in this case, which was proven in [20] for the homogeneous chains with \( N > 4. \) This fact is in favor of the discord as a measure of quantum correlations revealing more quantum properties than the entanglement.
Fig. 6 The distribution of the stationary pairwise discord $Q_{nm}$ among the virtual particles in the homogeneous spin chain-1/2 with $N = 41$ at the nearest neighbor interaction approximation. The initially polarized nodes are $a \ j = 1$, $b \ j = 7$. In both cases the shapes of destructions are similar to those obtained for the homogeneous chain, see Fig. 1.

4.3.1 Homogeneous chain

First, we consider the homogeneous chain (Fig. 6) and compare the discord distribution with that obtained in Sect. 3.1, Fig. 1.

Obviously, the shapes of the discord distributions are similar in both cases with the following quantitative differences.

1. The initially polarized node $j = 1$, Fig. 6a. All nodes are correlated, and the minimum pairwise discords correspond to pairs involving the end nodes. Comparing Figs. 6a and 1a we conclude that the discord is steeper in the case of initially polarized node, which means that the edge nodes are less correlated with the center nodes in this case. Consequently, the center nodes are better correlated with each other and the edge nodes are less sensitive to the perturbations of the center nodes. These perturbations must be large enough to effect the edge nodes.

2. If the initially polarized node is $j = 7$, we have (see Fig. 6b) three nonzero values for the elements $\rho_{nn}$, (i.e. $\rho_i, i = 1, 2, 3$) given by Eq. (56) and, consequently, three different values $J_i, i = 1, 2, 3$, for $J_{nn}$:

$$J_i = \frac{\tanh 5}{2}\rho_i, \quad i = 1, 2, 3.$$ (63)

Therewith

$$Q_{1}^{pol} = Q_{15}^{pol} \approx 0.00010, \quad Q_{2}^{pol} = Q_{24}^{pol} \approx 0.000092, \quad Q_{3}^{pol} = Q_{39}^{pol} \approx 0.00164,$$

$$Q_{4}^{pol} = Q_{12}^{pol} \approx 0.00031, \quad Q_{5}^{pol} = Q_{13}^{pol} \approx 0.00041, \quad Q_{6}^{pol} = Q_{23}^{pol} \approx 0.00123$$ (64)

All nodes are correlated accept for the nodes $n = 6i, i = 1, \ldots, 6$ because all the pairwise discords involving these nodes are zeros. Notice that the spread of the discord (i.e. the ratio of the difference between the maximum and minimal nonzero discords to the maximal discord) is larger in the case of a single polarized node, which follows from the comparison of Figs. 1b
and 6b. This means, in particular, that the nodes from the set \{6i + 1, 6i + 5, \ i = 0, 1, \ldots, 6\} are less sensitive to the perturbations of other virtual particles in the case of the initially polarized 7th node.

3. If the initially polarized node is \( j = 14 \), we have the only nonzero value \( \rho_{nn} \) (i.e. \( \rho_1 \)) given by Eq. (59) and

\[
J_1 = \frac{\tanh 5}{2} \rho_1 = \frac{\tanh 5}{56},
\]

\[
Q_{pol}^1 = 0.00092, \quad n = 3i - 1, 3i - 2, \ i = 1, \ldots, 13.
\]  

(65)

The cluster of correlated nodes is formed by the nodes \{3i - 1, 3i - 2; \ i = 1, 2, \ldots, 13\}.

4. If \( j = 21 \), then the only nonzero value of \( \rho_{nn} \) (i.e. \( \rho_1 \)) is given by Eq. (61) and

\[
J_1 = \frac{\tanh 5}{42},
\]

\[
Q_{pol}^1 = 0.00164 \quad n = 2i - 1, \quad i = 0, 1, \ldots, 21.
\]

(66)

Thus, the cluster of correlated nodes is represented by the family of odd nodes.

In general, the absolute value of the discord is significantly less in the case of a single initially polarized node, as follows from the comparison of the both graphs in Figs. 1 and 6.

4.3.2 Alternating chain

Similar to Sect. 4.2.1, the discord does not depend on the dimerization parameter \( \delta \) if the initially polarized node \( j \) is even. Comparing this discord with the discord for the alternating chain with initially excited node we conclude that the same remarks as for the homogeneous chain are valid in this case. Namely, the discord is steeper if \( j = 1 \), the spread of the discord is larger and the value of discord is smaller. A novelty is that at \( j = 41 \), unlike the discord in the chain with the initially excited spin \( j = 41 \), the node \( n = 21 \) is correlated with all other nodes, while other correlations are negligible, as demonstrated in Fig. 7 for the chain with \( \delta = 1/2 \).

**Fig. 7** The distribution of the stationary pairwise discord \( Q_{nm} \) in the alternating spin-1/2 chain with \( N = 41, \delta = 1/2 \) and the initially polarized node \( j = 41 \) at the nearest neighbor interaction approximation. The 21th node correlates with all others.
5 Conclusions

We study such representations of the density matrix associated with a quantum system of spin-1/2 particles which reveal the stationary distributed pairwise discord. This system is a system of virtual particles associated with the eigenstates of the Hamiltonian. In particular, if the nearest neighbor interaction approximation is used, this system of virtual particles is the system of $\beta$-fermions [20]. The systems with the stationary discord are convenient for the realization of the quantum operations. In addition, it is much simpler to prepare the desirable distribution of the discord, since it does not evolves. Using different coupling constants, different initial states and different Hamiltonians governing the spin dynamics we may handle the size of the cluster of coherent particles.

Emphasize, that the above virtual particles are not localized in the physical space, which creates a problem of “interaction” with these particles using the classical tools. However, this problem disappears in so-called “inner” parts of quantum algorithms where such interaction is absent. We assume that systems with stationary discord are most suitable namely for these algorithms.

Examples of homogeneous and non-homogeneous spin-1/2 chains (alternating, 3-alternating and completely inhomogeneous chain of ref. [21]) are considered with two types of the initial conditions: the single initially excited and single initially polarized node. The peculiarity of the initial state with the single initially excited node is that the both discord and entanglement are non zero in the above system of virtual particles in this case. We found (both analytically and numerically) that the stationary discord/entanglement distribution is defined by the position of the initially excited/polarized node. It is interesting that the shapes of discord and entanglement distributions are essentially the same in the case of initially excited node. In addition, this shapes remain essentially the same for the discord distribution in the case of initially polarized node. Set of peculiar subsystem of correlated virtual particles have been found. It is important that the subsystems of large numbers of virtual particles with equal pairwise discord are among them. Such subsystems might be proper candidates for the quantum registers.

It is shown that the remote DDIs only slightly deform the distribution of the discord in a quantum system, unlike the evolution of the pairwise quantum correlations in the system of physical spins and the state transfer process along the spin chains, which significantly depend on the interactions among remote nodes.

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6 Appendix: Minimization in Eq. (19)

Let us show that the minimum in Eq. (19) corresponds to $\eta = 0$, similar to ref. [20]. Equations (21) and (22) at $\eta = 0$ yield
\[ p_i(0) \equiv p_i|_{\eta=0} = \frac{1}{2}, \quad (67) \]

\[ \theta_i(0) \equiv \theta_i|_{\eta=0} = 2\sqrt{\rho_{nn}\rho_{mm} + \frac{1}{4}(1 - 2\rho_{mm})^2}, \quad i = 0, 1. \quad (68) \]

Consequently, using the definition of \( S_i \) given by Eq. (20), we conclude that \( S_1|_{\eta=0} = S_0|_{\eta=0} \equiv S(\theta_0(0)) \) and

\[ (p_0S_0 + p_1S_1)|_{\eta=0} = 2p_0(0)S(\theta_0(0)) = S(\theta_0(0)) = S\left(2\sqrt{\rho_{nn}\rho_{mm} + \frac{1}{4}(1 - 2\rho_{mm})^2}\right) \quad (69) \]

Similarly, Eqs. (21) and (22) at \( \eta = 1 \) yield

\[ p_0(1) = 1 - \rho_{nn}, \quad p_1(1) = \rho_{nn}, \quad (70) \]

\[ \theta_0(1) = \frac{|1 - 2\rho_{mm} - \rho_{nn}|}{1 - \rho_{nn}} \quad (71) \]

\[ \theta_1(1) = 1. \quad (72) \]

Again, using the definition of \( S_i \) given by Eq. (20) we have \( S_1|_{\eta=1} = 0 \) and we can write

\[ (p_0S_0 + p_1S_1)|_{\eta=1} = p_0(1)S(\theta_0(1)) = (1 - \rho_{nn})S\left(\frac{|1 - 2\rho_{mm} - \rho_{nn}|}{1 - \rho_{nn}}\right). \quad (73) \]

Thus we have to find the minimum of two quantities:

\[ \min\left( S\left(2\sqrt{\rho_{nn}\rho_{mm} + \frac{1}{4}(1 - 2\rho_{mm})^2}\right), (1 - \rho_{nn})S\left(\frac{|1 - 2\rho_{mm} - \rho_{nn}|}{1 - \rho_{nn}}\right) \right). \quad (74) \]

Representing the ratio of these two quantities as a two-dimensional surface in the space of the parameters \( \rho_{nn} \) and \( \rho_{mm} \) (\( \rho_{nn}, \rho_{mm} \leq 1, \rho_{nn} + \rho_{mm} \leq 1 \)) we conclude that the first of them (corresponding to \( \eta = 0 \)) is always less than the second one. Consequently the minimum in Eq. (19) is always at \( \eta = 0 \).

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