Entanglement in alternating open spin–1/2 chains with XY-Hamiltonian

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We investigate entanglement of spin pairs in alternating open spin chains in the equilibrium state in an external magnetic field. We calculate the reduced density matrix of spin pairs and estimate the concurrence with Wootter’s criteria. The obtained results demonstrate the dependence of the entanglement on the temperature, chain’s length, the positions of the spins, and the ratio of the spin-spin interaction constants.

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I. INTRODUCTION

A study of entangled states is an important direction in quantum information theory. A quantitative investigation of the degree of entanglement often poses considerable difficulties and is possible only in relatively simple cases. The problem becomes much simpler, if it is known how to diagonalize the Hamiltonian [1–3]. In particular, many interesting results were obtained for spin rings and infinite spin chains [4–6]. On the other hand, possible experimental realizations of qubits [7] involve finite open chains which were also used for the transfer of quantum states from one end of the chain to the other [8, 9]. Important results were obtained by Wang [10] who investigated open boundary effects on the ground-state entanglement in a homogeneous Heisenberg model. However, the models [4–6, 10] do not allow one to solve the qubit addressing problem which can be attacked in systems with several different Larmor frequencies. Such Larmor frequency variations naturally emerge in inhomogeneous systems with different constants of the spin-spin interaction (SSI) for different pairs of neighboring spins.

In this paper, we investigate entanglement in open alternating spin chains. Open alternating spin chains with XY–Hamiltonians can be used as a first step for the solution of the qubit addressing problem. Recently, the XY–Hamiltonian of an open finite alternating spin chain has been diagonalized [9, 11] on the basis of a generalization of the classical methods [1] for homogeneous chains. It was shown that the transfer of quantum states from one end to the other is possible with 100% fidelity for longer alternating chains than in the case of homogeneous chains [9].

The concurrence [12] is used as a quantitative measure of entanglement. A possibility of the exact diagonalization of the Hamiltonian [9] makes it possible to construct the reduced density matrix for any spin pair in a chain described by the equilibrium density matrix. Then entanglement can be investigated with Wootter’s criteria [12]. As a result, one can study the influence of the temperature, the chain length, the distance from the ends, and the ratio of the SSI constants on the entanglement of any spin pair in the chain.

The present paper is organized as follows. In Section II the model Hamiltonian of the open alternating spin chain is described and the eigenvalues of the Hamiltonian and its eigenvectors are given. In Section III we obtain the reduced density matrix for all pairs of the neighboring spins of the chain. We study the dependence of the spin pair entanglement on the temperature, chain’s length, spin positions and ratio of the SSI constants in Section IV.

II. THE MODEL

We consider an open alternating spin–1/2 chain with the XY–Hamiltonian in a strong external magnetic field. The Hamiltonian of the system can be written as

\[ H = \sum_{n=1}^{N} \omega_n I_{nz} + \sum_{n=1}^{N-1} D_{n,n+1}(I_{n,x} I_{n+1,x} + I_{n,y} I_{n+1,y}). \]  

(1)

Here, \( I_{n} \) are the spin–1/2 matrices (\( \alpha = x, y, z \)), and \( N \) is the number of the spins. The alternating Larmor frequencies are determined by the equation

\[ \omega_n = \begin{cases} \omega_1, & n \text{ is odd} \\ \omega_2, & n \text{ is even.} \end{cases} \]  

(2)

The alternating coupling constants are

\[ D_{n,n+1} = \begin{cases} D_1, & n \text{ is odd} \\ D_2, & n \text{ is even.} \end{cases} \]  

(3)

We assume that the number of the spins, \( N \), is odd. The Hamiltonian of Eq. (1) can be diagonalized [9, 11] on the basis of a generalization of the classical methods [1] for homogeneous chains.

The Jordan–Wigner transformation [1, 2] that maps
The new fermion operators $\gamma^\dagger_n$ and $\gamma_n$ can be written as

\[
I_{n,-} = I_{n,x} - iI_{n,y} = (-2)^{n-1} \left( \prod_{l=1}^{n-1} I_{l,z} \right) c_n, \quad (4)
\]
\[
I_{n,+} = I_{n,x} + iI_{n,y} = (-2)^{n-1} \left( \prod_{l=1}^{n-1} I_{l,z} \right) c_n^\dagger, \quad (5)
\]
\[
I_{n,z} = c_n^\dagger c_n - 1/2, \quad (6)
\]
where $c_n^\dagger$ and $c_n$ are creation and annihilation operators. As a result, the Hamiltonian in the matrix notation has the following form

\[
H = \frac{1}{2} c^\dagger (D + 2\Omega) c - \frac{1}{2} \sum_{n=1}^{N} \omega_n. \quad (7)
\]

Here we denote the row vector $c^\dagger = (c_1^\dagger, \ldots, c_N^\dagger)$, the column vector $c = (c_1, \ldots, c_N)^t$ (the superscript $t$ represents the transposition) and $D + 2\Omega$ is a three-diagonal matrix.

The diagonalization of the matrix $D + 2\Omega$ is performed by the unitary transformation

\[
D + 2\Omega = UA \ U^t, \quad A = \text{diag}\{\lambda_1, \ldots, \lambda_N\}. \quad (8)
\]

The new fermion operators $\gamma_n^\dagger$ and $\gamma_n$, which are introduced by the relationships

\[
c_n^\dagger = \sum_{k=1}^{N} u_{n,k}^* \gamma_k^\dagger, \quad c_n = \sum_{k=1}^{N} u_{n,k} \gamma_k, \quad (9)
\]
transform the Hamiltonian of Eq. (7) into the Hamiltonian

\[
H = \frac{1}{2} \sum_{k=1}^{N} \lambda_k \gamma_k^\dagger \gamma_k - \frac{1}{2} \sum_{n=1}^{N} \omega_n. \quad (10)
\]

This is a free fermion Hamiltonian with the energy levels $1/2\lambda_k$. Finally, the eigenvalues $\lambda_k$ and eigenvectors $|u_k\rangle = (u_{1k}, u_{2k}, \ldots, u_{Nk})^t$ of the Hamiltonian of Eq. (10) can be written as [11]

\[
\lambda_k = \begin{cases} 
\omega_1 + \omega_2 + \sqrt{\omega_1 - \omega_2)^2 + \Delta_k^2}, & k = 1, 2, \ldots, N-1 \\
2\omega_1, & k = N+1 \\
\omega_1 + \omega_2 - \sqrt{\omega_1 - \omega_2)^2 + \Delta_k^2}, & k = N+2, N+3, \ldots, N 
\end{cases} \quad (11)
\]

where

\[
\Delta_k = 1 + 2\delta \cos \left( \frac{2\pi k}{N+1} \right) + \delta^2, \quad \delta = D_2/D_1. \quad (12)
\]

For all the indices $k = 1, \ldots, N$ except the index $k = (N + 1)/2$ the eigenvector $|u_k\rangle$ has the elements

\[
u_{j,k} = \begin{cases} 
A_k \frac{D_{\lambda_k - 2\omega_1}}{\sqrt{\lambda_k - 2\omega_1)^2 + D_2^2\Delta_k}} \sin \left( \frac{\pi k(j-1)}{N+1} \right), & j = 1, 3, 5, \ldots, N \\
A_k \sin \left( \frac{\pi k(j+1)}{N+1} \right), & j = 2, 4, \ldots, N-1
\end{cases} \quad (13)
\]

with the normalization coefficient

\[
A_k = \frac{2|\lambda_k - 2\omega_1|}{\sqrt{\lambda_k - 2\omega_1)^2 + D_2^2\Delta_k}}. \quad (14)
\]

The elements of the eigenvector $|u_{(N+1)/2}\rangle$ read

\[
u_{j,(N+1)/2} = \begin{cases} 
B(-\delta)^{(N-j)/2}, & j = 1, 3, 5, \ldots, N \\
0, & j = 2, 4, \ldots, N-1
\end{cases} \quad (15)
\]

with the normalization coefficient

\[
B = \left( \frac{\delta^2 - 1}{\delta^{N+1} - 1} \right)^{1/2}. \quad (16)
\]

For $D_1 = D_2 = D$ and $\omega_1 = \omega_2 = \omega_0$ we obtain a homogeneous chain and the Hamiltonian of Eq. (10) can be written as [3]

\[
H = \sum_{k=1}^{N} \lambda_k \gamma_k^\dagger \gamma_k - \frac{1}{2} N\omega_0, \quad (17)
\]

with $\lambda_k = D \cos \frac{\pi k}{N+1} + \omega_0$ and eigenvector $|u_k\rangle$ has the elements

\[
u_{j,k} = \left( \frac{2}{N+1} \right)^{1/2} \sin \left( \frac{\pi k j}{N+1} \right), \quad j = 1, 2, \ldots, N. \quad (18)
\]

For homogeneous chains these expressions are valid both for odd and even $N$.

### III. THE REDUCED DENSITY MATRIX

In this section we consider a one–dimensional many–spin system in a thermodynamic equilibrium state. We describe an algorithm for obtaining the reduced density matrix for any spin pair. This algorithm will be applied in order to obtain the reduced density matrix of the nearest–neighbor spins $i$ and $i + 1$ for the open alternating chain with an odd number of the spins.

The density matrix, $\rho$, in the thermodynamic equilibrium system is

\[
\rho = e^{-\beta H}/Z, \quad (19)
\]
where $\beta = \hbar/kT$, $T$ is the temperature and $Z = \text{Tr}\{e^{-\beta H}\}$ is the partition function. The density matrix, $\rho$, can be written as

$$
\rho = \sum_{\xi_1,\xi_2,\ldots,\xi_N=0}^{3} \alpha_{ij}^{\xi_1,\xi_2,\ldots,\xi_N} x_1^{\xi_1} \otimes \ldots \otimes x_N^{\xi_N},
$$

(20)

where $N$ is a number of spins in the system, $\xi_k$ $(k = 1, 2, \ldots, N)$ is one of the values $\{0, 1, 2, 3\}$, $x_k^0 = I_k$ is the unit matrix of the dimension $2 \times 2$, $x_k^1 = i I_k$, $x_k^2 = k I_k$, and $\alpha_{ij}^{\xi_1,\xi_2,\ldots,\xi_N}$ is a numerical coefficient.

In order to obtain the reduced density matrix for spins $i, j$, we consider the system of all other spins as the environment. Averaging the density matrix, $\rho$, over the environment and taking into account that $\text{Tr}\{x_k^{\xi_k}\} = 0$ $(k = 1, 2, \ldots, N; \xi_k = 1, 2, 3)$ we find for the reduced density matrix, $\rho_{ij}$, of spins $i$ and $j$ the following expression

$$
\rho_{ij} = \sum_{\xi_i,\xi_j=0}^{3} \alpha_{ij}^{\xi_i,\xi_j} x_i^{\xi_i} \otimes x_j^{\xi_j},
$$

(21)

where the coefficient $\alpha_{ij}^{\xi_i,\xi_j}$ is defined as

$$
\alpha_{ij}^{\xi_i,\xi_j} = \frac{2^{N-2} \text{Tr}\{x_i^{\xi_i} x_j^{\xi_j}\}}{\text{Tr}\{(x_i^{\xi_i})^2 (x_j^{\xi_j})^2\}}.
$$

(22)

The calculations of the traces in Eq. (22) are performed in an $2^N$-dimension space. Here, the density matrix, $\rho$, and the density matrix, $\rho_{ij}$, are normalized to unity.

Since $[H, I_2] = 0$ one can see that

$$
\begin{align*}
\alpha_{ij}^{01} &= \alpha_{ij}^{02} = \alpha_{ij}^{20} = 0, \\
\alpha_{ij}^{13} &= \alpha_{ij}^{23} = \alpha_{ij}^{31} = \alpha_{ij}^{32} = 0.
\end{align*}
$$

(23)

Furthermore, $\alpha_{ij}^{12} = 4 \text{Tr}\{\rho I_2 I_j\} = 0$, $\alpha_{ij}^{21} = 4 \text{Tr}\{\rho I_2 I_j\} = 0$, and $\alpha_{ij}^{11} = 4 \text{Tr}\{\rho I_2 I_j\} = 4 \text{Tr}\{\rho I_2 I_j\} = \alpha_{ij}^{22}$ from the symmetry of the problem.

As a result, the structure of the reduced density matrix of two spins is given by

$$
\rho_{ij} = \begin{pmatrix}
a & 0 & 0 & 0 \\
b & x & 0 & 0 \\
0 & x & c & 0 \\
0 & 0 & 0 & d
\end{pmatrix},
$$

(24)

where $a = 1 + 4 \sum_{n=0}^{3} \alpha_{ij}^{n0}$, $b = 1 - 4 \sum_{n=0}^{3} \alpha_{ij}^{3n}$, $c = 1 - 4 \sum_{n=0}^{3} \alpha_{ij}^{3n}$, $d = 1 - 4 \sum_{n=0}^{3} \alpha_{ij}^{3n}$, and $x = \sum_{n=0}^{3} \alpha_{ij}^{n1}$. We calculate the coefficients $\alpha_{ij}^{03}, \alpha_{ij}^{30}, \alpha_{ij}^{33}$ and $\alpha_{ij}^{11}$ below.

### A. An open alternating chain with an odd number of spins

In order to calculate the coefficients $\alpha_{ij}^{03}, \alpha_{ij}^{30}, \alpha_{ij}^{33}$ and $\alpha_{ij}^{11}$ we use the diagonal form of the fermion Hamiltonian of Eq. (10) of the system. One finds that

$$
\alpha_{ij}^{00} = 1/4,
$$

(25)

$$
\alpha_{ij}^{20} = \text{Tr}\{\rho I_2 z\} = \sum_p u_{ip} e^{-\frac{\beta}{2} \lambda_p} \left( 1 + e^{-\frac{\beta}{2} \lambda_p} \right) - \frac{1}{2},
$$

(26)

$$
\alpha_{ij}^{30} = \text{Tr}\{\rho I_2 z\} = \sum_p u_{ip} e^{-\frac{\beta}{2} \lambda_p} \left( 1 + e^{-\frac{\beta}{2} \lambda_p} \right) - \frac{1}{2},
$$

(27)

$$
\alpha_{ij}^{33} = 4 \text{Tr}\{\rho I_2 z\} = 
$$

$$
4 \left[ \sum_m \sum_{n \neq m} u_{im} u_{jn} e^{-\frac{\beta}{2} \lambda_m} \left( 1 + e^{-\frac{\beta}{2} \lambda_m} \right) \left( 1 + e^{-\frac{\beta}{2} \lambda_n} \right) 
+ \sum_n u_{in} u_{jn} \sum_m u_{im} u_{jm} e^{-\frac{\beta}{2} \lambda_m} \left( 1 + e^{-\frac{\beta}{2} \lambda_m} \right) \left( 1 + e^{-\frac{\beta}{2} \lambda_n} \right) 
- 2 \left( \sum_k u_{ik}^2 e^{-\frac{\beta}{2} \lambda_k} + \sum_p u_{ip}^2 e^{-\frac{\beta}{2} \lambda_p} \right) \right] + 1.
$$

(28)

Our numerical simulations for the spin chains with 9 spins demonstrate that entanglement appears only between the nearest-neighbors even if SSI of all spins are taken into account. The following coefficients are sufficient for our investigations:

$$
\alpha_{i,i+1,1} = \alpha_{i,i+1,2} = 4 \text{Tr}\{\rho I_2 I_{i+1,x}\} = \text{Tr}\{\rho (c_i^{\dagger} c_{i+1} + c_i^{\dagger} c_{i+1} - c_i c_{i+1} - c_i c_{i+1})\} = 2 \sum_{n} u_{in} u_{i+1,n} e^{-\frac{\beta}{2} \lambda_n}.
$$

(29)

Introducing the notations

$$
C_1 = \frac{\omega_2 - \omega_1}{D_1}, \quad C_2 = \frac{\omega_2 + \omega_1}{D_1},
$$

$$
L_k = \begin{pmatrix}
1 & \ldots & 1 \\
C_1 + C_2 + \Delta_k & \ldots & C_1 + C_2 + \Delta_k \\
C_1 - C_2 + \Delta_k & \ldots & C_1 - C_2 + \Delta_k
\end{pmatrix},
$$

$$
f_k = A_k^2 = \begin{pmatrix}
4 \sum_{n=1}^{\Delta_k} \frac{1}{C_1 + \sqrt{C_1^2 + \Delta_k^2} + \Delta_k} \\
4 \sum_{n=1}^{\Delta_k} \frac{1}{C_1 - \sqrt{C_1^2 + \Delta_k^2} + \Delta_k}
\end{pmatrix},
$$

(30)

$$
(31)
$$
\[ R_k = A_k^2 \left( \frac{D_1}{\lambda_k - 2w_1} \right)^2 = \begin{cases} \frac{1}{N+1} \left( C_1 + \sqrt{C_1^2 + \Delta_k} \right)^2, & k = 1, \ldots, \frac{N-1}{2} \\ \frac{1}{N+1} \left( C_1 - \sqrt{C_1^2 + \Delta_k} \right)^2, & k = \frac{N+3}{2}, \ldots, N \end{cases} \]  

(32)

\[ \epsilon_k = \begin{cases} C_2 + \sqrt{C_2^2 + \Delta_k}, & k = 1, \ldots, \frac{N-1}{2} \\ C_2 - \sqrt{C_2^2 + \Delta_k}, & k = \frac{N+3}{2}, \ldots, N \end{cases} \]  

(33)

and

\[ g(\epsilon_k) = \frac{e^{-\tau \epsilon_k}}{1 + e^{-\tau \epsilon_k}}, \quad \tau = \frac{\beta D_1}{2}, \]  

(34)

we obtain explicit expressions for the coefficient \( \alpha^3_{i,i+1} \). Since the alternating chain is non–symmetric we obtain the different expressions for the coefficients at even and odd \( i \). At even \( i \) the coefficient \( \alpha^3_{i,i+1} \) is

\[ \alpha^3_{i,i+1} = 4 \left[ \sum_{m \neq \frac{N+1}{2}} \sum_{n \neq m, n \neq \frac{N+1}{2}} f_m R_n \sin^2 \left( \frac{\pi m i}{N+1} \right) S^2_{(n)}(n) g(\epsilon_m) g(\epsilon_n) + \sum_{m \neq \frac{N+1}{2}} f_m B^2(-\delta)^{N-i} \sin^2 \left( \frac{\pi m i}{N+1} \right) g(2w_1) g(\epsilon_m) \right] 

+ \left( \sum_{n} f_n L_n S_{\delta}(n) \sin \left( \frac{\pi n i}{N+1} \right) \right) \sum_{m} f_m L_m S_{\delta}(m) \sin \left( \frac{\pi n i}{N+1} \right) g(\epsilon_m) 

- \sum_{m \neq \frac{N+1}{2}} \sum_{n \neq m, n \neq \frac{N+1}{2}} f_m f_n L_n L_m S_{\delta}(m) S_{\delta}(n) \sin \left( \frac{\pi m i}{N+1} \right) \sin \left( \frac{\pi n i}{N+1} \right) g(\epsilon_m) g(\epsilon_n) 

- 2 \left\{ \sum_{k \neq \frac{N+1}{2}} f_k \sin^2 \left( \frac{\pi k i}{N+1} \right) g(\epsilon_k) + \sum_{p \neq \frac{N+1}{2}} R_p S^2_{\delta}(p) g(\epsilon_p) + B^2(-\delta)^{N-i} g(2w_1) \right\} + 1, \]  

(35)

where \( S_{\delta}(m) = \left[ \delta \sin \left( \frac{\pi m i}{N+1} \right) + \sin \left( \frac{\pi m (i+2)}{N+1} \right) \right] \). At odd \( i \) the coefficient \( \alpha^3_{i,i+1} \) is

\[ \alpha^3_{i,i+1} = 4 \left[ \sum_{m \neq \frac{N+1}{2}} \sum_{n \neq m, n \neq \frac{N+1}{2}} f_n R_m \sin^2 \left( \frac{\pi m (i+1)}{N+1} \right) Q^3_{(m)}(m) g(\epsilon_m) g(\epsilon_n) + \sum_{n \neq \frac{N+1}{2}} f_n B^2(-\delta)^{N-i} \sin^2 \left( \frac{\pi n (i+1)}{N+1} \right) g(2w_1) g(\epsilon_n) \right] 

+ \left( \sum_{n} f_n L_n Q_{\delta}(n) \sin \left( \frac{\pi n (i+1)}{N+1} \right) \right) \sum_{m} f_m L_m Q_{\delta}(m) \sin \left( \frac{\pi m (i+1)}{N+1} \right) g(\epsilon_m) 

- \sum_{m \neq \frac{N+1}{2}} \sum_{n \neq m, n \neq \frac{N+1}{2}} f_m f_n L_n L_m Q_{\delta}(m) Q_{\delta}(n) \sin \left( \frac{\pi m (i+1)}{N+1} \right) \sin \left( \frac{\pi n (i+1)}{N+1} \right) g(\epsilon_m) g(\epsilon_n) 

- 2 \left\{ \sum_{k \neq \frac{N+1}{2}} R_k Q^2_{\delta}(k) g(\epsilon_k) + B^2(-\delta)^{N-i} g(2w_1) + \sum_{p \neq \frac{N+1}{2}} f_p \sin^2 \left( \frac{\pi p (i+1)}{N+1} \right) g(\epsilon_p) \right\} + 1, \]  

(36)

where \( Q_{\delta}(m) = \left[ \delta \sin \left( \frac{\pi m (i-1)}{N+1} \right) + \sin \left( \frac{\pi m (i+1)}{N+1} \right) \right] \). Explicit expressions for the coefficients \( \alpha^3_{i,i+1} \), \( \alpha^{10}_{i,i+1} \) and \( \alpha^{11}_{i,i+1} \) can be obtained in a similar way.
B. The open homogeneous chain

The expressions of the previous Section simplify for homogeneous chains and can be written as follows

\[ \alpha_{ij}^{30} = \frac{2}{N+1} \sum_{k} \sin^{2} \left( \frac{i \pi k}{N+1} \right) g(\epsilon_{k}) - \frac{1}{2} \]  
\[ \alpha_{ij}^{33} = \frac{16}{(N+1)^{2}} \left\{ \sum_{k} \sum_{p \neq k} \sin^{2} \left( \frac{i \pi k}{N+1} \right) g(\epsilon_{k}) g(\epsilon_{p}) \right. 
\left. - \sum_{k \neq p} \sin \left( \frac{i \pi k}{N+1} \right) \sin \left( \frac{i \pi p}{N+1} \right) g(\epsilon_{k}) g(\epsilon_{p}) \right\} 
\left. - \frac{4}{N+1} \sum_{k} \sin^{2} \left( \frac{i \pi k}{N+1} \right) g(\epsilon_{k}) \right. 
\left. + \sum_{p} \sin^{2} \left( \frac{i \pi p}{N+1} \right) g(\epsilon_{p}) \right\} + 1, \]  
\[ \alpha_{i,i+1}^{11} = \frac{4}{N+1} \sum_{k} \sin \left( \frac{i \pi k}{N+1} \right) \sin \left( \frac{(i+1) \pi k}{N+1} \right) g(\epsilon_{k}), \]  
where \( D_{1} = D_{2} = D \), and the one-fermion spectrum \( \epsilon_{k} \) is defined as

\[ \epsilon_{k} = 2 \cos \frac{\pi k}{N+1} + \frac{2 \omega_{0}}{D}, \quad (k = 1, 2, \ldots, N). \]

We emphasize again that Eqs. (37)-(40) are valid for all \( N \).

IV. MEASURE OF ENTANGLEMENT

In this paper we restrict our attention to the analysis of the entanglement between two arbitrary spins in the chain. Here we consider the concurrence as a measure of entanglement [12].

Let \( A \) and \( B \) be a pair of qubits, and let the density matrix of the pair be \( \rho_{AB} \) which may be pure or mixed. Then the "spin-flipped" density matrix is determined as

\[ \tilde{\rho}_{AB} = (\sigma_{y} \otimes \sigma_{y}) \rho_{AB}^{*} (\sigma_{y} \otimes \sigma_{y}) \]  
where the asterisk denotes complex conjugation in the standard basis \( \{ |00\rangle, |01\rangle, |10\rangle, |11\rangle \} \) and the Pauli matrix \( \sigma_{y} = 2I_{y} \). The concurrence of the two-spin system with the density matrix \( \rho_{AB} \) is [12]

\[ C_{AB} = \max\{0, 2\lambda_{1} - \lambda_{2} - \lambda_{3} - \lambda_{4}\} \]
\[ \lambda = \max\{\lambda_{1}, \lambda_{2}, \lambda_{3}, \lambda_{4}\} \]  
where \( \lambda_{1}, \lambda_{2}, \lambda_{3}, \) and \( \lambda_{4} \) are the square roots of the eigenvalues of the product \( \rho_{AB} \tilde{\rho}_{AB} \). Since both \( \rho_{AB} \) and \( \tilde{\rho}_{AB} \) are positive operators, it follows that their product, though non-Hermitian, has only real and non-negative eigenvalues [13].

Using Eq. (24) one can find the expressions of \( \lambda_{1}, \lambda_{2}, \lambda_{3}, \lambda_{4} \) as follows

\[ \lambda_{1} = \lambda_{4} = \sqrt{ad}, \quad \lambda_{2,3} = |x \pm \sqrt{bc}|. \]  
Expressions for Eq. (43) yield all information necessary for the analysis of the pairwise entanglement for such chains.

V. NUMERICAL ANALYSIS OF THE CONCURRENCE IN SPIN PAIRS

As mentioned above, our numerical calculations in the nine-spin chain with the Hamiltonian of Eq. (1) lead to the conclusion that the concurrence is non-zero for nearest neighbors only. We focus below on entanglement of the nearest neighbors in the open alternating chain with the XY-Hamiltonian in the case of zero Larmor frequencies.

![Image](image.png)

FIG. 1: The concurrence of spins 2 and 3 versus the temperature for the number of spins \( N = 101 \) and \( D_{2}/D_{1} = 1.5 \). The inset displays the concurrence versus the temperature on a greater scale.

Using Eqs. (25)-(40), (43) we investigate numerically the dependence of the concurrence, \( C_{12} \), of the first and
FIG. 2: The nearest-neighbor concurrence versus the site number in the homogeneous chain for $N = 100$. The concurrence oscillates with a two–site period. The oscillations decay when the spin pair is far from the ends of the homogeneous chain.

Second spins on the temperature. Figure 1 shows that entanglement appears at $\beta D_1 \approx 1$. This corresponds to the temperature $T \approx 0.5 \mu K$ at $D_1 \approx 2 \pi \cdot 10^4 e^{-1}$. The temperature at which entanglement emerges in the pairs of neighboring spins depends on the ratio of the SSI constants, chain’s length and the distance from ends of the chain. It is interesting to note that ordered states of nuclear spins were observed at microkelvin temperatures [14].

Numerical results show (Fig. 2) that entanglement oscillates with the two–site period. The qualitative explanation of the numerical results is the following. Qubits 1 and N are situated at the chain ends. Since entanglement is non–zero only between the nearest–neighbors, the pair of qubits 1 and 2 and the pair of qubits N-1 and N have the maximal pairwise entanglement for the homogeneous chain. Spin 2 can be entangled both with spin 1 and with spin 3. Since spin 2 is strongly entangled with spin 1, the entanglement of spins 2 and 3 is weaker. As a result, spin 3 is strongly entangled with spin 4, etc. This explains the oscillator behavior of the concurrence displayed in Fig. 2. The oscillations decay when the spin pair is far from the ends of the homogeneous chain. These oscillations do not decay for alternating open chains as it is displayed in Fig. 3 at different ratios of the coupling constants, $D_2/D_1$. The oscillation of the entanglement from zero to values close to one is due to different coupling constants between spins in the alternating chain. In fact we have here the dimerised spin chain which can be considered qualitatively as a set of non–interacting spin pairs at $D_2/D_1 \geq 2$. The dependence of the concurrence on the ratio of the SSI is shown in Fig. 4. It is worth to notice that it is impossible to observe the influence of ends of the chain on the entanglement already at $D_2/D_1 = 1.5$.

FIG. 3: The nearest-neighbor concurrence versus the site number for $N = 17$ and $\beta D_1/2 = 30$ at the difference ratios of the SSI coupling constants; a: $D_2/D_1 = 1$; b: $D_2/D_1 = 1.17$; c: $D_2/D_1 = 3$. 
In Figs. 5 – 6 the dependence of the concurrences $C_{12}$ and $C_{23}$ on the length of the homogeneous chain consisting of an odd (even) number of spins is displayed. The concurrence $C_{12}$ decreases at even $N$ and increases at odd $N$ when $N$ increases. For the concurrence $C_{23}$ the situation is opposite. In order to explain these results it is necessary to take into account the influence of the ends of the chain on the entangled states. As a result, we obtain that the ends of the chain yield opposite contributions to the entanglement for the chain of an odd number of spins. For example, one can easily find in a chain consisting of 5 spins that spin 5 leads to a decrease of the entanglement of spins 1 and 2. This effect is diminished when the odd number of spins increases and then the entanglement of spins 1 and 2 increases. On the contrary, the second end of the chain increases the entanglement of spins 1 and 2 at an even number of spins. This leads to the calculated decrease of the concurrence (see Fig. 5) when the even number of spins increases. Analogously, it is possible to explain the growth (fall) of the concurrence of the entanglement of spins 2 and 3 in the dependence on the length of the chain consisting of an even (odd) number of spins (see Fig. 6). The maximums of the concurrence in Fig. 6 have a simple qualitative explanation. The growth of the concurrence up to its maximal value is determined by the decrease of the partial suppression of the SSI due to the flip–flop transitions at low temperatures. The state of spins 2 and 3 approaches to a separable one at low temperatures when the spins are trying to orient parallel to the local fields. Entanglement of such a state decreases when the temperature decreases.

VI. CONCLUSION

In the present work we investigate entanglement in alternating open chains. The developed methods of the diagonalization of the XY-Hamiltonian of open alternating spin chains allow us to study the pairwise entanglement for different parameters of the chain and its temperature. Similar methods can be applied for an investigation of the pairwise entanglement in open chains with periodic coupling constants [15]. Methods of exact diagonalization of the XY-Hamiltonian in such chains [15] allow a solution of different problems of quantum information theory for models of quantum registers taking into account the qubit addressing. However, the qubit addressing requires a large difference of the Larmor frequencies of
different spins in comparison with their SSI coupling constants. Our preliminary calculations demonstrate that the concurrence is close to zero at such conditions and the entangled states do not appear. The question is a subject of our further investigations.

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