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*S.I. Doronin, E.B. Fel'dman, A.N. Pyrkov**

Institute of Problems of Chemical Physics of RAS, 142432,
Chernogolovka, Moscow Region,, Russia
* *E-mail*: pyrkov@icp.ac.ru

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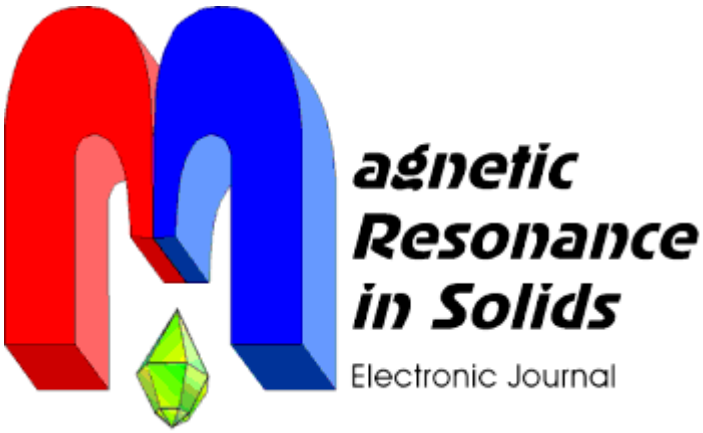

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S.I. Doronin, E.B. Fel'dman, A.N. Pyrkov*
Institute of Problems of Chemical Physics of RAS, 142432, Chernogolovka, Moscow Region, Russia
* *E-mail*: pyrkov@icp.ac.ru

We investigate entanglement of spin pairs in a one-dimension open chain of spins coupled by the dipole-dipole interactions (DDI) in the equilibrium state in the external magnetic field. We suggest a method of calculation of the reduced density matrix. Concurrence, the quantitative measure of the entanglement, is estimated with Wootter's criteria. Analytical and numerical methods are used in order to investigate the influence of the temperature, chain's length, distance between the spins and their distance from the chain's ends on their entanglement.

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1. Introduction

Quantum mechanics and quantum information theory form a theoretical basis for creation of quantum computers. Two types of quantum-mechanical states, separable and entangled, and the application of the quantum-mechanical superposition state as an elementary unit of information (qubit) leads to fantastic advantages of quantum computers in comparison with classical ones [1, 2]. Entangled states are the main resource of quantum computations and communications [3]. Generally, the concurrence [4] is used as a quantitative measure of entanglement. However, the concurrence can be fully investigated only in some simple cases. One of them is the quantum register representing a one-dimension open chain of spins coupled by the dipole-dipole interactions (DDI) in a strong external magnetic field. The XY-Hamiltonian of such system can be diagonalized [5-8]. A possibility of the exact diagonalization is very important in order to construct the reduced density matrix of any spin pair of the chain which is described by the equilibrium density matrix. Then entanglement is investigated with Wootter's criteria [4]. As a result, one can study the influence of the temperature, the chain length and its ends on the entanglement of any spin pair in the chain. These problems are solved in the present paper by analytical and numerical methods [7, 9-11].

2. The reduced density matrix of spin pairs in homogeneous chains

We consider a one-dimensional open chain consisting of N spins (s = 1/2) coupled by DDI in the external magnetic field. In the rotating reference frame [12], the Hamiltonian of the system (XY-Hamiltonian) is

$$H = D\sum_{n=1}^{N-1}(I_{nx}I_{n+1,x} + I_{ny}I_{n+1,y}), \tag{1}$$

where $I_{n\alpha}$ ($\alpha = x, y, z$) is the projection of the angular momentum operator of spin n on the axis α and D is the DDI coupling constant. In the thermodynamic equilibrium state the density matrix, ρ, of the system is

$$\rho = \frac{e^{-\beta\mathrm{H}}}{Z}, \tag{2}$$

where $\beta = \hbar/kT$, T is the temperature and $Z = \mathrm{Tr}\{e^{-\beta\mathrm{H}}\}$ the partition function. The density matrix ρ can be written as

$$\rho = \sum_{\xi_1,\xi_2\ldots\xi_N=0}^{3} \alpha_{12\ldots N}^{\xi_1\xi_2\ldots\xi_N} x_1^{\xi_1} \otimes \ldots \otimes x_N^{\xi_N}, \tag{3}$$

where ξ_k (k = 1,…, N) is one of the values {0, 1, 2, 3}, $x_j^0 = I_j$ is the unit matrix 2×2, $x_j^1 = I_{jx}$, $x_j^2 = I_{jy}$, $x_j^3 = I_{jz}$ (j = 1,…, N), and $\alpha_{12\ldots N}^{\xi_1\xi_2\ldots\xi_N}$ is the numerical coefficient.

In order to obtain the reduced density matrix for spins i, j we consider the system of all the other spins in the chain as the environment. Averaging the density matrix ρ over the environment and taking into account that $\mathrm{Tr}\{x_j^k\} = 0$ (j = 1,…, N; k = 1,2,3) we find for the reduced density matrix, ρ_{ij}, of spins i and j the following expression:

$$\rho_{ij} = \sum_{\xi_i,\xi_j=0}^{3} \alpha_{ij}^{\xi_i\xi_j} x_i^{\xi_i} \otimes x_j^{\xi_j}, \tag{4}$$

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

$$\alpha_{ij}^{\xi_i\xi_j} = \frac{\mathrm{Tr}\{\rho x_i^{\xi_i} x_j^{\xi_j}\}}{\mathrm{Tr}\{(x_i^{\xi_i})^2 (x_j^{\xi_j})^2\}}. \tag{5}$$

Using the exactly known diagonal representation of the Hamiltonian of Eq.(1) [6] one obtains the following expressions after laborious calculations

$$\alpha_{ij}^{00} = 1/4;\ \alpha_{ij}^{03} = \frac{1}{N+1}\sum_k \sin^2\left(\frac{j\pi k}{N+1}\right)\frac{e^{-\nu\varepsilon_k}}{1+e^{-\nu\varepsilon_k}} - 1/4;\ \alpha_{ij}^{30} = \frac{1}{N+1}\sum_k \sin^2\left(\frac{i\pi k}{N+1}\right)\frac{e^{-\nu\varepsilon_k}}{1+e^{-\nu\varepsilon_k}} - 1/4$$

$$\alpha_{ij}^{33} = \frac{4}{(N+1)^2}\Big\{\sum_k\sum_{p\neq k}\sin^2\left(\frac{i\pi k}{N+1}\right)\sin^2\left(\frac{j\pi p}{N+1}\right)\left(\frac{e^{-\nu\varepsilon_k}}{1+e^{-\nu\varepsilon_k}}\right)\left(\frac{e^{-\nu\varepsilon_p}}{1+e^{-\nu\varepsilon_p}}\right) -$$

$$\sum_k\sum_{p\neq k}\sin\frac{i\pi k}{N+1}\sin\frac{i\pi p}{N+1}\sin\frac{j\pi k}{N+1}\sin\frac{j\pi p}{N+1}\left(\frac{e^{-\nu\varepsilon_k}}{1+e^{-\nu\varepsilon_k}}\right)\left(\frac{e^{-\nu\varepsilon_p}}{1+e^{-\nu\varepsilon_p}}\right)\Big\} - \tag{6}$$

$$-\frac{1}{N+1}\Big\{\sum_k \sin^2\left(\frac{i\pi k}{N+1}\right)\frac{e^{-\nu\varepsilon_k}}{1+e^{-\nu\varepsilon_k}} + \sum_p \sin^2\left(\frac{j\pi p}{N+1}\right)\frac{e^{-\nu\varepsilon_p}}{1+e^{-\nu\varepsilon_p}}\Big\} + \frac{1}{4};$$

$$\alpha_{i,i+1}^{12} = \alpha_{i,i+1}^{21} = 0;\ \alpha_{i,i+1}^{11} = \alpha_{i,i+1}^{22} = \frac{2}{N+1}\sum_k \sin\frac{i\pi k}{N+1}\sin\frac{(i+1)\pi k}{N+1}\frac{e^{-\nu\varepsilon_k}}{1+e^{-\nu\varepsilon_k}},$$

where $\nu = \beta D$, and the one-fermion spectrum ε_k is defined as

$$\varepsilon_k = \cos\frac{\pi k}{N+1},\ (k = 1, 2,\ldots, N) \tag{7}$$

All other coefficients $\alpha_{ij}^{\xi_i\xi_j}$ equal to zero from the symmetry of the problem.

Using expressions of Eqs.(4, 6) we find a matrix representation of the reduced density matrix of nearest-neighbor spins *i* and *j*:

$$\rho_{i,i+1} = \begin{pmatrix} \frac{1}{4} + \alpha_{i,i+1}^{03} + \alpha_{i,i+1}^{30} + \alpha_{i,i+1}^{33} & 0 & 0 & 0 \\ 0 & \frac{1}{4} - \alpha_{i,i+1}^{03} + \alpha_{i,i+1}^{30} - \alpha_{i,i+1}^{33} & \alpha_{i,i+1}^{11} & 0 \\ 0 & \alpha_{i,i+1}^{11} & \frac{1}{4} + \alpha_{i,i+1}^{03} - \alpha_{i,i+1}^{30} - \alpha_{i,i+1}^{33} & 0 \\ 0 & 0 & 0 & \frac{1}{4} - \alpha_{i,i+1}^{03} - \alpha_{i,i+1}^{30} + \alpha_{i,i+1}^{33} \end{pmatrix}$$

The concurrence $C_{i,i+1}$ is defined as [4]

$$C_{i,i+1} = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{8}$$

where λ_p (p = 1, 2, 3, 4) are the square roots of the eigenvalues of the product matrix $R = \rho_{i,i+1}\tilde{\rho}_{i,i+1}$ in the descending order; the matrix $\tilde{\rho}_{i,i+1}$ is defined as $\tilde{\rho}_{i,i+1} = 1/16(I_{iy} \otimes I_{iy}\rho_{i,i+1}^{*} I_{iy} \otimes I_{iy})$. One can show that $0 \le C_{i,i+1} \le 1$. The system is non-entangled ("separable"), if its concurrence equals to zero.

3. Numerical analysis of the concurrence in spin pairs

Using expressions (6)-(8) we investigate numerically the dependence of the concurrence, C_{12}, of the first and the second spins on the temperature and the chain length. Figure 1 shows that the entanglement appears at $\beta D \approx 2$.This corresponds to the temperature interval $0.15 \le T \le 1\mu K$ at $D = 2\pi \cdot 10^4 c^{-1}$. Earlier, the ordered states of nuclear spins coupled by DDI in solids were observed at such temperatures [12].

Our numerical calculations show that the concurrence in the nine-spin chain is non-zero for nearest neighbors only when DDI of all spins are taken into account. The pair of qubits 1 and 2, and the pair of qubits *N*-1 and *N* have the maximal pairwise entanglement. 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 chain.

Analogously it is possible to explain the growth (fall) of the concurrence of the entanglement of spins 1 and 2 in the dependence on the length of the chain consisting of an odd (even) number of spins (Fig. 1). For this purpose it is

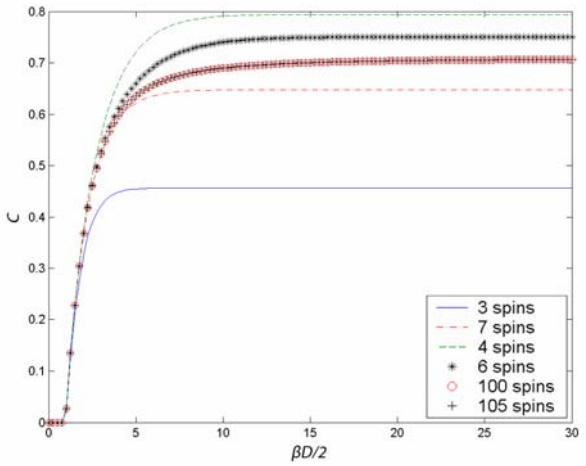

Fig.1. The concurrence of spins 1 and 2 versus the temperature for the number of spins *N* = 3, 4, 6, 7, 100, 105. The behavior of the concurrence C_{12} is different for chains with even and odd *N* when the system size increases. When *N* increases the concurrence C_{12} decreases at even *N* and increases at odd *N*.

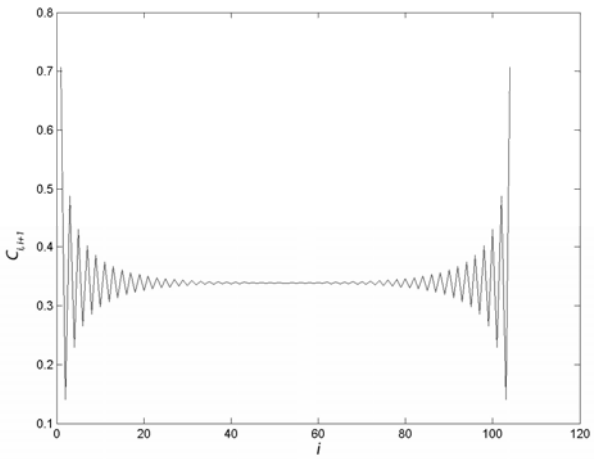

Fig.2. The nearest-neighbor concurrence versus the site number for *N* = 105.

necessary to take into account the influence of both 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 at an odd number of spins. For example, one can easily find in the 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 the entanglement of spins 1, 2 increases also. 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.1) when the even number of spins increases.

The presented numerical calculations show that a homogeneous open spin chain contains quantum correlations which are necessary in order to form pairwise entangled states. Thus, homogeneous chains consisting of spins 1/2 coupled by the dipole-dipole interaction (XY-Hamiltonian) allow us to investigate entangled states of spin pairs at different parameters of the system. One can modify entangled states changing the temperature, coupling constants and number of spins. The presented method of calculation of the reduced density matrix of the spin pair can be used also in a similar analysis of entangled states of the alternating spin chains. It is worth to notice that one can solve the qubit addressing problem in the alternating spin chains on the basis of the Larmor frequencies of different spins. The study of the entanglement in the alternating spin chains is the subject of our forthcoming paper.

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