Entanglement of dipolar coupling spins

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Abstract

Entanglement of dipole-dipole interacting spins 1/2 is usually investigated when the energy of interaction with an external magnetic field (the Zeeman energy) is greater than the energy of dipole interactions by three orders. Under this condition only a non-equilibrium state of the spin system, realized by pulse radiofrequence irradiations, results in entanglement.

The present paper deals with the opposite case: the dipolar interaction energy is the order of magnitude or even larger than the Zeeman one. It was shown that entanglement appears under the thermodynamic equilibrium conditions and the concurrence reaches the maximum when the external field is directed perpendicular to the vector connecting the nuclei. For this direction of the field and a system of two spins with the Hamiltonian accounting the realistic dipole-dipole interactions in low external magnetic field, the exact analytical expression for concurrence was also obtained. The condition of the entanglement appearance and the dependence of concurrence on the external magnetic field, temperature, and dipolar coupling constant were studied.

I. INTRODUCTION

Appreciation of the role of quantum entanglement [1–3] as a resource in quantum teleportation [4], quantum communication [5], quantum computation [6], and quantum metrology [7, 8] has stimulated intensive qualitative and quantitative research. Entanglement, as the quantum correlation, can bring up richer possibilities in the various fields of modern technology. Therefore, in the past few years great efforts have been done to understand and create entanglement. Entanglement between two quantum systems can be generated due to their interaction only [1–3, 9]. It has recently been shown that, in a chain of nuclear spins s = 1/2, which is described by the idealized XY model for a spin system under the thermodynamic equilibrium conditions, entanglement appears at very low temperatures $T \approx 0.5 \ \mu \text{K}$ [10].

In most real quantum systems, such as dipolar coupling spin system, specific conditions for creation of the entangled states are requested. In two-and three-spin [11] and manyspin [12] clusters of protons subjected to a strong magnetic field, truncated dipole-dipole interactions and multiple pulse radiofrequence irradiations, the entangled state of a spin pair emerges at temperatures $T \approx 20$ mK. In these papers the cases were considered where the energy of interaction of the spins with the external magnetic field (the Zeeman energy) is greater than the energy of dipole interactions by three orders [11, 12]. It was shown that at this condition only a non-equilibrium state of the spin system, realized by pulse radiofrequence irradiations, results in entanglement [12, 13].

The present paper deals with the case opposite to those considered previously [11, 12]: the dipolar interaction energy is the order of magnitude or even greater than the Zeeman one. We investigate entanglement of two spins coupled by the realistic dipole-dipole interactions in a low external magnetic field under the thermodynamic equilibrium conditions. We study dependence of the critical temperature and magnetic field at which entanglement appears in this system on a dipolar coupling constant.

II. HAMILTONIAN OF DIPOLAR COUPLING SPIN SYSTEM AND CONCUR-RENCE BETWEEN NUCLEAR SPINS 1/2

Let us consider a system of N spins coupled by long-range dipolar interactions and subjected to an external magnetic field, $\vec{H}_0 = H_0 \vec{z}$. The total Hamiltonian of this interacting system can be written as

$$H = H_z + H_{dd} \tag{1}$$

where the Hamiltonian H_z describes the Zeeman interaction between the nuclear spins and external magnetic field (here we used $\hbar = 1$)

$$H_z = \omega_0 \sum_{k=1}^N I_k^z,\tag{2}$$

 $\omega_0 = \gamma H_0$ is the energy difference between the excited and ground states of an isolated spin, γ is the gyromagnetic ratio of a spin, I_k^z is the projection of the angular spin momentum operator on the z- axes. The Hamiltonian H_{dd} describing dipolar interactions in an external magnetic field [14]:

$$H_{dd} = \sum_{j < k} \frac{\gamma^2}{r_{jk}^3} \{ \left(1 - 3\cos^2\theta_{jk} \right) \left[I_j^z I_k^z - \frac{1}{4} \left(I_j^+ I_k^- + I_j^- I_k^+ \right) \right] - \frac{3}{4} \sin 2\theta_{jk} \left[e^{-i\varphi_{jk}} \left(I_j^z I_k^+ + I_j^+ I_k^z \right) + e^{i\varphi_{jk}} \left(I_j^z I_k^- + I_j^- I_k^z \right) \right] - \frac{3}{4} \sin^2 \theta_{jk} \left[e^{-2i\varphi_{jk}} I_j^+ I_k^+ + e^{2i\varphi_{jk}} I_j^- I_k^- \right] \}$$

$$(3)$$

where r_{jk} , θ_{jk} , and φ_{jk} are the spherical coordinates of the vector \vec{r}_{jk} connecting the j-th and k-th nuclei in a coordinate system with the z-axis along the external magnetic field, \vec{H}_0 , I_j^+ and I_j^- are the raising and lowering spin angular momentum operators of the j-th spin. We consider the situation when it is necessary to take into account all the terms of the Hamiltonian of the dipole-dipole interactions, and not trusnekete any ones.

In the thermodynamic equilibrium the considered system is described by the density matrix

$$\rho = Z^{-1} \exp\left(-\frac{H}{k_B T}\right),\tag{4}$$

where $Z = Tr \{\exp(-H/k_BT)\}$ is the partition function, k_B is the Boltzamnn constant, and T is the temperature. We will analyze entanglement in the spin system described by the density matrix (4).

In order to quantify entanglement, the concurrence C is usually used [15]. For the maximally entangled states, the concurrence is C = 1, while for the separable states C = 0. The concurrence between the quantum states of two spins presented in the Hilbert space as a matrix 4×4 is expressed by the formula [15]

$$C = \max\left\{0, 2\lambda - \sum_{i=1}^{4} \lambda_i\right\}$$
(5)

where $\lambda = \max \{\lambda_1, \lambda_2, \lambda_3, \lambda_4\}$ and λ_i (i = 1, 2, 3, 4) are the square roots of the eigenvalues of the product

$$R = \rho \tilde{\rho} \tag{6}$$

with

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y) \,\bar{\rho} \,(\sigma_y \otimes \sigma_y) \tag{7}$$

where $\bar{\rho}$ the complex conjugation of the density matrix (4) and σ_y is the Pauli matrix

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{8}$$

III. ENTANGLEMENT IN PAIR OF SPINS

We examine dependence of the concurrence, C, between states of the two spins 1/2 on the magnetic field strength and its direction, dipolar coupling constant, and temperature. The numerical calculation of entanglement of the spins at arbitrary orientation of the magnetic field are performed using the software based on the Mathematica package. The results of the numerical calculation show that concurrence reaches its maximum at the case of $\theta = \frac{\pi}{2}$ and $\varphi = 0$ (Fig. 1) and we will consider this case below. This orientation of the spins allows us to obtain for concurrence as an exact analytical function of the temperature, magnetic field and dipolar coupling constant γ^2/r_{12}^3 . Using the exact diagonalization of the density matrix (4) we obtain the concurrence in the following form:

$$C(\beta, d) = \max\left\{0, \frac{A_{+} - A_{-} - e^{\frac{d}{2}}\cosh\frac{d}{4}}{\left(e^{\frac{d}{2}}\cosh\frac{d}{4} + \cosh\frac{\sqrt{16\beta^{2} + 9d^{2}}}{4}\right)}\right\},\tag{9}$$

where

$$A_{\pm} = \frac{1}{2} \sqrt{\frac{16\beta^2 + 9d^2 \cosh\frac{\sqrt{16\beta^2 + 9d^2}}{2} \pm 6d \sinh\frac{\sqrt{16\beta^2 + 9d^2}}{2} \sqrt{16\beta^2 + 9d^2 \cosh^2\frac{\sqrt{16\beta^2 + 9d^2}}{4}}}{16\beta^2 + 9d^2}},$$
(10)

with $\beta = \frac{\omega_0}{k_B T}$ and $d = \frac{\gamma^2}{r_{12}^3 k_B T}$.

At high temperature and low magnetic field ($\beta \ll 1$) and/or small dipolar coupling constant ($d \ll 1$) the expression in the figure brackets (9) becomes negative and, therefore, entanglement is zero. Equating this expression to zero we obtain the critical parameters: temperature T_c , strength of magnetic field H_c , and dipolar coupling constant at which the entanglement appears in a spin pair. Figure 2 presents the phase diagram in which the boundary between the entangled and separated states is determined from equation:

$$A_{+} - A_{-} - e^{\frac{d}{2}} \cosh \frac{d}{4} = 0.$$
(11)

For example, at d = 1 entanglement can be achieved at $\beta > 2.26$. To estimate the critical temperature let us consider fluorine with $\gamma = 4.0025 \frac{kHz}{G}$ and the dipolar interaction energy typically of order of a few kHz (in frequency units) [14]. Taking $H_0 = 3$ G we have $\omega_0 = 12$ kHz, which leads to $T_c = 0.33 \ \mu$ K. The estimated value of temperature is in good agreement with those reported early for the spin system s = 1/2 with the XY Hamiltonian in absence of a magnetic field [10]. Both models give also qualitatively similar dependences of concurrence on temperature but the model considered by us predicts appearance of entanglement in an external magnetic field higher than the critical value. It is interesting that the ordered states, such as antiferromagnetic, of nuclear spins were observed in a calcium-fluoride CaF_2 single crystal at $T = 0.34 \ \mu \text{K}$ [14, 16]. This structure is characterized by domains in the form of layers perpendicular to the external magnetic field. The magnetization inside the crystal is parallel to the external field and reverses its sign from a layer to a layer, while the total magnetization is zero. It is well know that when the magnetization reaches the maximum, all the spins are aligned along the field and entanglement is absent [2, 3]. Entanglement can appear if magnetization is less than its maximum. Therefore, it is reasonable to assume that simultaneously with the transition to the ordered state there arises entanglement of spins from different layers.

Figure 3 shows concurrence as a function of both parameters β and d at $\theta = \frac{\pi}{2}$ and $\varphi = 0$. At large temperature and low magnetic field concurrence is zero. One can see that the concurrence increases with the magnetic field and inverse temperature and reaches its maximum. Then the concurrence decreases. Figure 4 shows the concurrence as a function of the magnetic field at a constant temperature, (Fig. 4a) and as a function of the inverse temperature at a constant magnetic field (Fig. 4b). In the both cases concurrence remains zero up to a certain value of the magnetic field (Fig. 4a) or of the inverse temperature (Fig. 4b), which depends on the coupling constant. The following increase of the magnetic field or inverse temperature leads to eventually rising. In the case of increasing the magnetic field concurrence increases up to the maximum and then decreases as a magnetic field increases

(Fig.4a). Another behavior is observed at an increase of the inverse temperature (Fig. 4b): concurrence monotone grows with 1/T up to a steady value depending on a magnetic field and the following increase of the inverse temperature does not cause any change of concurrence.

IV. DISCUSSION AND CONCLUSIONS

It was obtained that in zero magnetic field the system is in a separable state. The system becomes entangled when the interaction energy of spins with the magnetic field are of the order of the dipolar interaction energy. Then, with increasing magnetic field the spin state tends to separable one. At a small dipolar coupling constant ($d \ll 1$) from the exact analytical solution (9) we obtain the following expression for the concurrency

$$C = \max\left\{0, -\frac{1}{2\cosh^2\frac{\beta}{2}}\right\}$$
(12)

Therefore, at these conditions the states of the system are always separable, C = 0. Entanglement appears in the course of increasing the dipolar coupling constant. To distinguish an entangled state from separable ones, it is important to determine an entanglement witness (EW) applicable to the considered quantum system [17, 18]. The determination of EW is one of the main problems of the experimental study of the entangled states. Internal energy [19], magnetic susceptibility [20], magnetization [21, 22], and intensity of MQ coherences [12, 23, 24] were used as EW in different quantum systems. With the aim to obtain the correlation between the nuclear magnetization and concurrence, using (4) and the definition of nuclear magnetization $M_z = Tr (\rho I_z)$, we obtain the exact expression for magnetization as a function of parameters β and d at $\theta_{12} = \frac{\pi}{2}$ and $\varphi_{12} = 0$:

$$M_z = \frac{-4\beta \sinh \frac{\sqrt{16\beta^2 + 9d^2}}{4}}{(16\beta^2 + 9d^2) \left(\cosh \frac{\sqrt{16\beta^2 + 9d^2}}{4} + e^{\frac{d}{2}} \cosh \frac{d}{4}\right)}$$
(13)

As example, at d = 3, the relation between the concurrence and magnetization can be fitted by C = -0.71(M + 0.26) (Figure 5).

Concurrence, the measure of entanglement between the states of the two spins, depends on the orientation of the magnetic field relative to vector \vec{r} connecting the nuclei. At $\theta = 0$ and π the states are separable and the concurrence reaches its maximum at the case of $\theta = \frac{\pi}{2}$ (Fig. 1). This effect can open a way to manipulate with the spin state by a rotation of the magnetic field or a sample.

In conclusion, investigation of entanglement in a spin 1/2 system under the thermodynamic equilibrium conditions showed that the entangled state can be achieved by application of a low external field when the Zeeman interaction energy is the order of or even less than the dipolar interaction one. It was estimated that for magnetic field $H_0 = 3$ G, the entangled state in a two-spin system arises at temperature $T \leq 0.33 \ \mu\text{K}$. The correlation between concurrence and nuclear magnetization is considered and it was shown that concurrence is well fitted by a linear dependence on the magnetization in the temperature and magnetic field range up to a deviation of the magnetization from Curie's law ($\beta = 3.32$, Fig. 5).

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A. Figure Captions:

Fig. 1 (Color online) Concurrence as a function of the parameter $\beta = \omega_0/k_B T$ and magnetic field direction at $\varphi = 0$ and d = 3.

Fig. 2 The phase diagram. Line presents boundary between the entangled and separated states in the plane $\beta - d$.

Fig. 3 (Color online) Concurrence as a function of the ratios of the magnetic field strength (ω_0) and dipolar coupling constant $(\frac{\gamma^2}{r_{12}^3})$ to k_BT .

Fig. 4 (Color online) Concurrence vs. magnetic field at T = const (a) and vs. temperature at H = const (b) for various dipole interaction constants. (a): black solid line - d = 0.5; red dashed line - d = 2; blue doted line - d = 10. Magnetic field is given in units of $\frac{k_BT}{\gamma}$. (b) black solid line - $\frac{d}{\beta} = 3$; red dashed line - $\frac{d}{\beta} = 5$; blue doted line - $\frac{d}{\beta} = 10$. Temperature is given in units of $\frac{\gamma^2}{r_{12}^2 k_B}$.

Fig. 5 (Color online) Absolute value of magnetization (black solid line) and concurrence (red dash line) as a function of $\beta = \frac{\omega_0}{k_B T}$. Fitting of the concurrence (blue dash-dot line) by

C = -0.71(M + 0.26) at d = 3.









