Entanglement in nuclear quadrupole resonance

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Abstract Entangled quantum states are an important element of quantum information techniques. We determine the requirements for states of quadrupolar nuclei with spins >1/2 to be entangled. It was shown that entanglement is achieved at low temperature by applying a magnetic field to quadrupolar nuclei possessing quadrupole moments, which interact with the electric field gradient produced by the charge distribution in their surroundings.

Keywords Nuclear quadrupole resonance · Entanglement

1 Introduction

Quantum entanglement [1–3], the most characteristic feature of quantum mechanics, is one of the central concepts in quantum information theory and is the feature that distinguishes it most significantly from the classical theory. Entanglement is now viewed as a physical resource, which provides a means to perform quantum computation and quantum communication [4, 5]. It should be emphasized that property of entanglement can be considered regardless of the nature of qubits [6, 7]. Entangled states may appear in various systems of interacting quantum particles, such as phonons, ions, electron, nuclear spins, and of a single particle interacting with environment [7–13] and in systems of interacting qubits [1–3].

One of the most intensively investigated systems is clusters of coupling nuclear spins [1–3] which received considerable attention as a platform for the practical implementation of a quantum computer (QC) by using nuclear magnetic resonance...
(NMR) technique [14–17]. The strength of the coupling (such as dipole-dipole, scalar or exchange interactions) between different spins and the interaction of the spins with the environment determine the decoherence time. Short decoherence times limit possible calculation times of the QC [18]. Later it has been proposed to use quadrupole nuclei, thus eliminating the requirement of interaction between spins and decreasing interaction of qubits with environment [19–25].

It was shown that a spin $\frac{3}{2}$ system is equivalent to a system of two magnetization vectors [26, 27] and can be represented using the Pauli spin matrices $2 \times 2$ [28]. It means that a single spin 3/2 is isomorphic to a system consisting of two dipolar coupling spins 1/2, which can be considered as qubits. This was experimentally confirmed by using NQR technique with quadrupole splitting [21, 22]. The feasibility of quantum computing based on a pure (without external magnetic fields) NQR technique was theoretically investigated in detail in [23]. Using the resonance excitation technique and the level-crossing method, three quantum logic gates were proposed: a controlled NOT, SWAP and NOT$_2$. Thus the method to synthesize qubits from a set of the spin states of a single particle with spin higher than 1/2 has been developed. It is logical to raise the question of entanglement of these qubits.

Our present purpose is to investigate entanglement between the quantum states of quadrupole nuclei. We consider a nucleus with spin $\frac{3}{2}$ being in an internal electric field gradient (EFG) and an external magnetic field when the quadrupole interaction energy is of the order of the magnitude or even greater than the Zeeman one. Results of computer simulations of entanglement dynamics are presented for real spin systems with a non-equidistant energy spectrum.

2 NQR in magnetic field

Let us consider a quadrupole nucleus with spin $I$ ($I > 1/2$) in thermodynamic equilibrium with the density matrix

$$\rho = Z^{-1} \exp \left( - \frac{\mathcal{H}}{k_B T} \right).$$

(1)

Here $k_B$ is the Boltzmann constant, $T$ is the lattice temperature, $Z = \text{Tr} \left\{ \exp \left( - \frac{\mathcal{H}}{k_B T} \right) \right\}$ is the partition function. In the general case, the Hamiltonian $\mathcal{H}$ can consist of the Zeeman ($\mathcal{H}_M$) and the quadrupole ($\mathcal{H}_Q$) parts,

$$\mathcal{H} = \mathcal{H}_M + \mathcal{H}_Q.$$  

(2)

The Zeeman interaction between the applied magnetic field, $\vec{H}_0$ and nuclear spin is the external factor for a crystal and the direction of this field is chosen as the $z$-axis of the laboratory frame, $\vec{H}_0 = H_0 \hat{z}$, where $H_0$ is the strength of the external magnetic field. The part of the Hamiltonian describing this interaction is

$$\mathcal{H}_M = -\gamma H_0 I_z,$$

(3)

where $\gamma$ is the gyromagnetic ratio of the nucleus with spin $I$, $I_z$ is the projection of the individual spin angular momentum operator $\vec{I}$ on the $z$-axis.

Quadrupole coupling exists between a non-spherical nuclear charge distribution and an electric field gradient (EFG) generated by the charge distribution in its
surroundings. It is possible to reduce the EFG symmetric tensor to a diagonal form by finding the principal axes frame (PAF) with the Z- and X-axis directed along the maximum and minimum of EFG, respectively, $|V_{ZZ}| \geq |V_{YY}| \geq |V_{XX}|$, where $V_{\xi\xi} = \frac{\partial^2 V}{\partial \xi^2}$ ($\xi = X, Y, Z$) and $V$ is the potential of the electric field. In the laboratory frame the quadrupolar Hamiltonian can be presented in the following form

$$
H_Q = \frac{eQq_{ZZ}}{4I(2I-1)} U(\theta, \varphi) \left[ 3I_z^2 - \vec{I}^2 + \frac{\eta}{2} \left( I_+^2 - I_-^2 \right) \right] U^+(\theta, \varphi),
$$

where

$$
U(\theta, \varphi) = e^{-i\varphi I_z} e^{-i\theta I_y} e^{i\varphi I_z},
$$

$eQq_{ZZ}$ is the quadrupole coupling constant of EFG, $I_{\pm}$ are the raising and lowering operators of the spin, and $\theta$ and $\varphi$ refer to the polar and azimuthal angles determining the orientation of the laboratory frame $z$-axis in the PAF coordinate system. The asymmetry parameter $\eta$ is defined as

$$
\eta = \frac{V_{YY} - V_{XX}}{V_{ZZ}},
$$

which may vary between 0 and 1.

Using the Hamiltonian 2 the density matrix 1 can be represented as a function of parameters $\alpha = \frac{\gamma H_0}{k_B T}$ and $\beta = \frac{eQq_{ZZ}}{4I(2I-1)k_B T}$:

$$
\rho = Z^{-1} \exp \left\{ -\alpha I_z - \beta U(\theta, \varphi) \left[ 3I_z^2 - \vec{I}^2 + \frac{\eta}{2} \left( I_+^2 - I_-^2 \right) \right] U^+(\theta, \varphi) \right\}.
$$

The density matrix 7 can be employed to obtain information on the dependence of entanglement on the magnetic field, quadrupole coupling constant, orientation of the crystal principal axis in the laboratory frame, and temperature.

Below we consider entanglement in a system of spins 3/2. A suitable system for studying by NQR technique is a high temperature superconductor $YBa_2Cu_3O_{7-\delta}$ containing the $^{63}Cu$ and $^{65}Cu$ nuclei with spin $\frac{3}{2}$ possessing quadrupole moments $Q = -0.211 \times 10^{-24}$ cm$^2$ and $-0.195 \times 10^{-24}$ cm$^2$, respectively [29]. There are two different locations of copper ions in this structure: the first are the copper ion sites at the center of an oxygen rhombus-like plane while the second one is five-coordinated by an apically elongated rhombic pyramid. The four-coordinated copper ion site, EFG is highly asymmetric ($\eta \geq 0.92$) while the five-coordinated copper ion site, EFG is nearly axially symmetric ($\eta = 0.14$). The quadrupole coupling constant ($eQq_{ZZ}$) of $^{63}Cu$ in the four-coordinated copper ion site is 38.2 MHz and in the five-coordinated copper ion site is 62.8 MHz [29].

3 Reduced density matrix and measures of entanglement

An important measure of entanglement is the concurrence [30]. For the maximally entangled states, the concurrence is $C = 1$, while for the separable states $C = 0$. The
concurrence of a quantum system with the density matrix presented in the Hilbert space as a matrix $4 \times 4$ is expressed by the formula [30]:

$$C = \max \left\{ 0, 2\nu - \sum_{i=1}^{4} \nu_i \right\}$$

where $\nu = \max \{\nu_1, \nu_2, \nu_3, \nu_4\}$ and $\nu_i$ $(i = 1, 2, 3, 4)$ are the square roots of the eigenvalues of the product

$$R = \rho_{\text{red}} \tilde{\rho}_{\text{red}},$$

where $\rho_{\text{red}} = Tr_{\text{partial}}(\rho)$ is the reduced density matrix, $Tr_{\text{partial}}(...)$ is the partial trace, and

$$\tilde{\rho}_{\text{red}} = G\tilde{\rho}_{\text{red}} G$$

where $\tilde{\rho}_{\text{red}}(\alpha, \beta)$ is the complex conjugation of the reduced density matrix $\rho_{\text{red}}$ and

$$G = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}. \quad (11)$$

An another important measure of entanglement is the entanglement entropy. In order to implement this measure of entanglement we first map the Hilbert space of a spin $3/2$ which is four dimensional onto the Hilbert space of two spins $1/2$, $S_A$ and $S_B$ [31]. The entropy of entanglement is defined as [32, 33]:

$$E = -Tr (\rho_A \log_2 \rho_A) = -Tr (\rho_B \log_2 \rho_B). \quad (12)$$

Here $\rho_A$ is the partial trace of $\rho_A = Tr_B(\rho)$ over subsystem $B$, and $\rho_B$ has a similar meaning.
Concurrence and the entanglement of formation vs. magnetic field at $T = \text{const}$ for various quadrupole interaction constants: \textit{black solid line}—$\beta = 2$; \textit{red dashed line}—$\beta = 6$; \textit{green dotted line}—$\beta = 8$; \textit{blue dash-doted line}—$\beta = 12$

This entropy is related to the concurrence $C$ by the following equation [30]

$$E(x) = -x \log_2 x - (1 - x) \log_2 (1 - x),$$

where $x = \frac{1}{2} \left( 1 + \sqrt{1 + C^2} \right)$.

The numerical simulations of entanglement of the spin states were performed for the special case $I = 3/2$ using the software based on the Mathematica package. In equilibrium the states of the system determined by Eq. 7 are separable without applying external magnetic filed ($\alpha = 0$) at any temperature. At high temperature ($\beta < 1$) and low magnetic field strength ($\alpha < 1$) the concurrence is zero. Entanglement appears in the course of temperature decrease and increasing the magnetic field.

The concurrence and the entanglement of formation dependences on the magnetic field, quadrupole coupling constant, and temperature are qualitatively independent of the angles. As an example, we present below the concurrence as a function of the parameters $\alpha$ and $\beta$ for the concurrence maximum for a spin in the five-coordinated copper ion site ($\eta = 0.14$) at $\theta = 0.94$ and $\varphi = 0$ (Fig. 1). The concurrence increases with the magnetic field strength and inverse temperature and reaches a maximum value. For low temperatures we obtain that concurrence and the entanglement of
formation increase with the magnetic field strength and then decrease with increasing magnetic field strength (Fig. 2). Another dependence of the concurrence on temperature is observed (Fig. 3). With a decrease of temperature below a critical value the concurrence monotonically increase till a limiting value. The critical temperature and limiting value are determined by a ratio of the Zeeman and quadrupole coupling energies, $\alpha/\beta$.

4 Discussion and conclusions

The obtained results show that the entangled states can be generated between the states of a single nuclear spin $\frac{3}{2}$. From a point of view of quantum information processing the considered system is isomorphic to a system consisting of two dipolar coupling spins $\frac{1}{2}$. The same quantum logical gates can be realized using both systems. Therefore the obtained entanglement can be considered as entanglement between qubits formed by states of a single particle. On the other hand, a single spin 3/2 isomorphic to a system consists of two dipolar coupling spins 1/2 and entanglement between the states of a spin 3/2 can be considered as entanglement between two effective spins 1/2. The behavior of entanglement of a spin 3/2 is very similar to that of a system consisting of two dipolar coupling spins $\frac{1}{2}$ [34]. It was obtained that in zero magnetic field the states of both spin systems, two spins $\frac{1}{2}$ and spin $\frac{3}{2}$, are in separable states. These systems become entangled with increasing magnetic field. Then, with a further increase of the magnetic field the spin states of the both systems tend to a separable one.

It has recently been shown that, in a system of nuclear spins $s = 1/2$, which is described by the idealized XY model and dipolar coupling spin system under thermodynamic equilibrium conditions, entanglement appears at very low temperatures $T \approx 0.5 \div 0.3 \mu$ K [34, 35]. In a non-equilibrium state of the spin system, realized by pulse radiofrequency irradiations, estimation of the critical temperature at which entanglement appears in a system of spins $\frac{1}{2}$ gives $T \leq 0.027$ K [36]. The calculation for $^{63}Cu$ in the five-coordinated copper ion site of $YBa_2Cu_3O_{7-\delta}$ at $\alpha/\beta = 1$, $\eta = 0.14$ and $eQq_{zz} = 62.8$ MHz, gives that the concurrence appears at $\beta = 0.6$ (Fig. 3). This $\beta$ value corresponds to temperature $T \approx 5$ mK. This estimated
value of critical temperature is three orders greater than the critical temperature estimated for the two dipolar coupling spins under thermodynamic equilibrium [34].

In conclusion, this investigation has shown that entanglement can be achieved by applying a magnetic field to a single spin 3/2 at low temperature. Concurrence and the entanglement of formation depend on the orientation between the external magnetic field and PAF axes. At $\theta = 0$ and $\pi$ the states are separable at any condition. At $\eta = 0.14$ the concurrence and the entanglement of formation reach their maximum value at $\theta = 0.94$ and $\phi = 0$ and $\pi$. This effect can open a way to manipulate the spin states by a rotation of the magnetic field or of the sample.

References