Multiple quantum spin dynamics of entanglement

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The dynamics of entanglement is investigated on the basis of exactly solvable models of multiple quantum (MQ) NMR spin dynamics. It is shown that the time evolution of MQ coherences of systems of coupled nuclear spins in solids is directly connected with dynamics of the quantum entanglement. We studied analytically the dynamics of entangled states for two- and three-spin systems coupled by the dipole-dipole interaction. In this case the dynamics of the quantum entanglement is uniquely determined by the time evolution of MQ coherences of the second order. The real part of the density matrix describing MQ dynamics in solids is responsible for MQ coherences of the zeroth order while its imaginary part is responsible for the second order. Thus, one can conclude that the dynamics of the entanglement is connected with transitions from the real part of the density matrix to the imaginary one, and vice versa. A pure state which generalizes the Greenberger-Horne-Zeilinger (GHZ) and *W* states is found. Different measures of the entanglement of this state are analyzed for tripartite systems.

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I. INTRODUCTION

Solid state NMR is one of the most promising candidates for realization of a quantum computer and quantum-information processing (QIP). Several such schemes have been suggested [1–8]. Possibilities for the experimental realizations of quantum algorithms and theoretical investigations of QIP are connected with multiple quantum (MQ) NMR. Contrary to the usual NMR, MQ NMR spectroscopy uses not only adjacent but all possible transitions between Zeeman levels of the system of interacting spins in an external magnetic field. This allows one to gain more detailed information on dynamical processes in solids. Further progress in the understanding of multiple-spin MQ dynamics was achieved with experimental investigations of MQ NMR dynamics of quasi-one-dimensional distributions of clusters of uniformly spaced proton spins in hydroxyapatite $Ca_5OH(PO_4)_3$ and related fluorine-containing apatites [9,10]. These materials represent a possible base for QIP devices [6,7]. Thus, investigations of the quantum entanglement with MQ NMR methods are of current interest. The existence of entanglement is a necessary condition for exponential speed-up during quantum computations [11]. It has been investigated and discussed in the literature whether the NMR scheme with pseudopure states is "true" quantum computation [11,12].

Numerical methods [13–15] and exactly solvable models [16–19] have been applied to the theoretical analysis of MQ dynamics. In this paper, we investigate the dynamics of entangled states on the basis of MQ NMR methods. The results obtained show that the time evolution of MQ coherences of nuclear spins 1/2 coupled by dipole-dipole interactions (DDI's) is directly connected with the dynamics of quantum entanglement. Exact solutions are presented for two and three spin-1/2 nuclei. For these systems the periodic dynamics of quantum entanglement is uniquely determined by the time evolution of the intensity of MQ coherences of the second order. We suppose that the intensity of MQ coherence of the second order can be considered as a measure of entanglement. In particular, it is significant that the entanglement and intensity of MQ coherence of the second order are equal to zero at the moment of time $\tau=0$. At the same time, the intensity of MQ coherence of the zeroth order is maximal at $\tau=0$. In the course of the time evolution an exchange between MQ coherences of the zeroth and second orders takes place while their sum is a constant of motion [20]. When the intensity of MQ coherence of the zeroth order is decreasing and becoming minimal, the entanglement achieves its maximum value and so does the intensity of MQ coherence of the second order. After that, the entanglement decreases, and so on. It has been shown [13] that the real part of the density matrix describing MQ dynamics in solids is responsible for MQ coherences of the zeroth order while its imaginary part is responsible for the second order. It is possible to conclude that the dynamics of the entanglement is connected with the transitions between the real and imaginary parts of the density matrix.

II. MQ DYNAMICS

MQ spin dynamics in solids is described by the Liouville–von Neumann equation

$$i\frac{d\rho}{d\tau}=[H,\rho(\tau)], \tag{1}$$

where the nonsecular average dipolar Hamiltonian H is given by [16]

$$H=-\frac{1}{2}\sum_{j<k} D_{jk}(I_j^+I_k^+ + I_j^-I_k^-) \tag{2}$$

and $I_j^{\pm}$ are the raising and lowering spin angular momentum operators of spin j. The dipolar coupling constant D_{jk} between spins j and k is given by

$$D_{jk}=\frac{\gamma^2\hbar}{2r_{jk}^3}(1-3\cos^2\theta_{jk}), \tag{3}$$

where r_{jk} is the distance between spins j and k, θ_{jk} the angle between the internuclear vector $\vec{r}_{jk}$ and the external magnetic field $\mathbf{H}_0$, and γ the gyromagnetic ratio. The angle θ_{jk} is the same for all spin pairs. In linear chains we assume that $\theta_{jk}=0$.

If the spin system is in thermal equilibrium with the lattice at $\tau=0$, then the solution of Eq. (1) in the high-temperature approximation is

$$\rho(\tau)=e^{-iH\tau}\rho(0)e^{iH\tau}. \tag{4}$$

Here $\rho(0)$ is the initial density matrix:

$$\rho(0)=\sum_{j}^{N} I_{zj}, \tag{5}$$

where I_{zj} is the projection of the spin j angular momentum on the direction z of the external field $\mathbf{H}_0$. According to [16] the density matrix $\rho(\tau)$ can be expanded as

$$\rho(\tau)=\sum_{n} \rho_n(\tau), \tag{6}$$

where $\rho_n(\tau)$ is the contribution to $\rho(\tau)$ due to MQ coherences of order n. If only the nearest neighbors interact, the profile of MQ coherences consists of zero and two quantum coherences [17,15]. At the same time, MQ NMR spectra consist of MQ coherences of arbitrary even orders ($n=0, \pm 2, \pm 4, \pm 6, \ldots, |n|\leqslant N$, where N is the number of spins) as the DDI's of all spins are taken into account. While the intensities of MQ coherences of order $n=4k$ ($0\leqslant 4k\leqslant N$) are determined by the real part of the density matrix $\rho(\tau)$ only, the intensities of MQ coherences of order $n=4k+2$ ($2\leqslant 4k+2\leqslant N$) are determined by the imaginary part of $\rho(\tau)$ [13].

Special experimental methods [21–23] are used to separate the signals from the MQ coherences of various orders. In MQ NMR experiments the multiple quantum coherences are transformed into longitudinal magnetization. As a result, the intensities of the MQ coherences $J_n(\tau)$ can be measured. They can be expressed as [16]

$$J_n(\tau)=\mathrm{Tr}\rho_n(\tau)\rho_{-n}(\tau). \tag{7}$$

It is worth noticing that $\rho_{-n}(\tau)=\rho_n^{+}(\tau)$.

The sum of the intensities of the multiple quantum coherences does not depend on time [20]. Normalizing this sum to unity, we have

$$J_0(\tau)+2\sum_{n=2}^{N} J_n(\tau)=1. \tag{8}$$

III. DYNAMICS OF ENTANGLEMENT BETWEEN TWO SPIN NUCLEI

A pair of spins has four possible basis product states: $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$. In this basis the initial density matrix from Eq. (5) is

$$\rho(0)=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{9}$$

The density matrix $\rho(\tau)$ can be obtained from the analytical solution Eq. (4) [17,24]:

$$\rho(\tau)=\rho_0(\tau)+\rho_{\pm 2}(\tau) =\begin{pmatrix} \cos\varphi(\tau) & 0 & 0 & i\sin\varphi(\tau) \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -i\sin\varphi(\tau) & 0 & 0 & -\cos\varphi(\tau) \end{pmatrix}, \tag{10}$$

where $\varphi(\tau)=D_{12}\tau$ and $\rho_0(\tau)=\mathrm{Re}[\rho(\tau)]$, $\rho_{\pm 2}(\tau)=\rho_{+2}(\tau)+\rho_{-2}(\tau)=\mathrm{Im}[\rho(\tau)]$.

The normalized intensity of MQ coherences can be calculated from Eqs. (7) and (10):

$$J_0(\tau)=\cos^2\varphi(\tau), \tag{11}$$

$$J_2(\tau)=J_{+2}(\tau)+J_{-2}(\tau)=\sin^2\varphi(\tau). \tag{12}$$

The density matrix $\rho(\tau)$ of Eq. (10) can be expressed through the vector of the state

$$|\Psi\rangle=e^{i\pi/4}\cos[\varphi(\tau)/2]|00\rangle+e^{-i\pi/4}\sin[\varphi(\tau)/2]|11\rangle. \tag{13}$$

The projector is

$$\sigma(\tau)=|\Psi\rangle\langle\Psi| =\frac{1}{2}\begin{pmatrix} 1+\cos\varphi(\tau) & 0 & 0 & i\sin\varphi(\tau) \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -i\sin\varphi(\tau) & 0 & 0 & 1-\cos\varphi(\tau) \end{pmatrix}. \tag{14}$$

Comparing Eqs. (10) and (14), we have

$$\rho(\tau)=2\sigma(\tau)-E', \tag{15}$$

where

$$E'=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

is independent of time. Thus, the MQ dynamics of the two-spin systems can be described by the state vector (13).

Let us consider the dynamics of the entanglement of the bipartite system in the state of Eq. (13). The measure of the entanglement for a pure bipartite state can be defined as the von Neumann entropy of any of its two parts [25]:

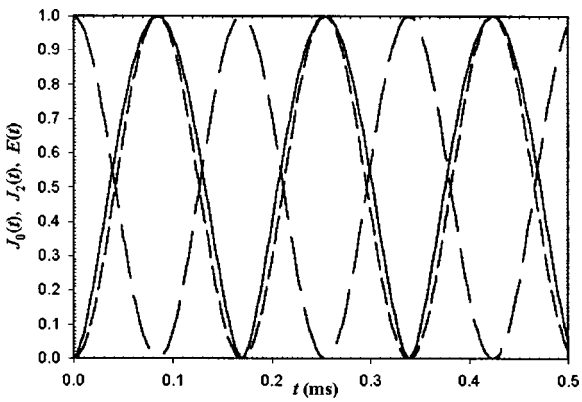

FIG. 1. Time dependence of the intensity of MQ coherences of the zeroth order $J_0(t)$ (long-dashed line), of the second order $J_2(t)$ [the square of the concurrence $C^2(t)$] (short-dashed line), and of entanglement $E(t)$ (solid line) for two spins coupled by DDI's with the dipolar coupling constant $D_{12}=2\pi 2950\ \mathrm{s}^{-1}$.

$$E=-\mathrm{Tr}\sigma_A \log_2 \sigma_A=-\mathrm{Tr}\sigma_B \log_2 \sigma_B, \tag{16}$$

where $\sigma_{A(B)}=\mathrm{Tr}_{B(A)}\sigma$ is the reduced density matrix.

If the quantum state is given by

$$|\Psi\rangle_{AB}=a|0\rangle_A\otimes|0\rangle_B+b|1\rangle_A\otimes|1\rangle_B, \tag{17}$$

then the operator σ_A can be written in the form (see Chap. 2.3.1 in Ref. [26])

$$\sigma_A=|a|^2|0\rangle_{A\ A}\langle 0|+|b|^2|1\rangle_{A\ A}\langle 1|. \tag{18}$$

In our case $|a|^2=\cos^2[\varphi(\tau)/2]$, $|b|^2=\sin^2[\varphi(\tau)/2]$, and we obtain

$$\sigma_A=\begin{pmatrix}\cos^2[\varphi(\tau)/2] & 0\\ 0 & \sin^2[\varphi(\tau)/2]\end{pmatrix}. \tag{19}$$

Thus, the entanglement resulting from Eq. (16) is

$$E(\tau)=-\cos^2[\varphi(\tau)/2]\log_2\{\cos^2[\varphi(\tau)/2]\} -\sin^2[\varphi(\tau)/2]\log_2\{\sin^2[\varphi(\tau)/2]\}. \tag{20}$$

Comparing solutions of Eqs. (11), (12), and (20) (see Fig. 1) it is possible to draw the conclusion that the dynamics of entanglement is directly correlated with the dynamics of the intensity of MQ coherences of the second order.

Let us consider the dynamics of the entanglement in terms of the concurrence, which can be determined as [27,28]

$$C(\psi)=\left|\sum_i \alpha_i^2\right|, \tag{21}$$

where α_i are the coefficients of the expansion of some state

$$|\psi\rangle=\sum_i^4 \alpha_i|e_i\rangle \tag{22}$$

in the following "magic basis" of completely entangled states:

$$|e_1\rangle=\frac{1}{\sqrt{2}}(|00\rangle+|11\rangle),\quad |e_2\rangle=\frac{1}{\sqrt{2}}i(|00\rangle-|11\rangle),$$

$$|e_3\rangle=\frac{1}{\sqrt{2}}i(|01\rangle+|10\rangle),\quad |e_4\rangle=\frac{1}{\sqrt{2}}(|01\rangle-|10\rangle). \tag{23}$$

Then the entanglement of $|\psi\rangle$ is [27,28]

$$E(\psi)=H\left[\frac{1}{2}(1+\sqrt{1-C^2})\right], \tag{24}$$

where H is the binary entropy function $H(x)=-x\log_2(x)-(1-x)\log_2(1-x)$.

Equation (13) can be rewritten in the form (22) as

$$|\Psi\rangle=\frac{1}{2}(e^{-i\varphi(\tau)/2}+ie^{-i\varphi(\tau)/2})\frac{1}{\sqrt{2}}(|00\rangle+|11\rangle) +\frac{1}{2}(e^{i\varphi(\tau)/2}-ie^{i\varphi(\tau)/2})\frac{1}{\sqrt{2}}i(|00\rangle-|11\rangle). \tag{25}$$

Thus $\alpha_1=(1/2)(e^{-i\varphi(\tau)/2}+ie^{-i\varphi(\tau)/2})$, $\alpha_2=(1/2)(e^{i\varphi(\tau)/2}-ie^{i\varphi(\tau)/2})$, $\alpha_3=\alpha_4=0$, and

$$C=|\alpha_1^2+\alpha_2^2|=|\sin\varphi(\tau)|. \tag{26}$$

Comparing Eqs. (12) and (26), it is possible to conclude that in the two-spin system the concurrence is connected with the intensity of MQ coherences of the second order by the relation

$$C^2(\tau)=J_2(\tau). \tag{27}$$

Note that the entanglement determined by Eqs. (20) and (24) is the same.

IV. THREE-SPIN CASE

It is known [13] that the operator $e^{i\pi I_z}$ is an integral of motion. Hence, the Hamiltonian $(2^N\times 2^N)$ matrix is reduced to two $2^{N-1}\times 2^{N-1}$ submatrices which correspond to odd and even numbers of the spins which are directed opposite to the applied magnetic field $\mathbf{H}_0$. If the number of spins is odd then both blocks give the same profiles of MQ coherences. One should solve the problem using one block of the density matrix and double the intensities of MQ coherences [13]. If the number of spins is even then the blocks give the different profiles of MQ coherences, but they can be calculated independently from one other [13].

For three-spin systems, there are eight possible product states: $|000\rangle$, $|001\rangle$, $|010\rangle$, $|011\rangle$, $|100\rangle$, $|101\rangle$, $|110\rangle$, $|111\rangle$. The density matrix is reduced to two blocks in the bases $|000\rangle$, $|011\rangle$, $|101\rangle$, $|110\rangle$ (for even number of individual spin states $|1\rangle$) and $|001\rangle$, $|010\rangle$, $|100\rangle$, $|111\rangle$ (for odd number of such spins).

The top block of the initial density matrix according to Eq. (5) is

$$\rho(0)=\begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}. \tag{28}$$

The time development of the density matrix can be expressed analytically [24]:

$$\rho(\tau)=\rho_0(\tau)+\rho_{\pm 2}(\tau)$$
$$=\begin{pmatrix} \frac{3}{2}+A & iR_{23} & iR_{13}B & iR_{12}B \\ -iR_{23}B & -\frac{1}{2}-R_{23}^2A & -R_{13}R_{23}A & -R_{12}R_{23}A \\ -iR_{13}B & -R_{13}R_{23}A & -\frac{1}{2}-R_{13}^2A & -R_{12}R_{13}A \\ -iR_{12}B & -R_{12}R_{23}A & -R_{12}R_{13}A & -\frac{1}{2}-R_{12}^2A \end{pmatrix}, \tag{29}$$

where $A=[\cos(D_{\rm eff}\,\tau)-1]$, $B=\sin(D_{\rm eff}\,\tau)$, and $R_{12}=D_{12}/D_{\rm eff}$, $R_{13}=D_{13}/D_{\rm eff}$, $R_{23}=D_{23}/D_{\rm eff}$. Here, $D_{\rm eff}=(D_{12}^2+D_{13}^2+D_{23}^2)^{1/2}$.

Let all three coupling constants be equal (the triangle ring) $D=D_{12}=D_{13}=D_{23}$. In this case, $D_{\rm eff}=\sqrt{3}D$, $R=R_{12}=R_{13}=R_{23}=1/\sqrt{3}$, and the density matrix simplifies to

$$\rho(\tau)=\begin{pmatrix} \frac{3}{2}+A & i\frac{1}{\sqrt{3}}B & i\frac{1}{\sqrt{3}}B & i\frac{1}{\sqrt{3}}B \\ -i\frac{1}{\sqrt{3}}B & -\frac{1}{2}-\frac{1}{3}A & -\frac{1}{3}A & -\frac{1}{3}A \\ -i\frac{1}{\sqrt{3}}B & -\frac{1}{3}A & -\frac{1}{2}-\frac{1}{3}A & -\frac{1}{3}A \\ -i\frac{1}{\sqrt{3}}B & -\frac{1}{3}A & -\frac{1}{3}A & -\frac{1}{2}-\frac{1}{3}A \end{pmatrix}, \tag{30}$$

where $A=[\cos\varphi(\tau)-1]$, $B=\sin\varphi(\tau)$, and $\varphi(\tau)=\sqrt{3}D\tau$.

Then the intensity of the normalized MQ coherences of the second order (for both blocks) can be calculated [24] from Eqs. (7) and (30) as

$$J_2(\tau)=\frac{2}{3}\sin^2\varphi(\tau). \tag{31}$$

The density matrix $\rho(\tau)$ of Eq. (30) can be expressed through the vector of the state

$$|\Psi\rangle=e^{i\pi/4}\cos[\varphi(\tau)/2]|000\rangle+\frac{1}{\sqrt{3}}e^{-i\pi/4}\sin[\varphi(\tau)/2]|011\rangle$$
$$+\frac{1}{\sqrt{3}}e^{-i\pi/4}\sin[\varphi(\tau)/2]|101\rangle$$
$$+\frac{1}{\sqrt{3}}e^{-i\pi/4}\sin[\varphi(\tau)/2]|110\rangle. \tag{32}$$

The projector is

$$\sigma(\tau)=|\Psi\rangle\langle\Psi|=\frac{1}{2}\begin{pmatrix} 2+A & i\frac{1}{\sqrt{3}}B & i\frac{1}{\sqrt{3}}B & i\frac{1}{\sqrt{3}}B \\ -i\frac{1}{\sqrt{3}}B & -\frac{1}{3}A & -\frac{1}{3}A & -\frac{1}{3}A \\ -i\frac{1}{\sqrt{3}}B & -\frac{1}{3}A & -\frac{1}{3}A & -\frac{1}{3}A \\ -i\frac{1}{\sqrt{3}}B & -\frac{1}{3}A & -\frac{1}{3}A & -\frac{1}{3}A \end{pmatrix}. \tag{33}$$

Comparing Eqs. (30) and (33), we have

$$\rho(\tau)=2\sigma(\tau)-\frac{1}{2}E, \tag{34}$$

where E is the unit matrix.

To find the connection between MQ dynamics and the dynamics of entanglement for a three-spin system, we shall analyze the entanglement properties of the pure state (32) through the state

$$|\Phi\rangle=a|000\rangle+b|011\rangle+c|101\rangle+d|110\rangle, \tag{35}$$

where $|a|^2+|b|^2+|c|^2+|d|^2=1$.

The density matrix of three particles A,B,C is $\sigma_{ABC}=|\Phi(ABC)\rangle\langle\Phi(ABC)|$. The two-particle and one-particle reduced density matrices are given by

$$\sigma_{BC}={\rm Tr}_A\sigma_{ABC},$$
$$\sigma_A={\rm Tr}_{BC}\sigma_{ABC}. \tag{36}$$

All other reduced density matrices are obtained analogously.

For the state (35) we have

$$\sigma_{BC}=\begin{pmatrix} |a|^2 & 0 & 0 & ab^* \\ 0 & |c|^2 & cd^* & 0 \\ 0 & dc^* & |d|^2 & 0 \\ ba^* & 0 & 0 & |b|^2 \end{pmatrix},$$
$$\sigma_A=\begin{pmatrix} |a|^2+|b|^2 & 0 \\ 0 & |c|^2+|d|^2 \end{pmatrix}. \tag{37}$$

The matrices σ_{AC}, σ_B, and σ_{AB}, σ_C are obtained from Eq. (37) by the changes $c \Leftrightarrow b$ and $c \Leftrightarrow d$ performed one after the other.

For analysis of the entanglement we use the approach advanced in Ref. [29]. We introduce the "spin-flipped" density matrix $\tilde{\sigma}_{BC} = (\sigma_y \otimes \sigma_y)\sigma^*_{BC}(\sigma_y \otimes \sigma_y)$, where σ^*_{BC} is the complex-conjugate matrix of σ_{BC} and σ_y is the standard y component Pauli matrix. As both σ_{BC} and $\tilde{\sigma}_{BC}$ are positive operators, it follows that the product $\sigma_{BC}\tilde{\sigma}_{BC}$, though non-Hermitian, also has only real and non-negative egenvalues [29].

Then

$$\sigma_{BC}\tilde{\sigma}_{BC} = \begin{pmatrix} 2|a|^2|b|^2 & 0 & 0 & 2|a|^2ab^* \\ 0 & 2|c|^2|d|^2 & 2|c|^2cd^* & 0 \\ 0 & 2|d|^2dc^* & 2|c|^2|d|^2 & 0 \\ 2|b|^2ba^* & 0 & 0 & 2|a|^2|b|^2 \end{pmatrix} \tag{38}$$

and the two nonzero eigenvalues of this matrix product are

$$\lambda_1^{BC} = 4|a|^2|b|^2, \quad \lambda_2^{BC} = 4|c|^2|d|^2. \tag{39}$$

Having executed the above-mentioned replacement, we obtain

$$\lambda_1^{AC} = 4|a|^2|c|^2, \ \ \lambda_2^{AC} = 4|b|^2|d|^2,$$

$$\lambda_1^{AB} = 4|a|^2|d|^2, \ \ \lambda_2^{AB} = 4|b|^2|c|^2.$$

The concurrence between two particles is defined in this case as $C = |\sqrt{\lambda_1} - \sqrt{\lambda_2}|$ [28] and the square of it is

$$C^2_{BC} = 4(|a||b| - |c||d|)^2, \quad C^2_{AC} = 4(|a||c| - |b||d|)^2,$$

$$C^2_{AB} = 4(|a||d| - |b||c|)^2. \tag{40}$$

The concurrence between the particle A and the pair BC can be calculated [29] as

$$C^2_{A\ (BC)} = \mathrm{Tr}\sigma_{AB}\tilde{\sigma}_{AB} + \mathrm{Tr}\sigma_{AC}\tilde{\sigma}_{AC} = 4 \det \sigma_A, \tag{41}$$

and is similar in the remaining cases.

We obtain

$$C^2_{A\ (BC)} = 4(|a|^2|c|^2 + |a|^2|d|^2 + |b|^2|c|^2 + |b|^2|d|^2),$$

$$C^2_{B\ (AC)} = 4(|a|^2|b|^2 + |a|^2|d|^2 + |b|^2|c|^2 + |c|^2|d|^2),$$

$$C^2_{C\ (AB)} = 4(|a|^2|b|^2 + |a|^2|c|^2 + |b|^2|d|^2 + |c|^2|d|^2). \tag{42}$$

One can easily verify that

$$\begin{aligned} C^2_{A\ (BC)} - C^2_{AB} - C^2_{AC} &= C^2_{B\ (AC)} - C^2_{AB} - C^2_{BC} \\ &= C^2_{C\ (AB)} - C^2_{AC} - C^2_{BC} \\ &= 16|a||b||c||d| = \tau_{ABC}, \end{aligned} \tag{43}$$

where the three-tangle [29] τ_{ABC} is the measure of three-particle entanglement.

Apparently, the pure state for the second block for an odd number of spins

$$|\Phi\rangle = d|001\rangle + c|010\rangle + b|100\rangle + a|111\rangle \tag{44}$$

has analogous measures of the entanglement.

It is interesting to compare measures of entanglement of the state given by Eq. (35) or Eq. (44) with those for other classes of pure states. One can see that these expressions generalize the states known as the Greenberger-Horne-Zeilinger (GHZ) [30] and W states [31]. Depending on the value of the coefficients they have measures of entanglement relevant for either the GHZ or W state.

For example, under the condition that $|a|^2 = |b|^2 = |c|^2 = |d|^2 = 1/4$, all pair concurrences C^2_{BC}, C^2_{AC}, and C^2_{AB} are equal to zero and $C^2_{A\ (BC)} = C^2_{B\ (AC)} = C^2_{C\ (AB)} = \tau_{ABC} = 1$ similar to the GHZ state [29]. In this case we have the maximal three-spin entanglement. However, the spins of each pair are classically correlated but not entangled. It also implies that when one of the spins is traced out then the remaining two are unentangled.

If only one of the coefficients a,b,c,d is zero we have a state analogous to the W state. This is obvious when $a=0$ but it is nontrivial in the remaining cases. In all these cases the three-tangle τ_{ABC} is equal to zero; the condition $C^2_{A\ (BC)} = C^2_{AB} + C^2_{AC}$ is also satisfied (analogously for B-AC and C-AB). This means that this case corresponds to the W state [29].

In the general case the state (35) or (44) has all the characteristics of the entanglement not equal to zero simultaneously. This property distinguishes these states from other known pure states.

Returning to the vector state of Eq. (32) we have time-periodic coefficients. Then miscellaneous states will be realized, including the completely separable state when $\sin[\varphi(\tau)/2] = 0$.

Three-spin states of Eqs. (35) and (44) can be generalized for an arbitrary number of spins. For example, the well-known Bell basis for the two-spin systems $|\psi^\pm\rangle = (1/\sqrt{2})(|00\rangle \pm |11\rangle)$, $|\phi^\pm\rangle = (1/\sqrt{2})(|01\rangle \pm |10\rangle)$ is also a special case of these states with an even and odd number of $|1\rangle$ single-spin states, respectively. The case when the total number of spins is even is different from the one with an odd number of spins. Two states transfer one to the other with a flip of all spins when their number is odd. The analogous procedure does not change these states for an even number of spins.

For our problem we have from Eqs. (32) and (39)

$$\lambda_1 = \lambda_1^{BC} = \lambda_1^{AC} = \lambda_1^{AB} = \frac{1}{3}\sin^2 \varphi(\tau),$$

$$\lambda_2 = \lambda_2^{BC} = \lambda_2^{AC} = \lambda_2^{AB} = \frac{4}{9}\sin^4[\varphi(\tau)/2] \tag{45}$$

and from Eqs. (40)–(43) we obtain

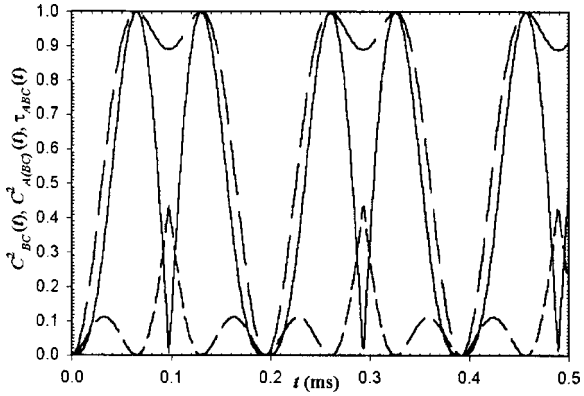

FIG. 2. Time dependence of the square of the pairwise concurrence $C^2_{BC}(t)$ (short-dashed line), the square of the concurrence $C^2_{A(BC)}(t)$ (long-dashed line), and the three-tangle $\tau_{ABC}(t)$ (solid line) for three spins coupled by DDI's with the dipolar coupling constant $D_{12}=D_{23}=D_{13}=2\pi 2950\ \mathrm{s}^{-1}$.

$$C^2_{BC}=C^2_{AC}=C^2_{AB}=(\sqrt{\lambda_1}-\sqrt{\lambda_2})^2$$
$$=\left(\frac{1}{\sqrt{3}}|\sin\varphi(\tau)|-\frac{2}{3}\sin^2[\varphi(\tau)/2]\right)^2,$$

$$C^2_{A\ (BC)}=C^2_{B\ (AC)}=C^2_{C\ (AB)}=2(\lambda_1+\lambda_2)$$
$$=2\left(\frac{1}{3}\sin^2\varphi(\tau)+\frac{4}{9}\sin^4[\varphi(\tau)/2]\right),$$

$$\tau_{ABC}=4\sqrt{\lambda_1\lambda_2}=\frac{8}{3\sqrt{3}}|\sin\varphi(\tau)|\sin^2[\varphi(\tau)/2]. \qquad (46)$$

If we have the condition $b=c=d\neq a$ as in our case, then it is enough to know only one eigenvalue λ_1 for the full solution of the problem of entanglement. Another eigenvalue λ_2 can be obtained from the expression

$$\lambda_1=2\sqrt{\lambda_2}-3\lambda_2. \qquad (47)$$

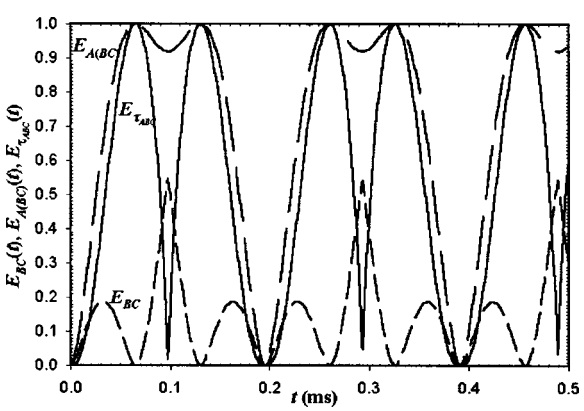

FIG. 3. Time dependence of the pairwise entanglement $E_{BC}(t)$ (short-dashed line), the entanglement $E_{A(BC)}(t)$ (long-dashed line), and the three-tangle entanglement $E\tau_{ABC}(t)$ (solid line) for three spins coupled by DDI's with the dipolar coupling constant $D_{12}=D_{23}=D_{13}=2\pi 2950\ \mathrm{s}^{-1}$.

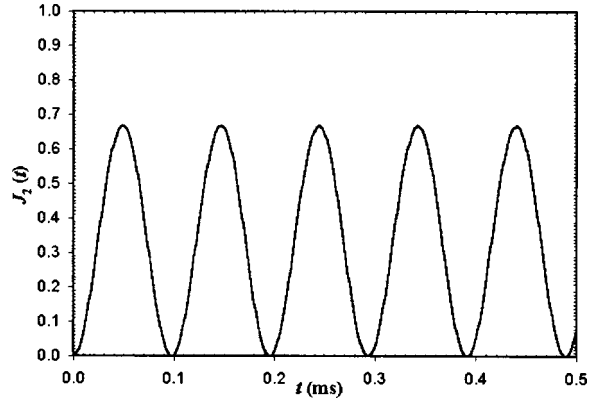

FIG. 4. Time dependence of the intensity of MQ coherence of the second order $J_2(t)$ for three spins coupled by DDI's with the dipolar coupling constant $D_{12}=D_{23}=D_{13}=2\pi 2950\ \mathrm{s}^{-1}$.

Comparing Eq. (31) with Eq. (45), we conclude that the intensity of MQ coherences of the second order coincides with the eigenvalue λ_1 (for both blocks with double λ_1)

$$J_2(\tau)=2\lambda_1. \qquad (48)$$

The same result was obtained before for a two-spin system in the previous section. Then we had one block only (the other block was zero) and $J_2(\tau)=C^2(\tau)=\lambda$ (the matrix $\sigma\tilde{\sigma}$ had one nonzero eigenvalue). Thus, it is possible to conclude that the intensity of MQ coherences of the second order is a generalized measure of entanglement for two- and three-spin systems. Many-spin systems demand further investigation.

Figure 2 shows the evolution of concurrences and the three-tangle for the three-spin ring. The evolution of the corresponding entanglements [Eq. (24)] has similar forms and they are represented in Fig. 3. All these curves can be obtained from the time evolution of the intensity of MQ coherences of the second order (Fig. 4) according to Eqs. (48), (47), (46), and (24).

From Figs. 2 and 3 we can see that completely separable states (all measures of the entanglement equal to zero) occur at times $\tau=0.1957$, 0.3914 ms, etc., when $\sin[\varphi(\tau)/2]=0$.

V. CONCLUSION

The dynamics of entanglement in solids where nuclei are coupled by DDI's can be investigated using the time evolution of MQ coherences. This is the main result of this paper. The intensities of MQ NMR coherences can be measured in macroscopic systems. Since experimental methods for the observation of these coherences have been developed, one can apply our results for the investigation of different schemes of quantum computers on the basis of MQ NMR in solids.

We proved that the dynamics of entanglement in two- and three-spin systems is determined by the time evolution of the MQ coherence of the second order, which can be described with the imaginary part of the density matrix. For systems with a larger number of spins, the situation is more complicated. The MQ dynamics of such systems includes the MQ coherences of higher orders. It is possible to assume that the

dynamics of entanglement in this case is determined by the intensities of MQ coherences of orders 2, 6, 10,..., $\leqslant N$, which can be described by the imaginary part [13] of the density matrix.

It is also worth noticing that we found a pure state which generalizes the well-known classes of pure states GHZ and *W*. The algorithm for construction of such states for an arbitrary number of spins is suggested. The difference between the cases of odd and even numbers of spins is elucidated. Different measures of the entanglement of this state are analyzed for tripartite systems.

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